

Electronic Supporting Information

Machine learning-aided engineering of a cytochrome P450 for optimal bioconversion of lignin fragments

Artur Hermano Sampaio Dias,^{ab} Yuanxin Cao,^a Munir S. Skaf^b and Sam P. de Visser^{*a}

^a Manchester Institute of Biotechnology and Department of Chemical Engineering,
The University of Manchester, 131 Princess Street, Manchester M1 7DN, United
Kingdom.

^b Institute of Chemistry and Centre for Computing in Engineering & Sciences, Uni-
versity of Campinas, Campinas, SP 13083-861, Brazil.

Email: sam.devisser@manchester.ac.uk

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Part 1: METHODS

Part 1.1 Model preparation and set-up

Initially, we took the guaethol-bound CYP255A and *p*-anisic acid-bound CYP199A4 structures from the Protein Data Bank (PDB, see Fig. S1),¹ where they are deposited under the PDB codes 5OMS² and 4DO1,³ respectively. We added hydrogen atoms to each structure using the H++ webserver considering pH 7 conditions.⁴ All protonation states of titratable residues were further manually inspected, and all carboxylate groups were in their deprotonated forms, while all Arg and Lys side chains were protonated. All His amino acid side chains were singly protonated on either the N_δ or N_ε atom. Thereafter, each system was manually converted into a Compound I (CpdI) structure by adding an oxygen atom to the heme at a distance of 1.686 Å above the iron atom, such that its four surrounding nitrogen atoms and this newly added oxygen atom created a pyramidal geometry.

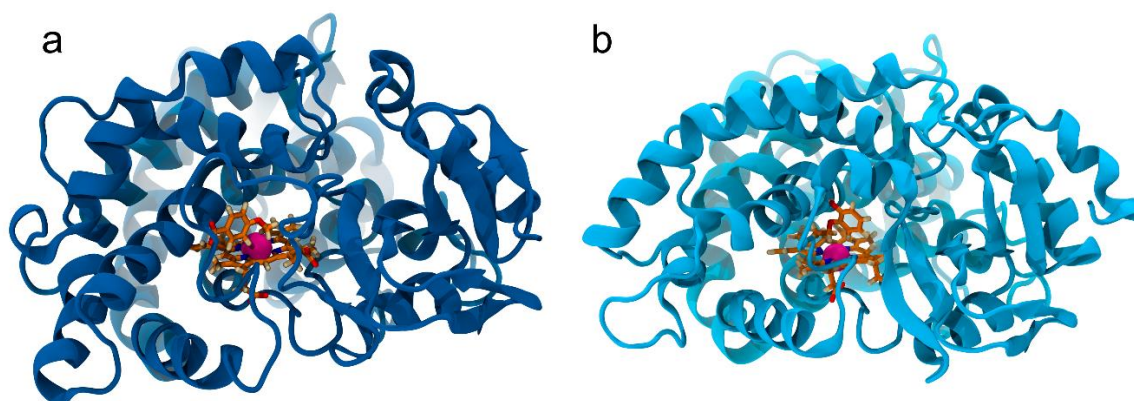


Fig. S1. P450 enzymes studied in this work: a) CYP199A4 bound to *p*-anisic acid; b) CYP255A bound to guaethol.

Prior to the molecular dynamics (MD) simulations, we applied the MCPB.py⁵ routine available in Amber 2018⁶ to generate force field parameters needed to simulate each heme complex. This set-up calculation took into consideration the first-coordination sphere ligands, that is, the porphyrin ring, the newly added distal oxo group, and the axial ligand whose sulfur atom belongs to a cysteine residue from the L-helix in each system. Once such parameters were generated, we used the LEaP module as available in Amber 2018 to solvate each structure with TIP3P water in separate rectangular boxes with 10 Å of padding in all directions and sodium and chloride ions to render a simulation box with net charge zero.⁷

Part 1.2 Molecular dynamics approaches

The protein and substrate (guaethol for CYP255A and 4-methoxybenzoate for CYP199A4) atoms were described by the ff14SB⁸ force field and each system was subjected to 10,000 steps of energy minimization, that is 5,000 of steepest descent followed by 5,000 of conjugate gradient. The energy-minimized structures were then heated and equilibrated in three consecutive steps at constant pressure for 40 picoseconds, in steps of 2 femtoseconds, each:

- i. Heating from 0 to 150 K with harmonic restraints of $10 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$ on all alpha-carbons as well as on heme, iron, distal oxo and substrate atoms.
- ii. Heating from 150 to 300 K with harmonic restraints of $5 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$ on all alpha-carbons as well as on heme, iron, distal oxo and substrate atoms.
- iii. Equilibration at 300 K with harmonic restraints of $5 \text{ kcal mol}^{-1} \text{ \AA}^{-2}$ only on heme, iron, distal oxo and substrate atoms.

The production runs lasted 100 ns and were free of restrictions at 300 K and 1 atm. For each system's run, we took into consideration two factors for picking out the configuration to move forward with QM calculations (Fig. S2):

- i. Frames with strong and stabilizing non-bonded forces between substrate and active site residues (number of hydrogen bonds in CYP199A4 and strength of van der Waals interactions, since they have strongly polar and non-polar active sites, respectively).
- ii. Frames whose active site residues configuration was the closest possible to the average structure throughout the entire run, RMSD-wise – this way we could sort out potential reactive configurations from the MD trajectories.

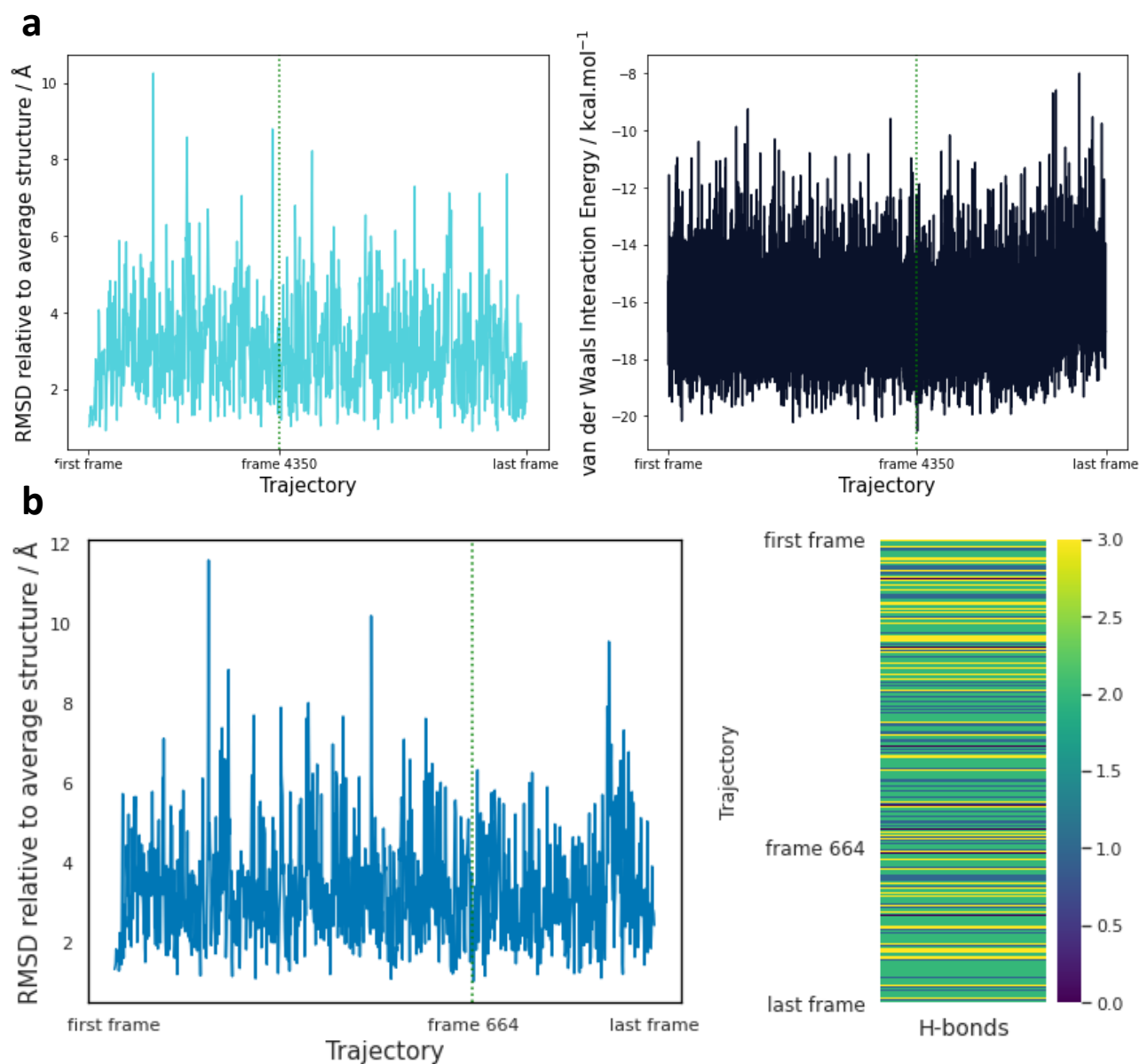


Fig. S2. Frame selection from the MD trajectories: a) For CYP255A, the production run frame 4350 was structurally similar to the average structure throughout the entire simulation and had the most stabilizing van der Waals interaction energy between substrate and active site residues, thus this frame was picked for the next DFT calculations; b) wildtype CYP199A4 production run frame 664 was structurally similar to the average structure throughout the entire simulation and had the maximum number of hydrogen bonds (3) between substrate and active site residues, therefore it was picked for the next DFT calculations.

Part 1.3 QM cluster model set-up

Once the most representative frame from each trajectory was selected, an active site cluster model was created using previous approaches.^{9,10} To do so, we selected the amino acid residues that make up the active site in each system and trimmed out all other atoms. Thus, CYP199A4 cluster model was composed by 255 atoms (Fig. S3a), namely including a truncated porphyrin ring with all side chains replaced by hydrogen atoms, the iron atom with its distal oxo and axial thiolate ligands, the *p*-anisic acid molecule, three water molecules, and the atoms of residues Ser₂₄₄, Arg₂₄₃, Arg₉₂, Ser₂₄₇, Ala₂₄₈, Gly₂₄₉, Phe₁₈₂, Val₁₈₃, Phe₂₉₈, Phe₁₈₅, Thr₂₅₂, Glu₉₉, Leu₉₈ and Ser₉₅ – and CYP255A cluster model was composed of 306 atoms (Fig. S3b) – the truncated porphyrin ring, the iron atom with its distal oxo and axial –SCH₃ ligands, the guaethol molecule, two water molecules, the side chain of residues Cys₃₅₆, Val₂₄₁, Tyr₂₄₂, Ile₈₀, Ile₈₁, Leu₂₄₄, Phe₃₉₅, Gly₂₄₅, Ala₂₄₆, Asn₂₄₈, Glu₂₄₉, Ile₂₉₂, Phe₇₅, Phe₁₆₉, Ala₂₉₅, Thr₂₉₆ as well as the backbone atoms of residues Leu₂₄₃ and Met₂₄₇. Protein residues were truncated by replacing the aliphatic C–C bond that is broken by C–H a capping atom. The net charge of the CYP255A QM-model was –1, whereas that of CYP199A4 was zero.

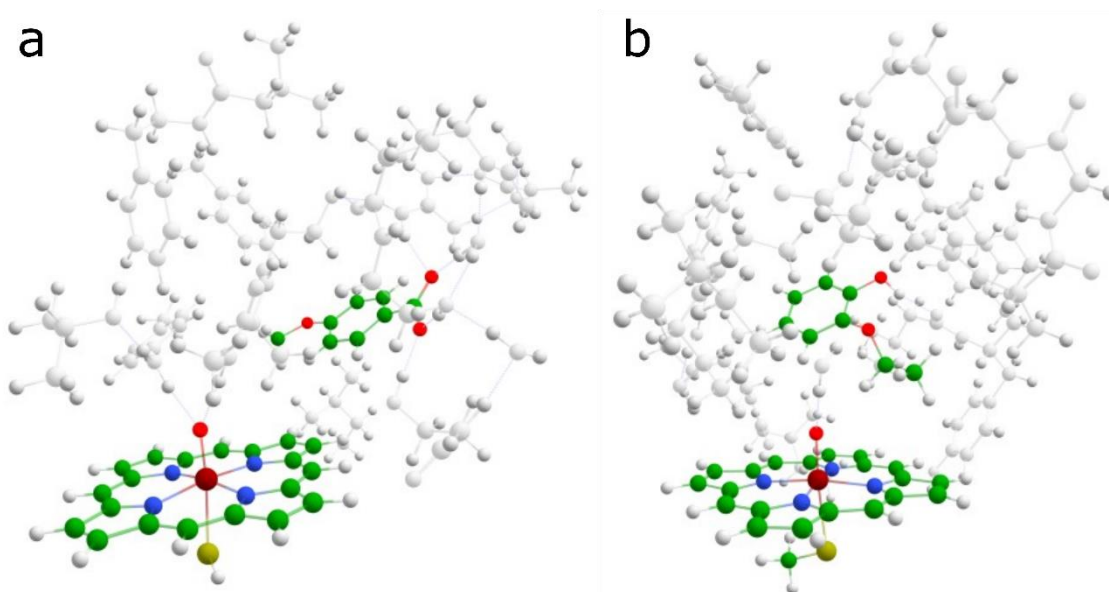


Fig. S3. QM Cluster Models investigated in this study, with protein and water residues coloured in white for clarity: a) CYP 199A4 reduced to its catalytic centre in 255 atoms; b) CYP255A active site assembled in 306 atoms.

For each individual system, we then carried out DFT calculations using the Gaussian-09 software package.¹¹ All structures – reactants, intermediates, products, and transition states – were optimized without constraints in the gas phase. Two spin states were taken into consideration for the reaction mechanisms studies, namely doublet ($S = 1/2$) and quartet ($S = 3/2$), which are henceforth identified by superscripts 2 and 4 in front of the label, respectively. The calculations were carried out using the unrestricted hybrid density functional UB3LYP with a split-valence basis set described with the LanL2DZ basis set with effective core potential on iron, and for the C, H, N, O, and S atoms the 6-31G* basis set was employed (basis set BS1).^{12,13} Potential energy scans were performed along various reaction coordinates to establish possible mechanisms and to obtain starting structures for the transition state searches along a particular degree of freedom. Full geometry optimizations for the transition state structures were performed and their outcome was confirmed by a frequency calculation. A single imaginary frequency involving the correct vibrational distortion confirmed the structure to be a transition state, while local minima were confirmed by finding real frequencies only.

To describe the energy landscape more accurately, we performed single-point calculations with a continuum polarized conductor model with a dielectric constant mimicking chlorobenzene, which is a good mimic for the active site of P450 systems ($\epsilon = 4.7$),¹⁴ and 6-311+G* basis set on H, C, N, O, and S atoms and LACV3P+ basis set with core potential on iron (basis set BS2).

Part 1.4 Mutant structures set-up

We created a set of mutants of CYP199A4 based on visual inspection of the crystal structure 4DO1, whereby the substrate-binding position and orientation was changed so that its reactivity would lead to changes in product distributions. This was tested, for instance, by moving the position of the active site Arg residue (Arg₉₂ in wildtype) as it is known to form a salt-bridge with the carboxylate group of the substrate. Further substrate position and orientation in the active site is achieved through hydrophobic interactions with aliphatic amino acid residues in the active site. The complete set of mutants and their respective mutations tested is as shown in Table S1.

Table S1. CYP199A4 mutations investigated in this work.

<i>Mutant</i>	<i>Mutations</i>
<i>A</i>	Arg92Val / Val295Lys
<i>B</i>	Ser244Ala / Ala248Ser
<i>C</i>	Ser244Ala / Ala248Thr
<i>D</i>	Arg92Leu / Leu396Arg
<i>E</i>	Arg92Leu / Leu396Lys
<i>F</i>	Arg92Leu / Leu98Lys
<i>G</i>	Arg92Leu / Leu98Arg
<i>H</i>	Arg92Ala / Arg243Ala / Ala248Ser

Each mutant was generated using VMD software package,¹⁵ and followed by steps of energy minimization and equilibration with explicit solvent in the same fashion as described above for the wildtype structures. Subsequently, *p*-anisic acid was inserted into the protein structures using molecular docking procedures as carried out with the AutoDock Vina software package¹⁶ using an approximately cubic search box of volume 1.363 nm³ centered exactly on the distal oxo ligand of CpdI. The maximum energy difference between the best binding mode and the worst one was set to 2 kcal mol⁻¹, the exhaustiveness of the search engine was set to maximum, and the maximum number of binding modes was set to 10.

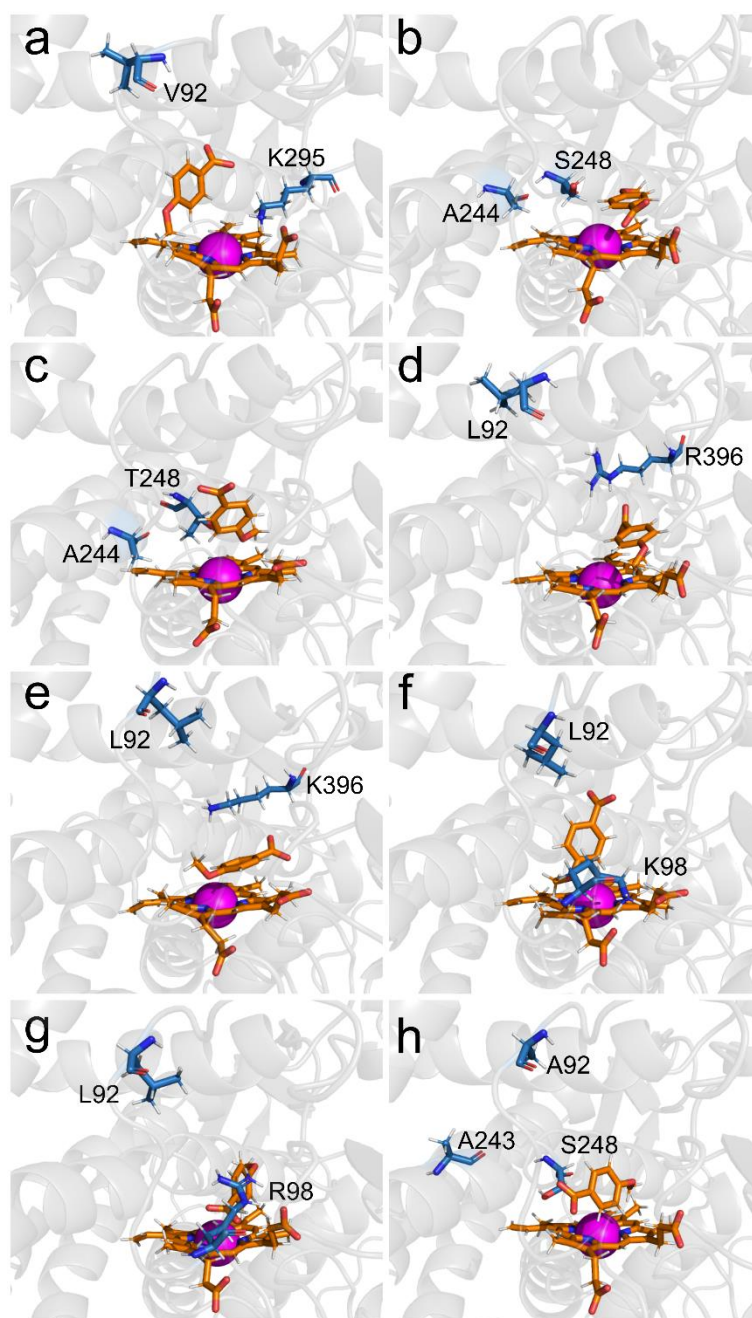


Fig. S4. Mutant CYP19A4 structures, after energy minimization, heating, and substrate docking but prior to MD simulations: a-h) mutants A-H (see Table S1).

The lowest-energy binding pose for each mutant was then solvated following the same procedures described above. Each CYP^{MUTANT}-substrate^{DOCKED} complex (Fig. S4) was subjected to energy minimization, heating, equilibration, and a production run following the same parameters aforementioned for the wildtype complex. In this case, each CYP^{MUTANT}-substrate^{DOCKED} production run lasted 1 μ s. Additionally, wildtype CYP199A4 had an additional 100 ns-run with the substrate positioned in an alternative configuration, which was obtained by re-docking *p*-anisic acid into the active site of CYP199A4 through the same procedure described above (Fig. S5).

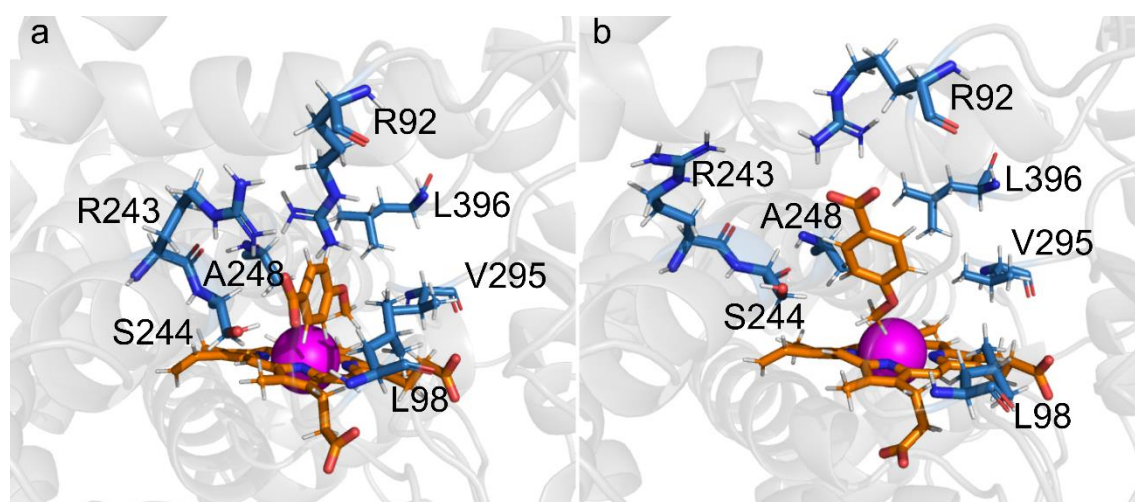


Fig. S5. Starting structures for the two wildtype CYP199A4 molecular dynamics runs: a) 4-methoxybenzoate positioned on the active site as it is found in the 4DO1 PDB entry; b) *p*-anisic acid docked onto the active site following the best solution proposed by AutoDock Vina.

Part 1.5 Machine-learning aided mutant selection

In order to find mutants with different regioselectivity of reaction with *p*-anisic acid, we applied an unsupervised machine learning strategy, which was carried out as follows: Firstly, we divided each CYP^{MUTANT}-substrate^{DOCKED} production run into 10 bins of 100 ns each. We analyzed each trajectory bin, including the two wildtype 100 ns bins in terms of 13 geometrical and force field-related collective variables (Fig. S6 and Parts 2.2 and 2.3):

1. The distance between O_{CpdI} and C8_{SUBSTRATE};
2. The distance between O_{CpdI} and C3_{SUBSTRATE};
3. The distance between O_{CpdI} and C7_{SUBSTRATE};
4. The distance between N(A)_{HEME} and C8_{SUBSTRATE};
5. The distance between N(B)_{HEME} and C8_{SUBSTRATE};
6. The distance between N(C)_{HEME} and C8_{SUBSTRATE};
7. The distance between N(D)_{HEME} and C8_{SUBSTRATE};
8. The RMSD_{SUBSTRATE} relative to its average structure throughout the run;
9. The van der Waals interaction energy between substrate and the main phenylalanine residues of the active site – Phe₁₈₂, Phe₁₈₅ and Phe₂₉₈;
10. The electrostatic interaction energy between substrate and all protein residues within 8 Å of O_{CpdI};
11. The active site fluctuation, measured as the RMSF of all protein residues within 8 Å of O_{CpdI};
12. The angle Fe-O3_{SUBSTRATE}-C1_{SUBSTRATE};
13. The dihedral S_{AXIAL}-Fe-O_{CpdI}-C4_{SUBSTRATE}.

and between-cluster distances – lower values indicate better clustering, and a value of 0 indicates perfect clustering.²¹

Having reached convergence on the optimal number, n , of clusters for our datapoints (see figure S30), we applied the K -Means algorithm as implemented in Scikit-learn package,²² setting its hyperparameter “number of clusters” equal to n . The t-Distributed Stochastic Neighbour Embedding (TSNE)²³ was used to bring the multi-dimensional data into a bidimensional plot. The best mutant was selected according to the Jaccard Similarity²⁴: This score was calculated for each CYP199A4 variant (WT and mutants) pair, following the rationale that, if two variations are grouped in the same cluster, they behave similarly, and thus lead to a similar product distribution. Therefore, we searched for the mutant whose datapoints were not clustered with any wildtype datapoint.

Finally, the selected mutant was subjected to DFT calculations using a QM cluster model and calculations were performed as described above for aromatic hydroxylation and O -demethylation of the substrate. To do so, we selected the best frame from the molecular dynamics trajectory, trimmed it to create a QM-cluster model, and ran full DFT calculations with it, all following the same criteria as stated above for the wildtype CYPs.

Part 1.6 Evolutionary Scale Modelling on Mutants

We then applied the Evolutionary Scale Model (ESM) approach on wildtype and mutant structures to understand their structural similarities.

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Part 2: MOLECULAR DYNAMICS SIMULATIONS AND MACHINE LEARNING APPROACHES

Part 2.1 Molecular Dynamics Trajectory of CYP255A

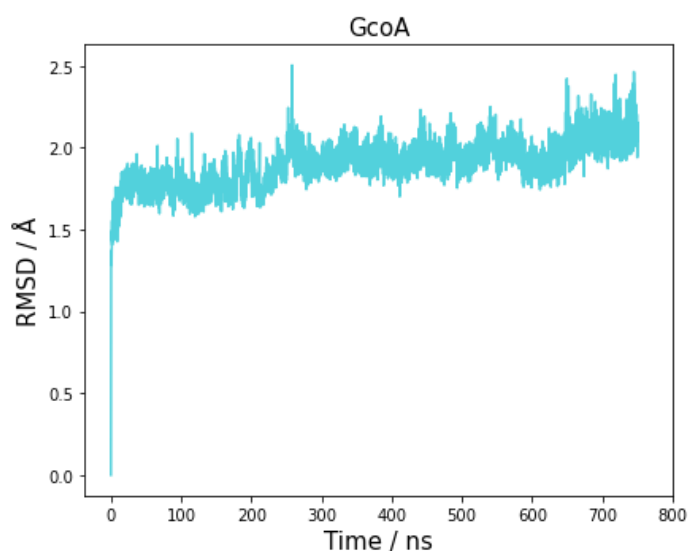


Fig. S7. All-atoms RMSD of the CYP255A receptor (protein+heme) throughout 750 ns of MD production run.

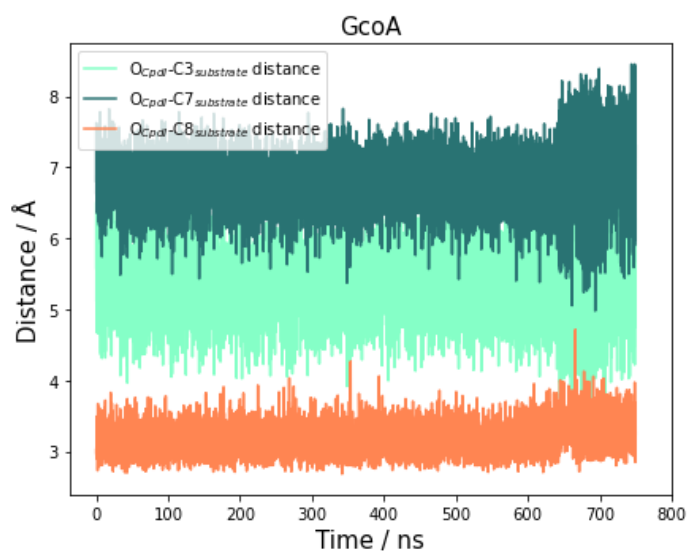


Fig. S8. Euclidean distance between O_{CpdI} and atoms C3, C7, and C8 of substrate in the CYP255A system throughout 750 ns of MD production run.

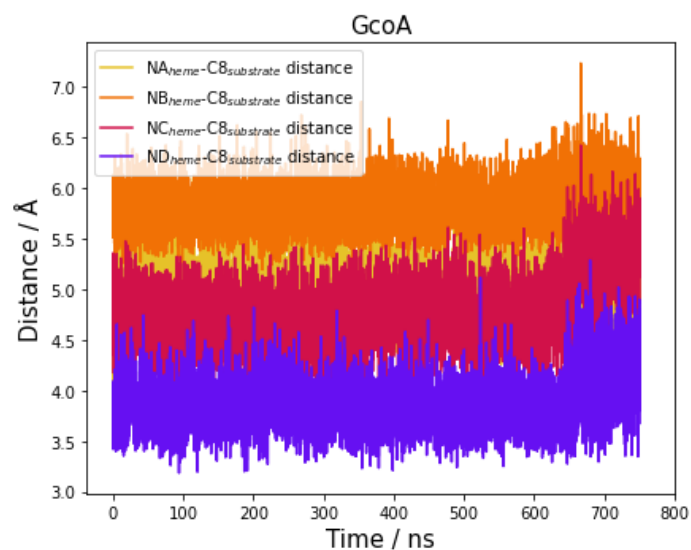


Fig. S9. Euclidean distance between $C8_{\text{substrate}}$ and the four nitrogen atoms in the porphyrin ring of the CYP255A system throughout 750 ns of MD production run.

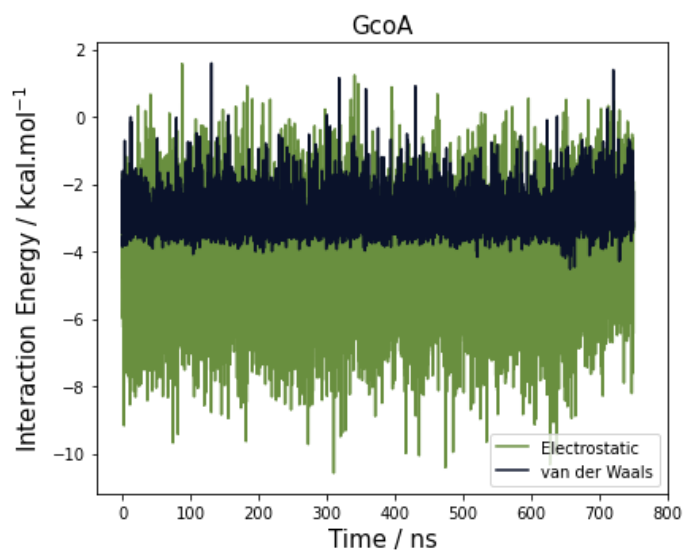


Fig. S10. Interaction energies between substrate and the active site residues in CYP255A throughout 750 ns of production run. Electrostatic interaction energies between substrate and active site residues (all within 8 Å from O_{CpdI}) are depicted in green, while van der Waals interaction energies between substrate and the three aromatic residues in the active site (Tyr_{242} , Phe_{349} and Phe_{395}) are depicted in dark blue.

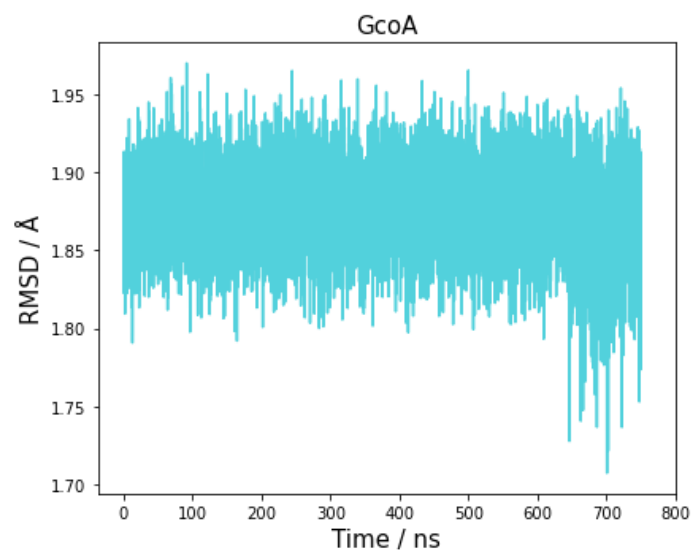


Fig. S11. All-atoms RMSD of the substrate (guaethol) in CYP255A throughout 750 ns of MD production run.

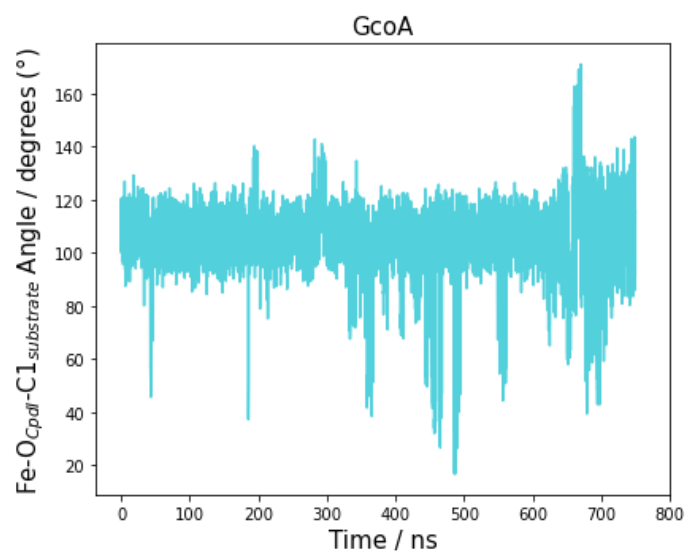


Fig. S12. Angle between Fe, O_{Cpdl} and $C1_{substrate}$ in the CYP255A system throughout 750 ns of MD production run.

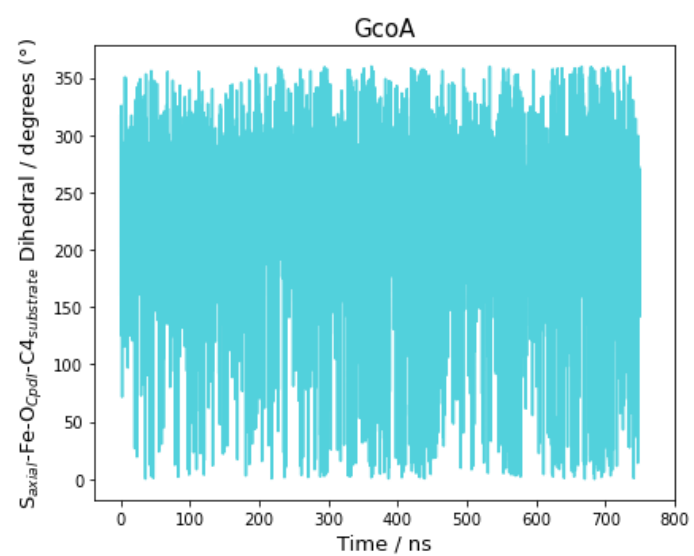


Fig. S13. Dihedral angle between S_{axial} , Fe, O_{Cpdl} and $C4_{substrate}$ in the CYP255A system throughout 750 ns of MD production run.

Part 2.2 Molecular Dynamics Trajectory of Wildtype CYP199A4 Structures

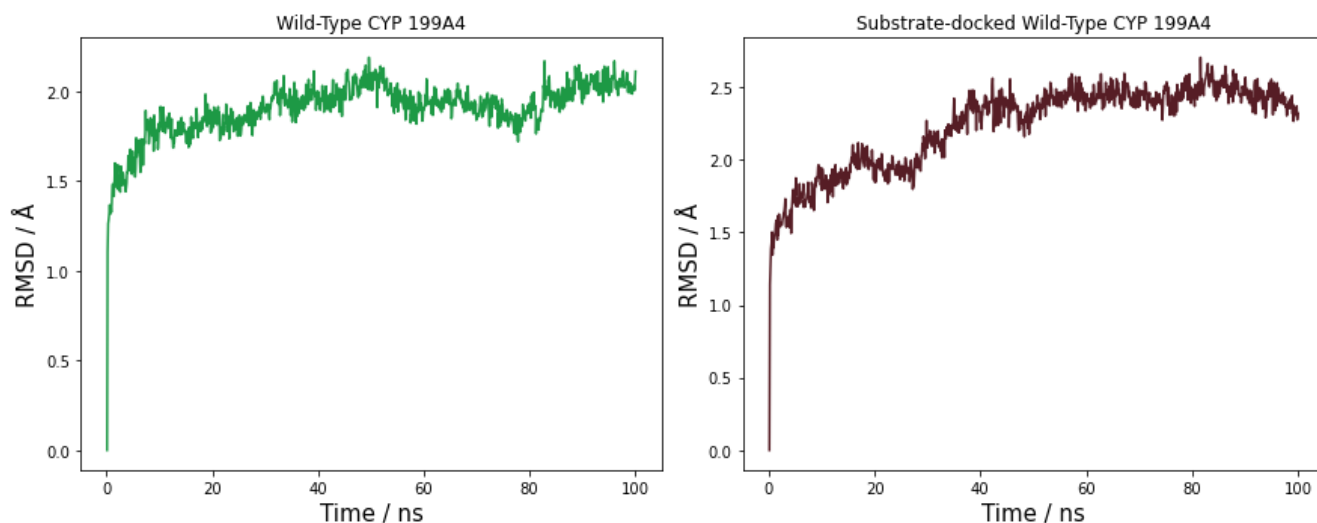


Fig. S14. All-atoms RMSD of wildtype CYP199A4 receptors (protein+heme) throughout 100 ns of MD production run. Left: CYP199A4 whose substrate started MD in its crystallographic configuration. Right: CYP199A4 whose substrate was re-docked onto the catalytic site before the MD simulation.

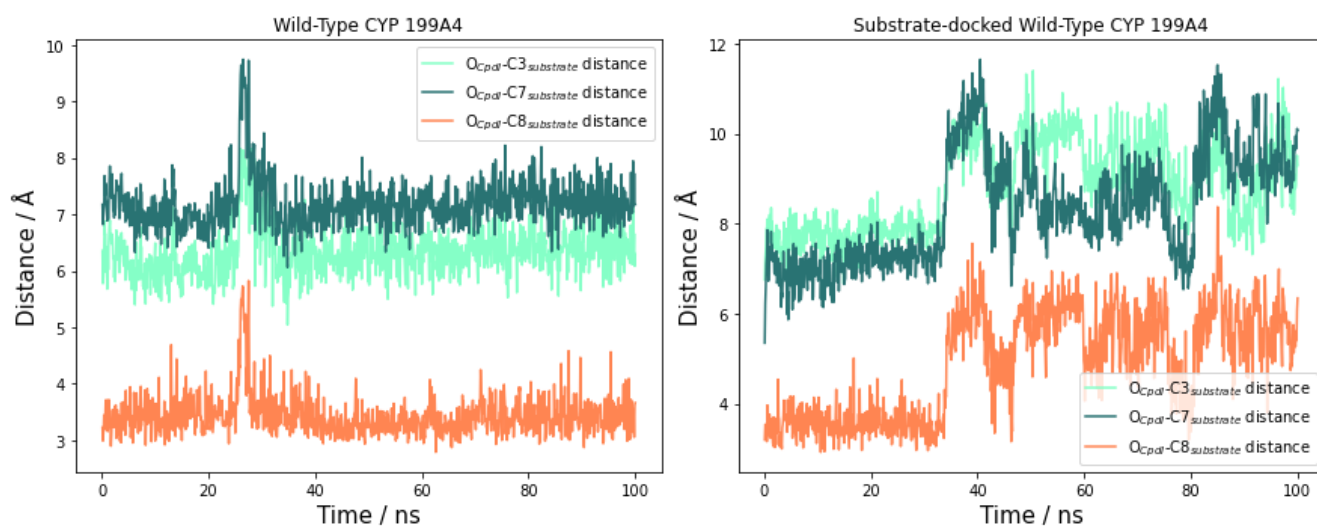


Fig. S15. Euclidean distance between O_{CpdI} and atoms C3, C7, and C8 of substrate in wildtype CYP199A4 systems throughout 100 ns of MD production run. Left: CYP 199A4 whose substrate started MD in its crystallographic configuration. Right: CYP199A4 whose substrate was re-docked onto the catalytic site prior to the MD simulation.

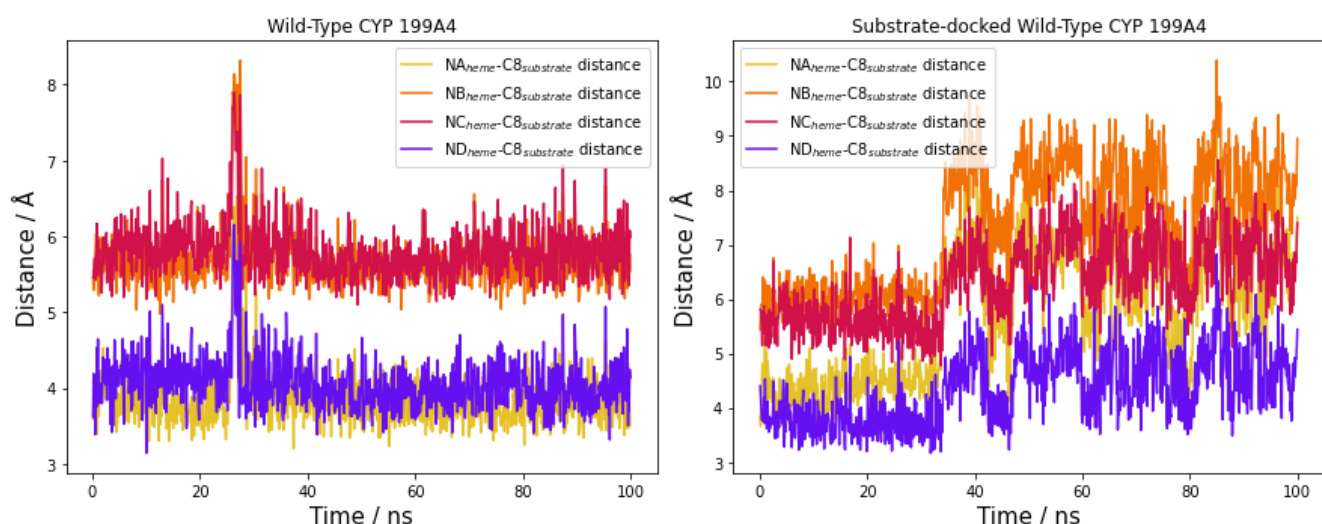


Fig. S16. Euclidean distance between C8_{substrate} and the four nitrogen atoms in the porphyrin ring of wildtype CYP199A4 systems throughout 100 ns of MD production run. Left: CYP199A4 whose substrate started MD in its crystallographic configuration. Right: CYP199A4 whose substrate was re-docked onto the catalytic site prior to the MD simulation.

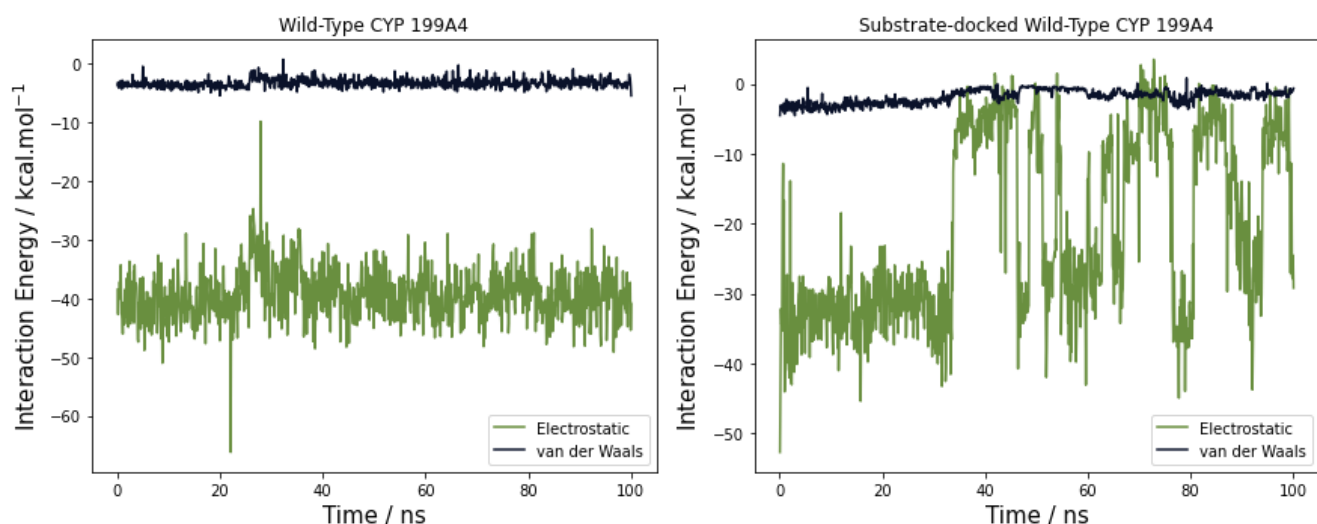


Fig. S17. Interaction energies between substrate and wildtype CYP199A4's active site residues throughout 100 ns of production run. Electrostatic interaction energies between substrate and active site residues (all within 8 Å from O_{CpdI}) are depicted in green, while van der Waals interaction energies between substrate and the three phenylalanine residues in the active site (Phe₁₈₂, Phe₁₈₅ and Phe₂₉₈) are depicted in dark blue. Left: CYP199A4 whose substrate started MD in its crystallographic configuration. Right: CYP199A4 whose substrate was re-docked onto the catalytic site prior to the MD simulation.

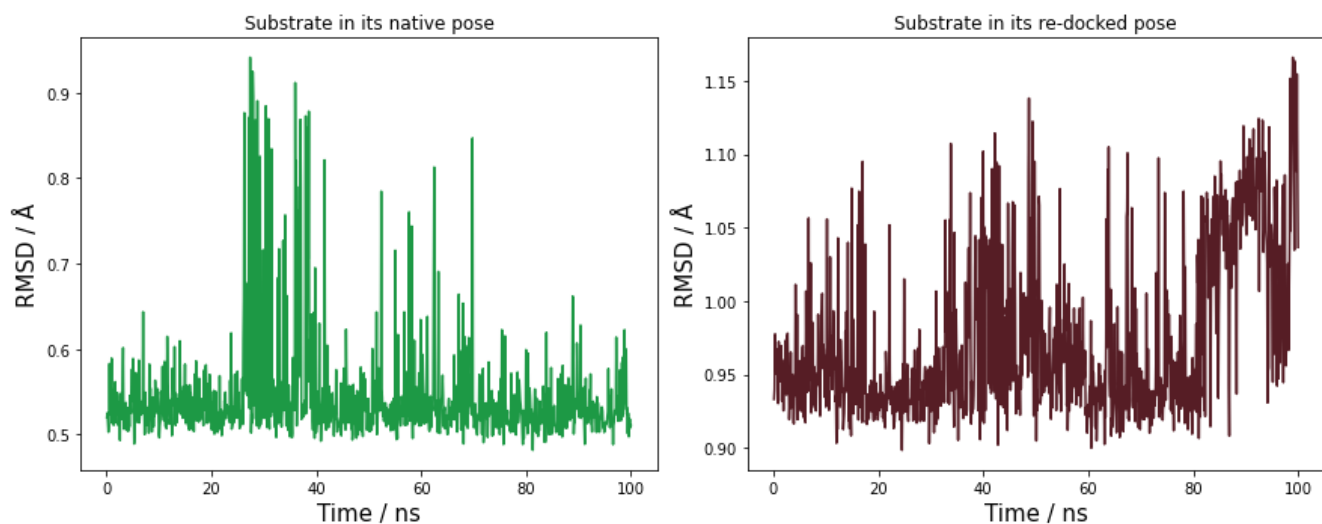


Fig. S18. All-atoms RMSD of wildtype CYP199A4 substrates (4-methoxybenzoate) throughout 100 ns of MD production run. Left: native substrate as in its crystallographic configuration (PDB ID: 4DO1). Right: substrate that was re-docked onto the catalytic site prior to the MD simulation.

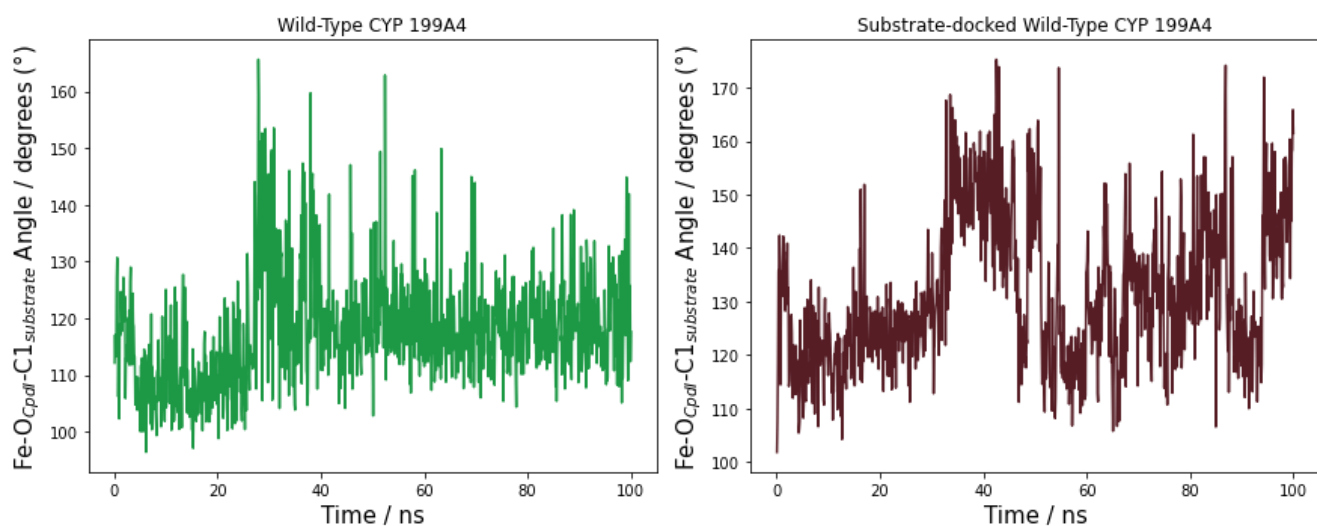


Fig. S19. Angle between Fe, O_{CpdI} and C1_{substrate} in the wildtype CYP199A4 structures throughout 100 ns of MD production run. Left: native substrate as in its crystallographic configuration (PDB ID: 4DO1). Right: substrate that was re-docked onto the catalytic site prior to the MD simulation.

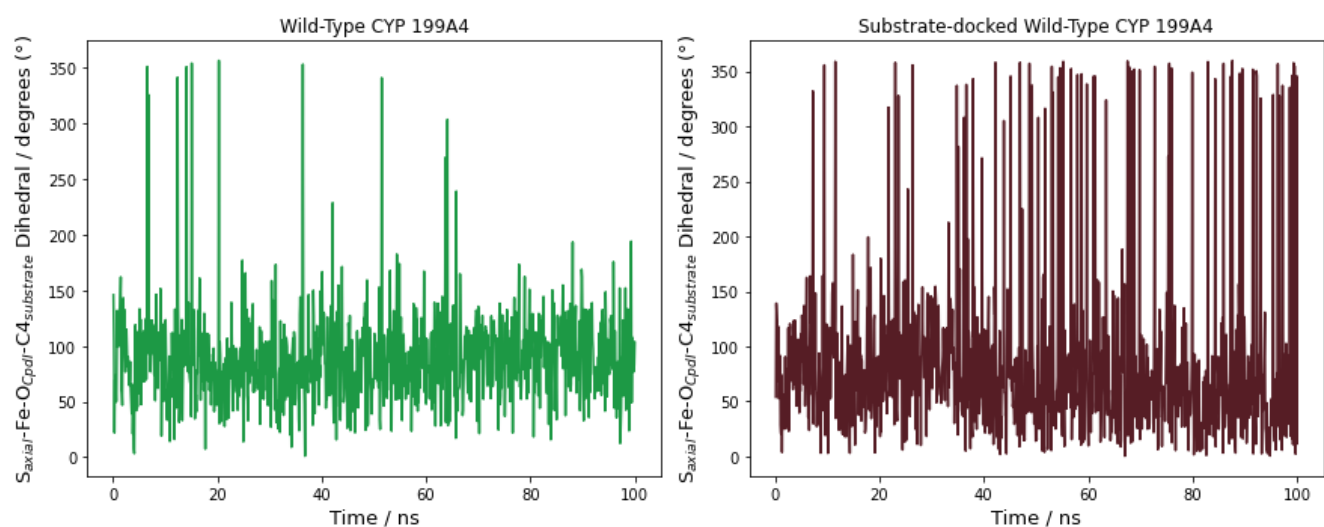


Fig. S20. Dihedral angle between S_{axial} , Fe, O_{CpdI} and $C1_{substrate}$ in the wildtype CYP199A4 structures throughout 100 ns of MD production run. Left: native substrate as in its crystallographic configuration (PDB ID: 4DO1). Right: substrate that was re-docked onto the catalytic site prior to the MD simulation.

Part 2.3 Molecular Dynamics Trajectory of Mutant CYP19A4 Structures

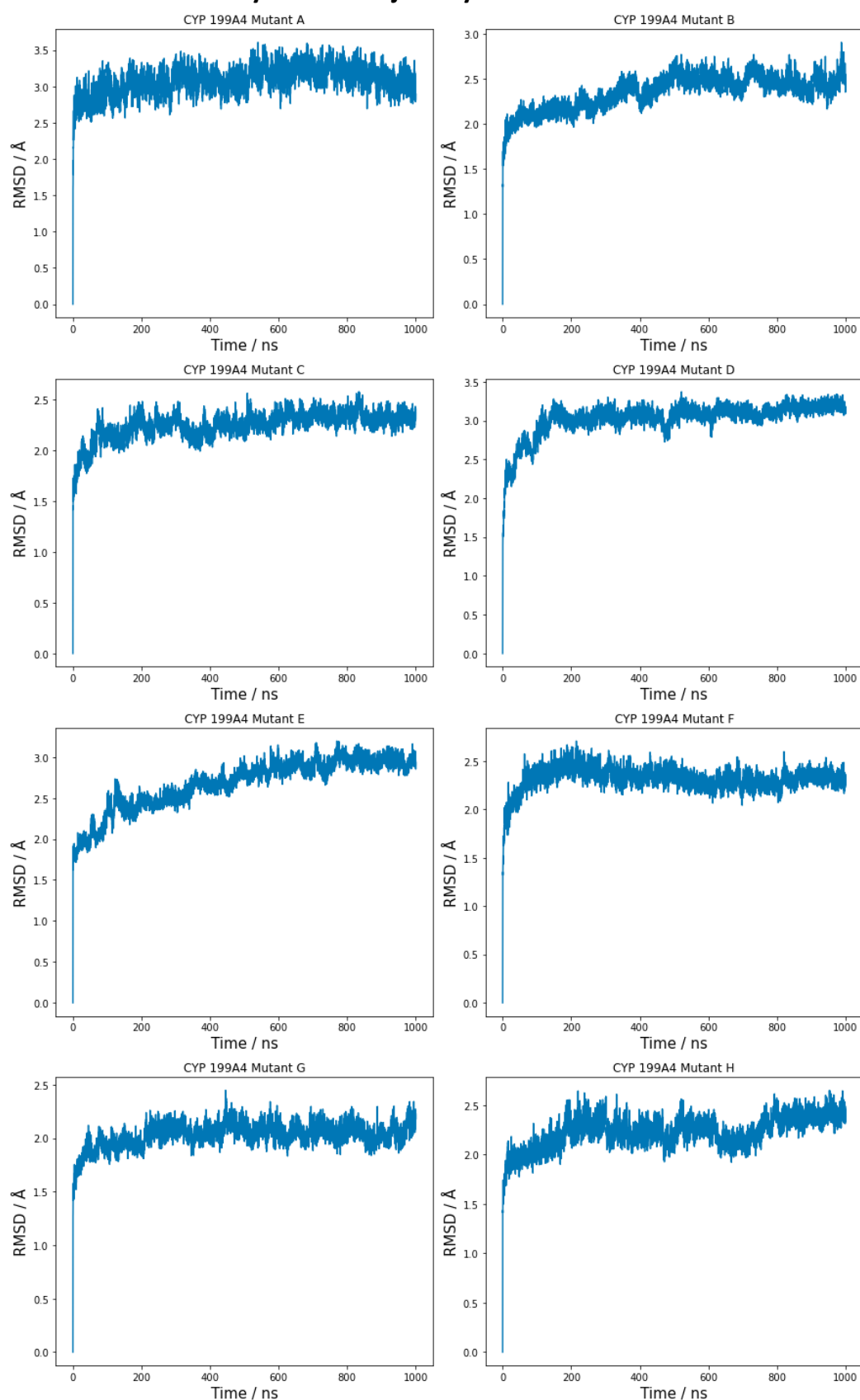


Fig. S21. All-atoms RMSD of mutant CYP19A4 structures (protein+heme) throughout 1 μ s of MD production run. Top-Down and Left-Right: mutants A-H.

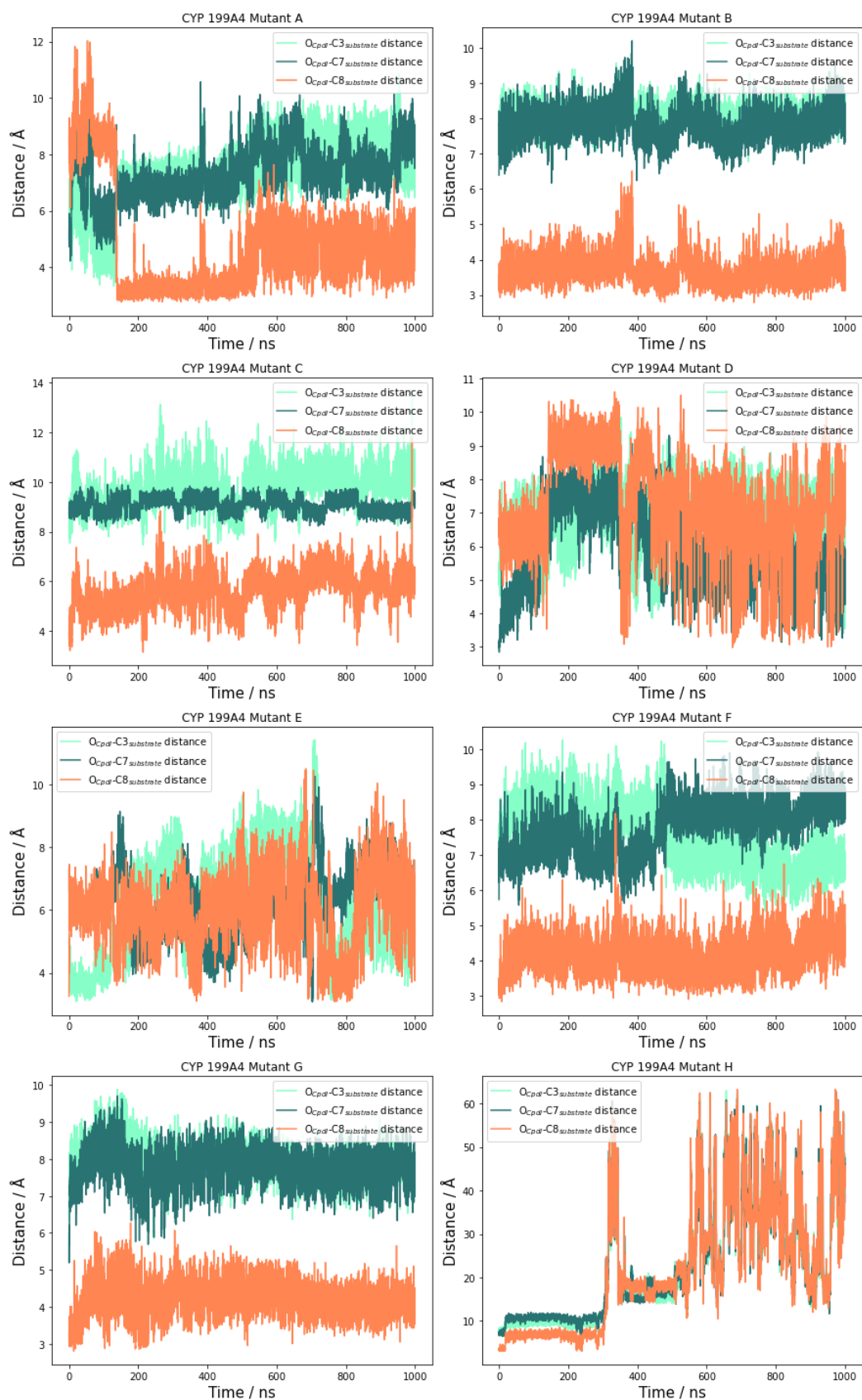


Fig. S22. Euclidean distance between O_{CpdI} and atoms C3, C7, and C8 of substrate in mutant CYP19A4 systems throughout 1 μ s of MD production run. Top-Down and Left-Right: mutants A-H.

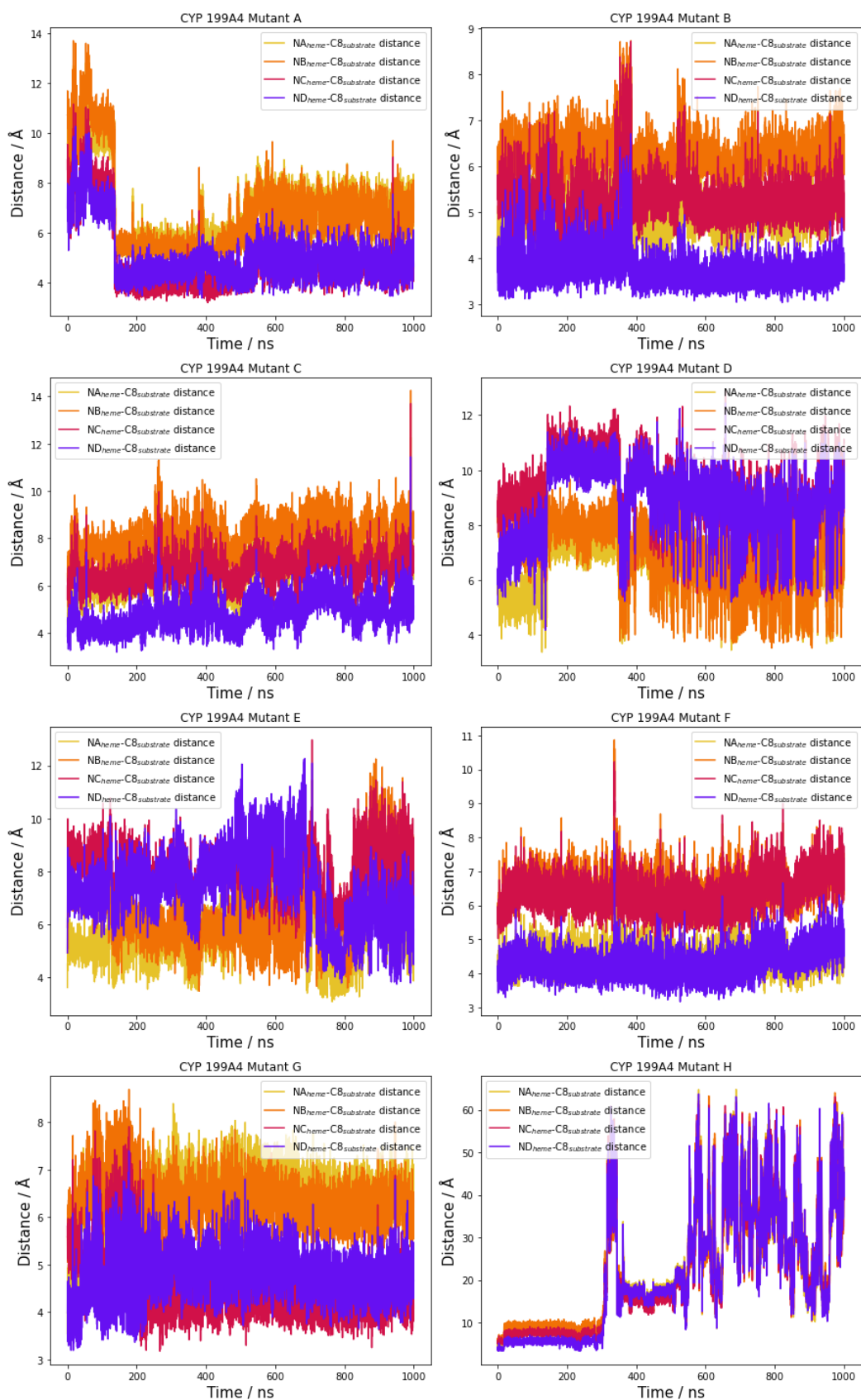


Fig. S23. Euclidean distance between $C8_{\text{substrate}}$ and the four nitrogen atoms in the porphyrin ring of mutant CYP199A4 systems throughout 1 μs of MD production run. Top-Down and Left-Right: mutants A-H.

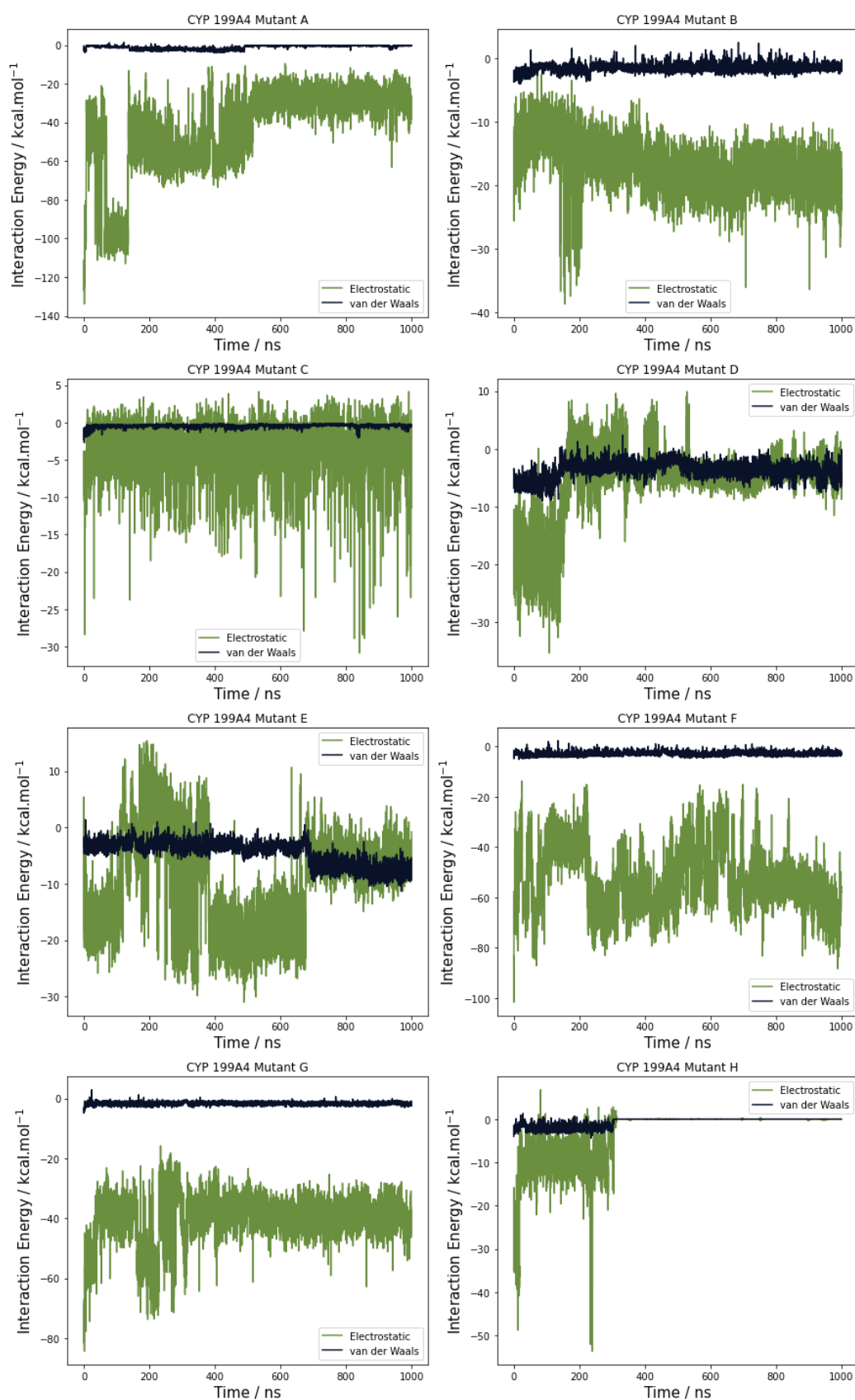


Fig. S24. Interaction energies between substrate and mutant CYP199A4's active site residues throughout 1 μ s of production run. Electrostatic interaction energies between substrate and active site residues (all within 8 Å from O_{CpdI}) are in green, while van der Waals interaction energies between substrate and the three phenylalanine residues in the active site (Phe₁₈₂, Phe₁₈₅ and Phe₂₉₈) are depicted in dark blue. Top-Down and Left-right: mutants A-H.

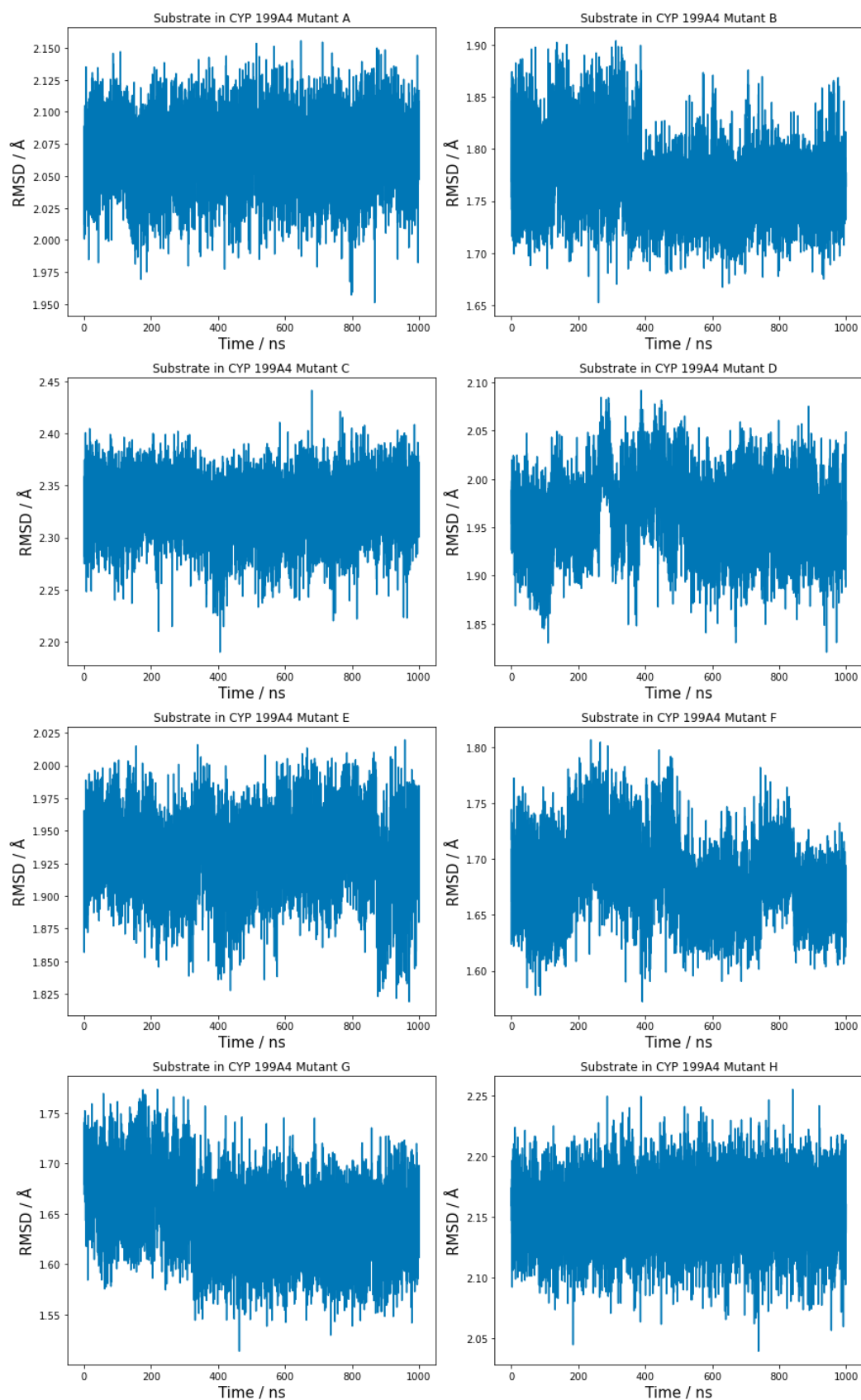


Fig. S25. All-atoms RMSD of substrate (4-methoxybenzoate) in all mutant CYP199A4 systems throughout 1 μ s of MD production run. Top-Down and Left-Right: mutants A-H.

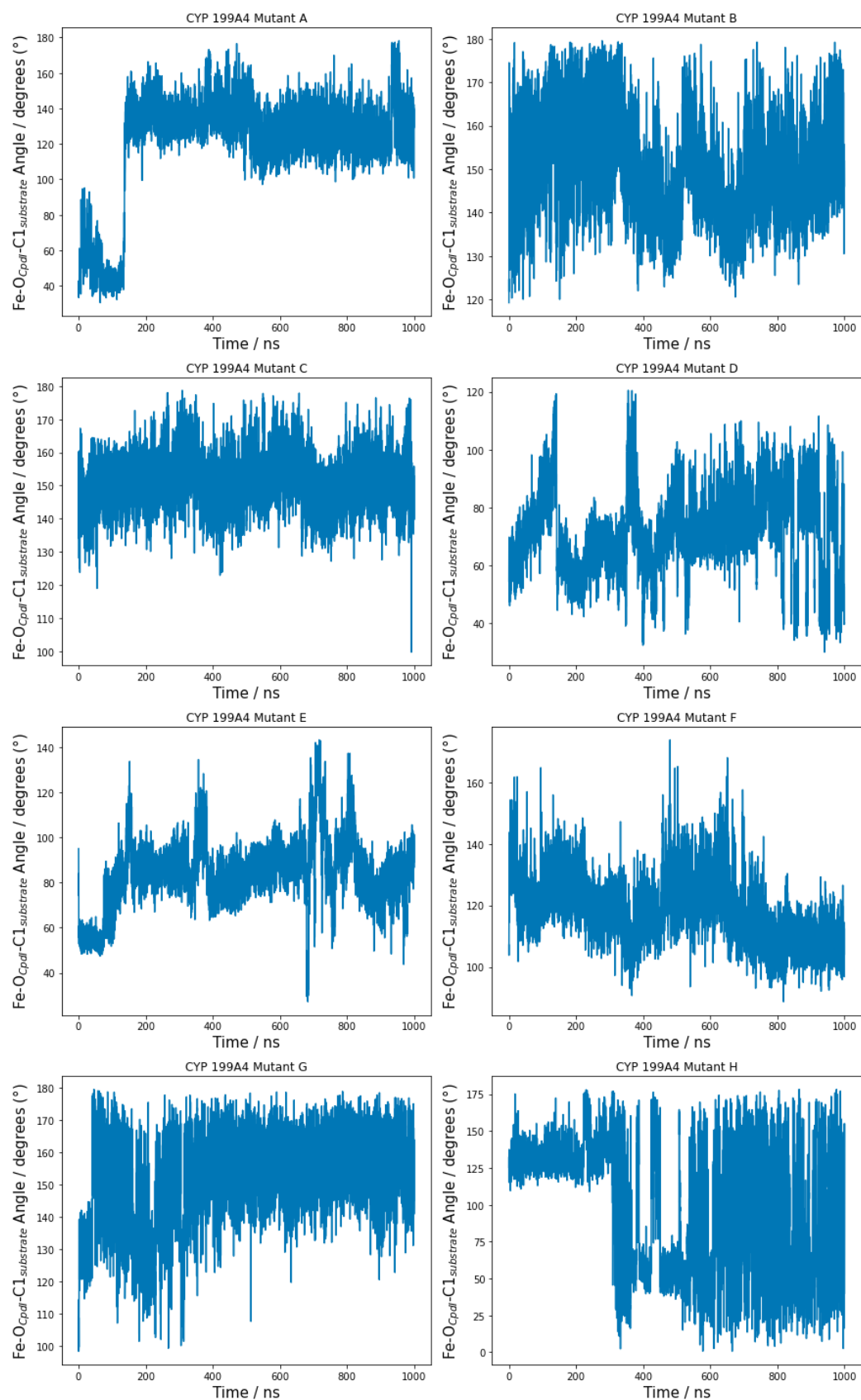


Fig. S26. Angle between Fe, O_{CpdI} and C1_{substrate} in the mutant CYP199A4 structures throughout 1 μ s of MD production run. Top-Down and Left-Right: mutants A-H.

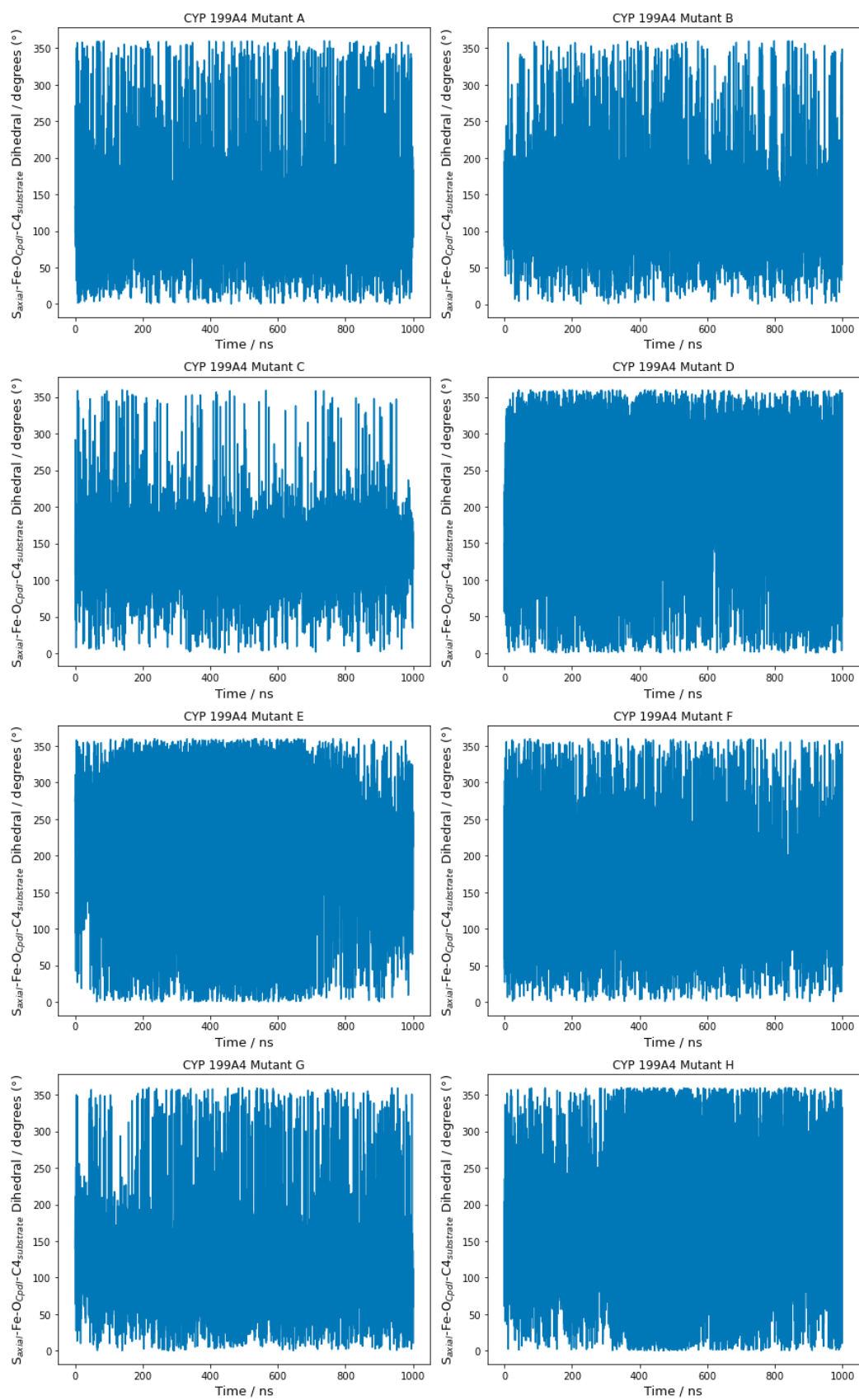


Fig. S27. Dihedral angle between S_{axial} , Fe, O_{Cpdl} and $C1_{substrate}$ in the mutant CYP199A4 structures throughout 1 μ s of MD production run. Top-Down and Left-Right: mutants A-H.

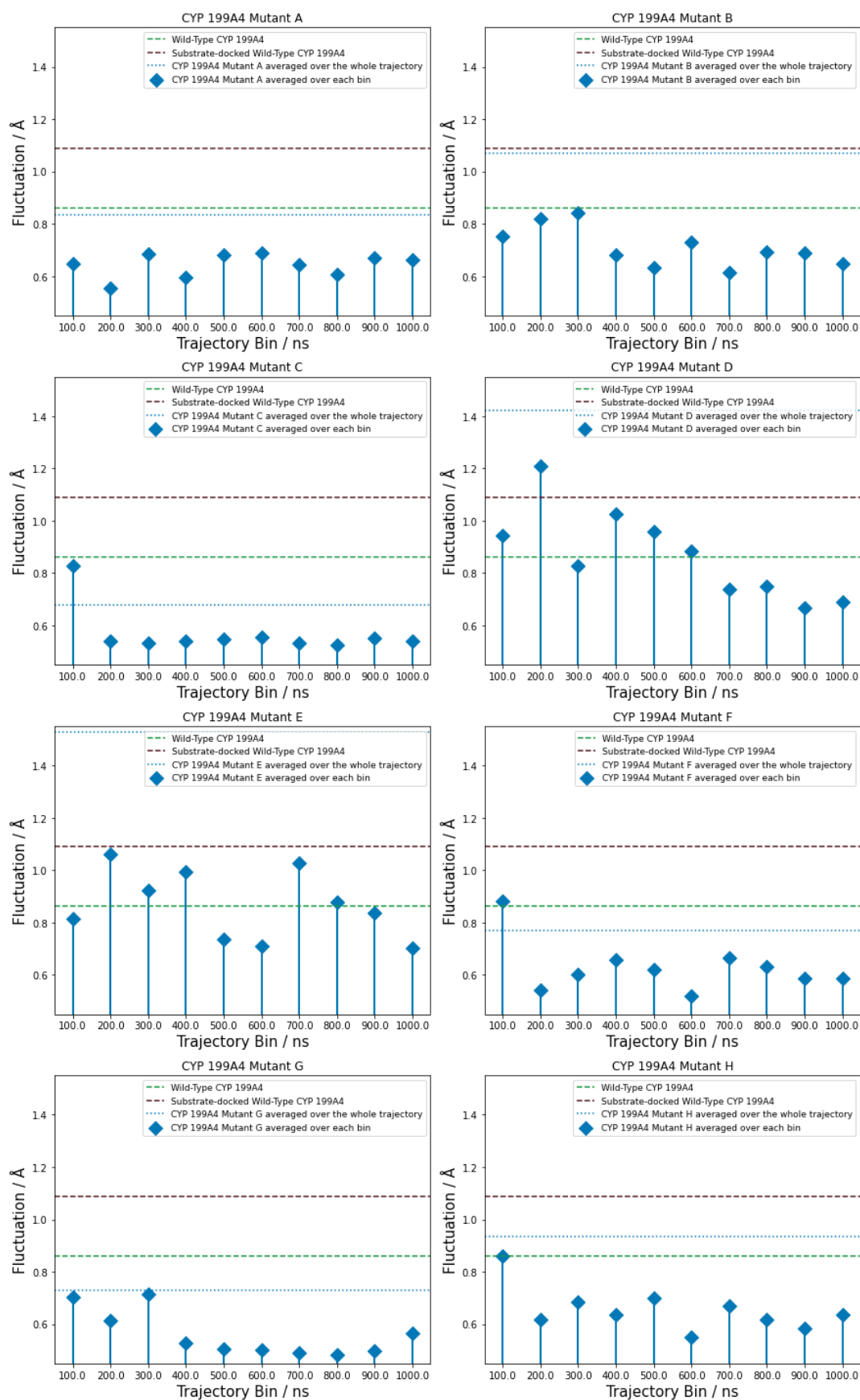


Fig. S28. RMSF of active site residues (all within 8 Å of O_{CpdI}) from mutant CYP199A4 structures throughout 1 μ s of MD production run. For comparison purposes, in each subplot there are horizontal lines that mark the RMSF of active site residues of the two wildtype CYP199A4 structures over their respective 100 ns-long MD runs Top-Down and Left-Right: mutants A-H.

Part 2.4 Unsupervised Learning for CYP199A4 Mutant Selection

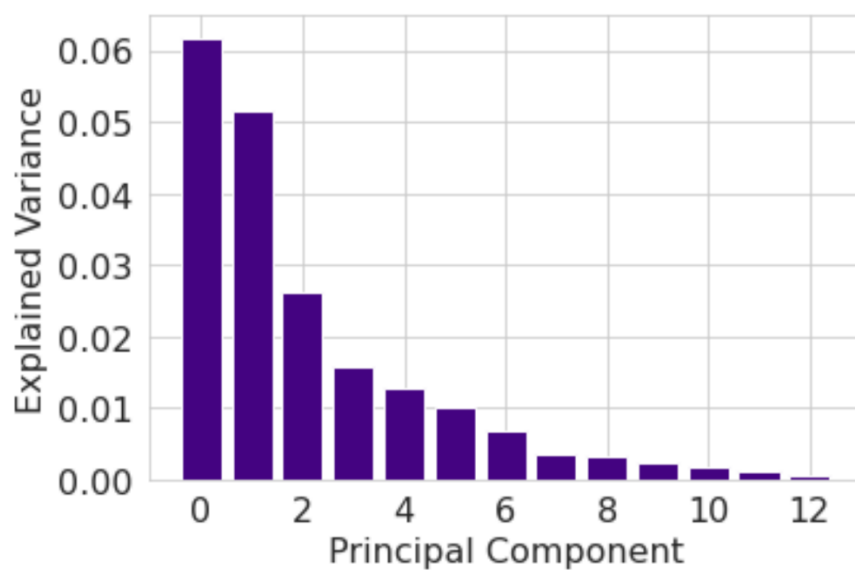


Fig. S29. Explained variance of the CYP199A4 dataset. Principal components which explained less than 0.01 of variance were discarded moving forward into the next steps. Thus, the intrinsic dimension of the dataset was determined to be 6.

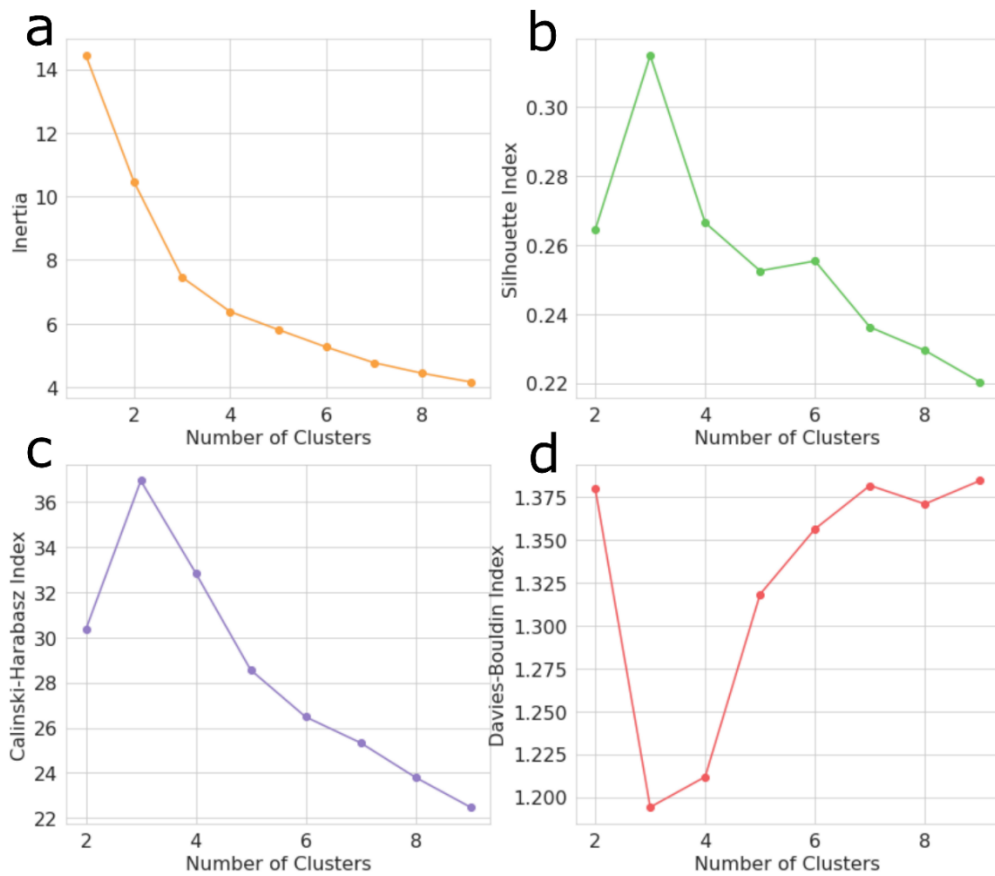


Fig. S30. Clustering metrics used to investigate the optimal grouping of datapoints from our CYP19A4, PCA-transformed, dataset: a) Inertia, or the within-cluster sum of squares, starts to moderately level off at $n=3$; b) Silhouette index, which indicate better clustering at higher values; c) Calinski-Harabasz index, just like the Silhouette, peaks at $n=3$ and represents better cluster separation at this value; d) and Davies-Bouldin index, which indicates higher quality clusters with lower values, bottoms at $n=3$. In conclusion, the optimal division of the data is splitting it into three distinct clusters.

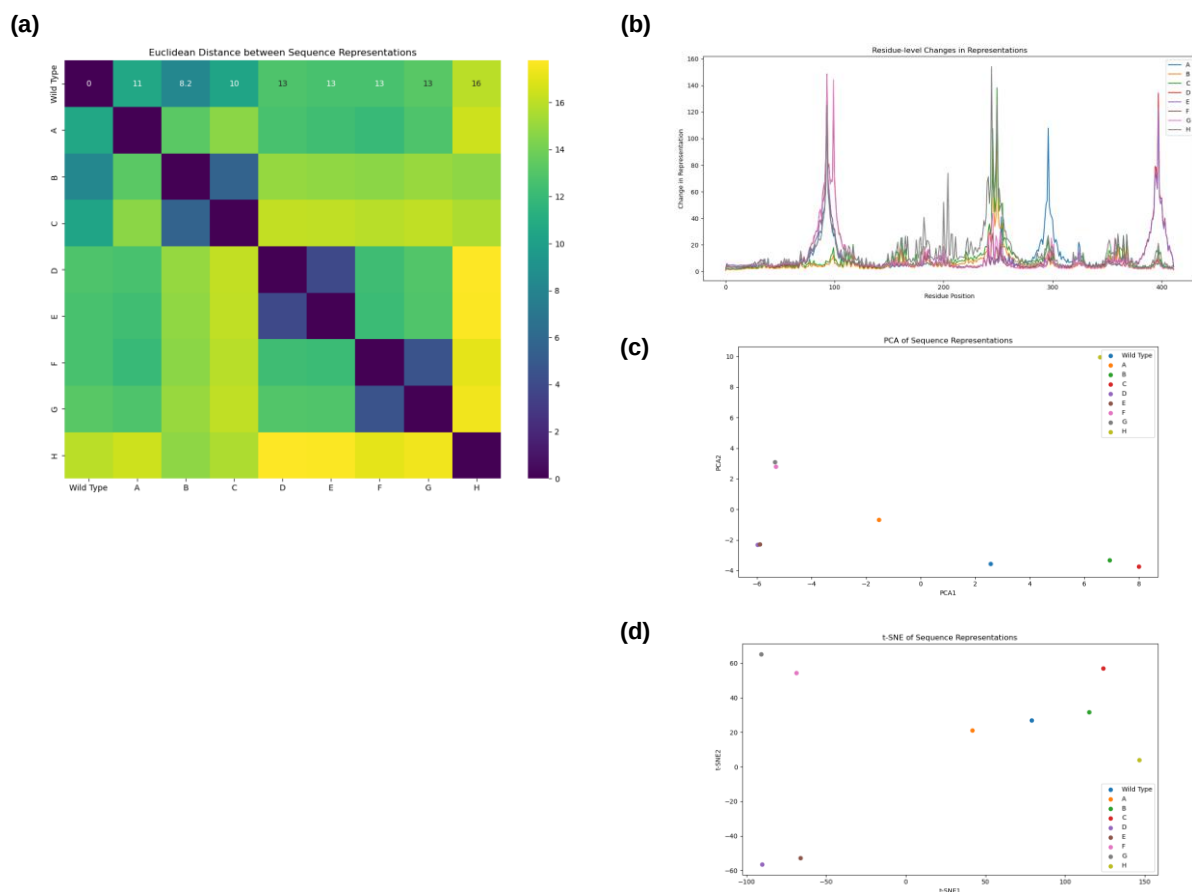


Fig. S31. Environmental sequence modelling of WT and eight selected mutants: a) Euclidian distance plot between WT and mutant selections. This Figure shows minor structural changes upon mutation and are expected to have little impact on structure and function; b) Residue levels plot, which highlights the key residues that are affected by the mutations; c) PCA plot comparing WT and mutant structures; d) t-SNE plot comparing WT and mutant structures.

Part 3: QM CLUSTER CALCULATIONS

Part 3.1 CYP255A system

Part 3.1.1 QM cluster energies, charges, and spin densities

Table S2: Absolute (free) energies (in au) of UB3LYP/BS1 optimized geometries of GcoA cluster model as obtained in Gaussian-09. Also shown are the degree of spin contamination in the structures (S^2 values).

	E [BS1, au]	ZPE	G [au]	E [BS2, au]	S^2
^2RC	-7135.13	2.60	-7132.79	-7137.08	1.7778
^4RC	-7135.13	2.60	-7132.79	-7137.08	3.7814
$^2\text{TS1}$	-7135.11	2.59	-7132.78	-7137.05	1.8098
$^4\text{TS1}$	-7135.12	2.59	-7132.78	-7137.06	3.8161
$^2\text{IM1}$	-7135.15	2.60	-7132.81	-7137.09	1.7694
$^4\text{IM1}$	-7135.15	2.60	-7132.81	-7137.08	3.7880
$^2\text{PR1}$	-7135.25	2.61	-7132.90	-7137.17	0.8807
$^4\text{PR1}$	-7135.25	2.61	-7132.90	-7137.18	3.7920

Table S3: Relative (free) energies (in au) of UB3LYP/BS1 optimized geometries of CYP255A cluster model as obtained in Gaussian-09.

	ΔE	$\Delta E + \text{ZPE}$	ΔG	$\Delta E [\text{BS2}]$	$\Delta E [\text{BS2}] + \text{ZPE}$	$\Delta G [\text{BS2}]$
^2RC	0.00	0.00	0.00	0.00	0.00	0.00
^4RC	0.08	0.11	-0.17	0.17	0.20	-0.08
$^2\text{TS1}$	7.88	4.49	4.36	4.00	10.71	10.58
$^4\text{TS1}$	3.91	0.74	0.99	9.09	5.92	6.17
$^2\text{IM1}$	-18.16	-17.50	-14.30	-5.64	-4.97	-1.78
$^4\text{IM1}$	-17.60	-17.07	-14.67	-5.12	-4.59	-2.19
$^2\text{PR1}$	-78.21	-74.16	-69.33	-60.75	-56.69	-51.87
$^4\text{PR1}$	-76.06	-72.49	-68.97	-62.39	-58.82	-55.30

Table S4: Group charges and spin densities (in au) of UB3LYP/BS1 optimized geometries of CYP255A cluster model as obtained in Gaussian-09.

(a) Charges

	Fe	O	Por	Axial	SubH	Prot	Total
² RC	0.50	-0.48	-0.26	0.04	-0.48	-0.32	-1.00
⁴ RC	0.49	-0.48	-0.26	0.04	-0.48	-0.32	-1.00
² TS1	0.44	-0.63	-0.23	0.10	-0.21	-0.48	-1.00
⁴ TS1	0.40	-0.64	-0.25	0.14	-0.18	-0.48	-1.00
² IM1	0.32	-0.78	-0.14	0.09	-0.01	-0.48	-1.00
⁴ IM1	0.32	-0.78	-0.14	0.08	-0.01	-0.48	-1.00
² PR1	0.25	-0.68	-0.32	0.07	0.26	-0.57	-1.00
⁴ PR1	0.43	-0.68	-0.35	-0.09	0.26	-0.57	-1.00

(b) Spin densities

	Fe	O	Por	Axial	SubH	Prot	Total
² RC	1.28	0.81	-0.25	-0.66	0.00	-0.19	1.00
⁴ RC	1.20	0.83	0.17	0.60	0.00	0.20	3.00
² TS1	0.85	-0.35	0.29	0.67	-0.46	0.00	1.00
⁴ TS1	1.06	0.59	0.20	0.62	0.52	0.00	3.00
² IM1	1.03	0.06	-0.52	-0.56	0.95	0.05	1.00
⁴ IM1	0.91	0.12	0.44	0.54	0.95	0.05	3.00
² PR1	1.16	0.00	-0.11	-0.04	0.00	0.00	1.00
⁴ PR1	2.41	0.00	0.05	0.54	0.00	0.00	3.00

Part 3.1.2: Cartesian coordinates of optimized geometries

²Reactant / LS_React

C	-0.812574000000	9.893979000000	2.891643000000
H	-1.884782000000	9.681273000000	2.964519000000
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C	1.596470000000	6.707046000000	4.570532000000
H	2.204653000000	5.915799000000	4.999575000000
C	2.165298000000	7.625678000000	3.682799000000
H	3.215585000000	7.546828000000	3.413925000000
C	1.378740000000	8.642807000000	3.135132000000
H	1.829935000000	9.360924000000	2.453065000000
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H	-10.368776000000	1.695186000000	4.361000000000
C	-8.359027000000	2.213291000000	3.825778000000
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O	1.571112000000	6.479878000000	-2.160035000000
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H	1.209599000000	6.702796000000	0.979925000000
C	3.138041000000	7.041436000000	0.151781000000
H	3.495643000000	7.040885000000	-0.882843000000
C	4.003127000000	6.075138000000	0.975708000000
O	5.003967000000	6.493755000000	1.547583000000
N	3.605866000000	4.771853000000	0.981384000000
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H	3.900948000000	1.972135000000	-4.580512000000
C	2.997828000000	3.904164000000	-4.257910000000
H	1.981825000000	3.495249000000	-4.283711000000
H	3.013633000000	4.737626000000	-3.545853000000
H	3.247986000000	4.293318000000	-5.247396000000

C	5.452485000000	3.308176000000	-4.144057000000
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C	8.635580000000	2.508846000000	-2.759936000000
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C	8.713306000000	-1.166416000000	1.668013000000
O	9.420488000000	-0.836305000000	2.617885000000
N	7.459095000000	-1.673105000000	1.825114000000
H	6.854150000000	-1.985919000000	1.063549000000
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N	7.334403000000	-1.650434000000	-2.829503000000
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H	7.378501000000	-3.649212000000	-2.182012000000
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H	5.531308000000	-4.463923000000	-3.495782000000
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C	3.375484000000	-7.208353000000	-3.287627000000
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C	3.544219000000	-9.055601000000	-4.441823000000
C	2.332016000000	-6.145850000000	-2.885867000000
H	1.499533000000	-6.653644000000	-2.368322000000
H	2.805775000000	-5.477573000000	-2.155126000000
C	1.772006000000	-5.309476000000	-4.044059000000
H	1.181370000000	-5.915386000000	-4.742044000000
H	1.132084000000	-4.498818000000	-3.677443000000
H	2.587643000000	-4.847875000000	-4.615129000000
C	2.073270000000	-4.485116000000	1.529937000000
H	2.497130000000	-4.576938000000	2.534801000000
C	1.983467000000	-2.999065000000	1.136463000000
H	2.987874000000	-2.571778000000	1.072272000000
H	1.508365000000	-2.886828000000	0.154432000000
H	1.392811000000	-2.437764000000	1.866041000000
C	0.694276000000	-5.109863000000	1.550624000000
O	-0.105709000000	-4.924121000000	2.480015000000
N	0.360929000000	-5.858748000000	0.463020000000
H	1.025289000000	-5.924380000000	-0.296604000000
C	-0.973496000000	-6.404867000000	0.289139000000
H	-1.331731000000	-6.740616000000	1.265844000000
C	-1.967038000000	-5.375492000000	-0.274935000000
H	-1.811972000000	-4.433419000000	0.267121000000
C	-1.797506000000	-5.130871000000	-1.766897000000
H	-2.528644000000	-4.400405000000	-2.129480000000
H	-0.811985000000	-4.706217000000	-1.980077000000
H	-1.924981000000	-6.064536000000	-2.329063000000

O	-3.275172000000	-5.893985000000	0.042857000000
H	-3.933572000000	-5.347023000000	-0.419186000000
C	-7.916776000000	-1.711014000000	-4.260604000000
H	-7.786893000000	-2.794763000000	-4.193451000000
H	-8.821298000000	-1.474858000000	-4.828735000000
S	-6.479102000000	-0.928372000000	-5.054338000000
C	6.615724000000	-5.542094000000	2.196857000000
H	7.619384000000	-5.132978000000	2.016684000000
H	6.019965000000	-5.334676000000	1.301265000000
C	6.004611000000	-4.909052000000	3.424998000000
C	5.241904000000	-3.735603000000	3.310294000000
H	5.071586000000	-3.317829000000	2.320461000000
C	4.713810000000	-3.111910000000	4.444053000000
H	4.130096000000	-2.200891000000	4.333014000000
C	4.930293000000	-3.654043000000	5.714082000000
H	4.526124000000	-3.164116000000	6.597005000000
C	5.674214000000	-4.829186000000	5.838726000000
H	5.844533000000	-5.265066000000	6.820716000000
C	6.204064000000	-5.447057000000	4.704108000000
H	6.785659000000	-6.360858000000	4.811597000000
O	-3.049052000000	-1.602960000000	-2.704303000000
Fe	-4.379925000000	-1.447698000000	-3.640265000000
N	-5.362815000000	-2.948561000000	-2.716991000000
N	-3.731886000000	-2.738439000000	-5.045786000000
N	-5.280448000000	-0.119236000000	-2.410291000000
C	-6.417104000000	-1.683072000000	-0.892359000000
C	-4.653799000000	-4.820643000000	-4.138018000000
C	-2.518973000000	-1.178908000000	-6.497823000000
C	-4.394673000000	1.970546000000	-3.338122000000
C	-6.078041000000	-2.862122000000	-1.549950000000
C	-3.916169000000	-4.095986000000	-5.063914000000
C	-2.851475000000	-0.002154000000	-5.843591000000
C	-5.135656000000	1.248538000000	-2.415855000000
C	-6.475857000000	-4.177540000000	-1.112776000000
C	-3.217294000000	-4.680946000000	-6.183832000000
C	-2.424093000000	1.310494000000	-6.262980000000
C	-5.861067000000	1.829972000000	-1.310195000000
C	-5.998621000000	-5.061162000000	-2.037717000000
C	-2.604368000000	-3.658001000000	-6.838206000000
C	-2.954058000000	2.196372000000	-5.375910000000
C	-6.427847000000	0.800761000000	-0.622933000000
C	-5.303166000000	-4.282494000000	-3.033752000000
C	-2.935841000000	-2.449862000000	-6.120536000000
C	-3.704474000000	1.424917000000	-4.413393000000
C	-6.050066000000	-0.411907000000	-1.309937000000
N	-3.635192000000	0.090679000000	-4.720065000000
H	-7.017567000000	-1.745266000000	0.010658000000
H	-4.700651000000	-5.897323000000	-4.268706000000
H	-1.884788000000	-1.101178000000	-7.375251000000
H	-4.345485000000	3.046693000000	-3.205773000000
C	-0.130744000000	1.197036000000	-2.837637000000
C	-1.120952000000	-1.144142000000	3.097183000000
C	-1.682028000000	-1.713809000000	1.950538000000
C	-0.231091000000	-0.075091000000	2.984575000000
C	-1.327179000000	-1.227061000000	0.690642000000
C	-0.852125000000	0.932271000000	-1.529032000000
C	0.120122000000	0.419373000000	1.725597000000
C	-0.411556000000	-0.178060000000	0.570062000000
O	1.017749000000	1.465029000000	1.654834000000
O	0.071966000000	0.229528000000	-0.662464000000
H	-1.359025000000	-1.548291000000	4.076938000000
H	-2.347826000000	-2.567314000000	2.040610000000
H	0.218895000000	0.381796000000	3.861623000000
H	-1.714317000000	-1.688402000000	-0.212892000000
H	-1.746933000000	0.320965000000	-1.689577000000
H	-1.146397000000	1.868440000000	-1.038927000000
H	0.779191000000	1.781931000000	-2.667746000000
H	0.142607000000	0.251812000000	-3.316251000000
H	-0.784160000000	1.751774000000	-3.518640000000
H	0.731995000000	2.117361000000	0.972425000000
O	-2.971965000000	-4.877448000000	2.764312000000

H	-1.992562000000	-4.910014000000	2.729935000000
H	-3.250837000000	-5.324014000000	1.940887000000
O	-0.178996000000	-2.258786000000	-2.545043000000
H	-1.132774000000	-2.092638000000	-2.670644000000
H	0.104350000000	-1.582494000000	-1.907317000000
H	-8.028972000000	-1.317385000000	-3.243381000000
H	-1.799141000000	1.508344000000	-7.124412000000
H	-2.855939000000	3.274628000000	-5.360858000000
H	-1.980818000000	-3.697298000000	-7.722072000000
H	-3.202275000000	-5.737985000000	-6.416747000000
H	-6.103812000000	-6.138657000000	-2.059372000000
H	-7.056317000000	-4.379972000000	-0.221678000000
H	-5.924166000000	2.892221000000	-1.106615000000
H	-7.044952000000	0.813564000000	0.265775000000
H	-0.630862000000	10.831988000000	3.432761000000
H	-0.918317000000	-7.277951000000	-0.369950000000
H	3.302299000000	8.040677000000	0.565771000000
H	6.720802000000	-6.627068000000	2.316236000000
H	2.384293000000	-3.790865000000	9.035605000000
H	8.008352000000	4.532494000000	-2.671141000000
H	-9.198048000000	-0.266079000000	4.944413000000
H	-6.419310000000	-2.511235000000	2.324521000000
H	2.747441000000	-4.997647000000	0.836295000000
H	4.531728000000	-6.973327000000	-1.457681000000
H	4.843302000000	-8.504320000000	-2.311620000000
H	-0.743798000000	4.851550000000	3.007624000000
H	7.728174000000	-3.392402000000	-3.885825000000

⁴Reactant / HS_React

C	-0.819145000000	9.892778000000	2.882253000000
H	-1.891490000000	9.680569000000	2.954481000000
H	-0.578563000000	10.080793000000	1.829250000000
C	0.010919000000	8.764103000000	3.451738000000
C	-0.545198000000	7.833445000000	4.339579000000
H	-1.597030000000	7.913111000000	4.607057000000
C	0.234959000000	6.815296000000	4.896229000000
H	-0.214126000000	6.110536000000	5.591640000000
C	1.587216000000	6.706144000000	4.565588000000
H	2.194719000000	5.915133000000	4.996039000000
C	2.157582000000	7.624919000000	3.678984000000
H	3.208381000000	7.546277000000	3.412039000000
C	1.371895000000	8.641939000000	3.129855000000
H	1.824260000000	9.360152000000	2.448662000000
C	-9.377999000000	-0.126076000000	3.877113000000
H	-10.280751000000	-0.697023000000	3.623988000000
C	-9.638200000000	1.378727000000	3.610433000000
H	-10.372681000000	1.689475000000	4.370125000000
C	-8.363572000000	2.208756000000	3.833613000000
H	-7.923964000000	2.002357000000	4.817468000000
H	-7.606511000000	1.979666000000	3.073857000000
H	-8.570900000000	3.282733000000	3.786503000000
C	-10.285577000000	1.623975000000	2.231695000000
H	-9.589651000000	1.315271000000	1.445014000000
H	-11.155104000000	0.957800000000	2.140213000000
C	-10.744351000000	3.068799000000	2.001137000000
H	-9.901864000000	3.768854000000	1.968975000000
H	-11.277571000000	3.158374000000	1.047681000000
H	-11.425539000000	3.404618000000	2.794375000000
C	-8.228489000000	-0.729102000000	3.069324000000
O	-8.215475000000	-0.709441000000	1.832993000000
N	-7.239330000000	-1.300892000000	3.798494000000
H	-7.293031000000	-1.257806000000	4.805366000000
C	-6.074826000000	-1.960092000000	3.205492000000
H	-5.365845000000	-1.202701000000	2.843457000000
C	-5.370375000000	-2.911630000000	4.186157000000
H	-4.536672000000	-3.350384000000	3.622901000000
C	-4.767786000000	-2.154518000000	5.383311000000
H	-4.171149000000	-1.299337000000	5.043943000000
H	-5.537127000000	-1.774867000000	6.072822000000
H	-4.104251000000	-2.799312000000	5.966640000000
C	-6.291052000000	-4.075789000000	4.611169000000

H	-7.106681000000	-3.700914000000	5.248567000000
H	-6.775101000000	-4.478567000000	3.710057000000
C	-5.558061000000	-5.217391000000	5.326536000000
H	-5.138226000000	-4.892472000000	6.285707000000
H	-6.240283000000	-6.050695000000	5.533820000000
H	-4.735010000000	-5.588724000000	4.706341000000
C	1.432713000000	-3.252683000000	9.130167000000
H	1.059259000000	-3.414404000000	10.147371000000
H	1.653185000000	-2.181414000000	9.027340000000
C	0.433900000000	-3.714964000000	8.092603000000
C	0.811637000000	-3.852039000000	6.748084000000
H	1.840095000000	-3.647460000000	6.456157000000
C	-0.105010000000	-4.261768000000	5.779158000000
H	0.198974000000	-4.367721000000	4.741199000000
C	-1.425030000000	-4.549710000000	6.143731000000
H	-2.132962000000	-4.877912000000	5.387215000000
C	-1.812834000000	-4.422631000000	7.478854000000
H	-2.832901000000	-4.657463000000	7.776128000000
C	-0.890088000000	-4.006585000000	8.443074000000
H	-1.199773000000	-3.913495000000	9.482669000000
C	-1.055017000000	4.081645000000	2.274853000000
H	-0.585398000000	3.142505000000	2.577408000000
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H	-3.045474000000	4.911023000000	2.055980000000
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H	-4.187442000000	2.803598000000	1.332799000000
H	-2.847966000000	3.198513000000	0.253253000000
C	-3.045240000000	3.562212000000	3.724324000000
H	-4.137554000000	3.493749000000	3.782169000000
H	-2.633011000000	2.588191000000	4.014357000000
H	-2.712549000000	4.303273000000	4.461448000000
C	-0.467956000000	4.456970000000	0.924711000000
O	0.315252000000	3.733491000000	0.288306000000
N	-0.813383000000	5.680223000000	0.435131000000
H	-1.555147000000	6.184361000000	0.903426000000
C	-0.432583000000	6.102365000000	-0.909865000000
H	-0.592024000000	5.267381000000	-1.599504000000
C	-1.289626000000	7.307006000000	-1.368157000000
H	-1.130103000000	8.143525000000	-0.674279000000
H	-0.890415000000	7.617834000000	-2.338751000000
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C	-3.661083000000	7.303272000000	-0.440142000000
H	-3.310487000000	7.875774000000	0.417516000000
C	-5.001464000000	6.924636000000	-0.491654000000
H	-5.689585000000	7.170765000000	0.310766000000
C	-5.476682000000	6.213880000000	-1.598159000000
O	-6.789771000000	5.835938000000	-1.589918000000
H	-6.991319000000	5.352942000000	-2.407149000000
C	-4.608486000000	5.919586000000	-2.656592000000
H	-4.982043000000	5.400787000000	-3.537596000000
C	-3.267946000000	6.294946000000	-2.582306000000
H	-2.602805000000	6.050080000000	-3.407329000000
C	1.064381000000	6.442523000000	-1.048251000000
O	1.574520000000	6.480108000000	-2.162101000000
N	1.726777000000	6.713895000000	0.108444000000
H	1.208463000000	6.702241000000	0.977419000000
C	3.138137000000	7.040790000000	0.152189000000
H	3.497196000000	7.040924000000	-0.881931000000
C	4.002295000000	6.074124000000	0.976625000000
O	5.002403000000	6.492521000000	1.549941000000
N	3.605107000000	4.770803000000	0.981223000000
H	2.724421000000	4.520367000000	0.545782000000
C	4.422745000000	3.715678000000	1.597640000000
H	5.396386000000	4.176553000000	1.774846000000
C	3.840457000000	3.241082000000	2.944421000000
H	3.544074000000	4.154270000000	3.477540000000
H	2.917400000000	2.664000000000	2.796868000000
C	4.817607000000	2.454150000000	3.846026000000
H	5.722171000000	3.070180000000	3.961677000000
C	4.195029000000	2.273050000000	5.239965000000

H	3.933170000000	3.237552000000	5.694024000000
H	3.280177000000	1.668068000000	5.185690000000
H	4.890369000000	1.761775000000	5.915384000000
C	5.245244000000	1.094380000000	3.271279000000
H	5.895148000000	0.569294000000	3.980001000000
H	4.374555000000	0.453418000000	3.081171000000
H	5.810750000000	1.184514000000	2.339285000000
C	4.670388000000	2.648670000000	0.512252000000
O	5.705825000000	2.667303000000	-0.154869000000
N	3.655423000000	1.778576000000	0.251599000000
H	2.890403000000	1.663620000000	0.912798000000
C	3.842441000000	0.684395000000	-0.700180000000
H	4.568868000000	-0.058072000000	-0.351228000000
H	2.873724000000	0.182786000000	-0.801736000000
C	4.285078000000	1.148285000000	-2.086696000000
O	5.051277000000	0.470397000000	-2.776565000000
N	3.750048000000	2.309368000000	-2.544541000000
H	3.158614000000	2.844478000000	-1.922632000000
C	4.012265000000	2.812403000000	-3.889813000000
H	3.903695000000	1.969519000000	-4.580834000000
C	3.000979000000	3.901824000000	-4.258596000000
H	1.984813000000	3.493325000000	-4.284795000000
H	3.016868000000	4.735342000000	-3.546613000000
H	3.251663000000	4.290789000000	-5.248025000000
C	5.455326000000	3.305173000000	-4.143242000000
O	5.779217000000	3.591727000000	-5.293150000000
N	6.289064000000	3.378976000000	-3.073753000000
H	5.953123000000	3.139131000000	-2.144517000000
C	7.707616000000	3.640172000000	-3.227655000000
H	7.885949000000	3.833128000000	-4.289428000000
C	8.637523000000	2.508242000000	-2.756238000000
O	9.807429000000	2.769164000000	-2.490709000000
N	8.091348000000	1.263053000000	-2.685701000000
H	7.094423000000	1.157603000000	-2.846886000000
C	8.813303000000	0.168661000000	-2.036602000000
H	9.874289000000	0.400669000000	-2.133461000000
C	8.432452000000	0.081577000000	-0.537531000000
H	8.651280000000	1.052913000000	-0.079222000000
H	7.350450000000	-0.071491000000	-0.452855000000
C	9.177394000000	-1.032127000000	0.221206000000
H	9.035134000000	-1.991856000000	-0.290339000000
H	10.250717000000	-0.823696000000	0.242056000000
C	8.715281000000	-1.166979000000	1.672219000000
O	9.421278000000	-0.836191000000	2.622715000000
N	7.461446000000	-1.675005000000	1.828241000000
H	6.857568000000	-1.988255000000	1.066100000000
H	7.136933000000	-1.828264000000	2.772923000000
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O	9.591967000000	-1.878282000000	-3.043215000000
N	7.338430000000	-1.651422000000	-2.826042000000
H	6.583533000000	-1.105568000000	-2.425631000000
C	7.083108000000	-3.070443000000	-3.064240000000
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C	5.620290000000	-3.375996000000	-3.397652000000
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C	4.587766000000	-2.881671000000	-2.361696000000
H	4.505838000000	-1.793677000000	-2.416429000000
H	3.608878000000	-3.298851000000	-2.625240000000
C	4.930980000000	-3.284286000000	-0.917308000000
O	4.751990000000	-4.492079000000	-0.592794000000
O	5.377900000000	-2.383781000000	-0.142678000000
C	4.067485000000	-7.781610000000	-2.038163000000
H	3.343741000000	-8.298855000000	-1.391878000000
C	3.377015000000	-7.211733000000	-3.286285000000
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H	1.998307000000	-8.874063000000	-3.601594000000
H	2.326672000000	-7.940981000000	-5.072433000000
H	3.546384000000	-9.058153000000	-4.441672000000
C	2.333480000000	-6.149093000000	-2.885006000000

H	1.500019000000	-6.656907000000	-2.368988000000
H	2.806481000000	-5.481588000000	-2.153027000000
C	1.775465000000	-5.311457000000	-4.043218000000
H	1.185799000000	-5.916660000000	-4.742644000000
H	1.135119000000	-4.501073000000	-3.676785000000
H	2.592064000000	-4.849539000000	-4.612645000000
C	2.075133000000	-4.488034000000	1.529487000000
H	2.499525000000	-4.580910000000	2.534052000000
C	1.985926000000	-3.001688000000	1.137152000000
H	2.990386000000	-2.574442000000	1.073303000000
H	1.510963000000	-2.888739000000	0.155134000000
H	1.395270000000	-2.440737000000	1.867007000000
C	0.695772000000	-5.112023000000	1.550539000000
O	-0.104125000000	-4.924815000000	2.479686000000
N	0.362244000000	-5.862076000000	0.463750000000
H	1.026504000000	-5.928204000000	-0.295949000000
C	-0.972306000000	-6.408165000000	0.290627000000
H	-1.330822000000	-6.741506000000	1.268035000000
C	-1.965491000000	-5.379803000000	-0.275984000000
H	-1.809857000000	-4.436396000000	0.263628000000
C	-1.795902000000	-5.139187000000	-1.768621000000
H	-2.526285000000	-4.408886000000	-2.133072000000
H	-0.809909000000	-4.716150000000	-1.982764000000
H	-1.924310000000	-6.074219000000	-2.328289000000
O	-3.273805000000	-5.896853000000	0.043277000000
H	-3.932081000000	-5.349785000000	-0.418870000000
C	-7.913725000000	-1.701216000000	-4.252134000000
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C	6.619216000000	-5.545467000000	2.198100000000
H	7.622662000000	-5.135649000000	2.018349000000
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C	6.007152000000	-4.912836000000	3.425986000000
C	5.244053000000	-3.739672000000	3.310968000000
H	5.074035000000	-3.321939000000	2.321075000000
C	4.715201000000	-3.116170000000	4.444477000000
H	4.131298000000	-2.205302000000	4.333174000000
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H	4.526470000000	-3.168550000000	6.597327000000
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C	6.206113000000	-5.450849000000	4.705164000000
H	6.787980000000	-6.364443000000	4.812931000000
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Fe	-4.382275000000	-1.432881000000	-3.632863000000
N	-5.359888000000	-2.939282000000	-2.711376000000
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C	-6.416175000000	-1.679839000000	-0.885095000000
C	-4.650569000000	-4.806773000000	-4.139060000000
C	-2.520680000000	-1.157629000000	-6.490847000000
C	-4.404822000000	1.983029000000	-3.327353000000
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C	-5.877591000000	1.835505000000	-1.305204000000
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C	-2.934699000000	-2.430371000000	-6.116089000000
C	-3.711537000000	1.440684000000	-4.402360000000
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C	-1.681017000000	-1.715792000000	1.946010000000
C	-0.232837000000	-0.074279000000	2.979393000000
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C	-0.847131000000	0.926521000000	-1.535800000000
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O	1.017039000000	1.464484000000	1.649126000000
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H	-1.361606000000	-1.546164000000	4.072651000000
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H	0.215511000000	0.384471000000	3.856311000000
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O	-2.971027000000	-4.877476000000	2.763503000000
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H	-3.249401000000	-5.324883000000	1.940328000000
O	-0.175006000000	-2.269646000000	-2.547120000000
H	-1.128492000000	-2.103282000000	-2.674691000000
H	0.107145000000	-1.592805000000	-1.909499000000
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H	-3.193888000000	-5.718617000000	-6.417203000000
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H	3.301691000000	8.039788000000	0.567030000000
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H	8.009059000000	4.531494000000	-2.667891000000
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H	-6.422822000000	-2.513306000000	2.327495000000
H	2.748631000000	-5.000517000000	0.835173000000
H	4.531743000000	-6.978717000000	-1.455164000000
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H	-0.750311000000	4.848076000000	3.000458000000
H	7.733694000000	-3.393170000000	-3.882173000000

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C	4.693328000000	9.956730000000	-2.893843000000
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C	1.409064000000	8.078478000000	-3.453309000000
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C	2.358993000000	8.973456000000	-2.955479000000
H	2.059798000000	9.710469000000	-2.213379000000
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C	9.640245000000	-0.348722000000	-2.291310000000
H	9.081494000000	0.424935000000	-2.830905000000
H	9.915668000000	0.055561000000	-1.307999000000
H	10.570481000000	-0.531700000000	-2.844398000000
C	6.644325000000	-3.874556000000	-2.464407000000
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C	4.177341000000	-4.216931000000	-2.678663000000
H	3.567217000000	-3.415071000000	-3.114928000000
C	3.493299000000	-5.575769000000	-2.922511000000
H	2.517939000000	-5.504393000000	-2.421422000000
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H	2.613717000000	-6.709923000000	-4.572918000000
C	4.272356000000	-6.733752000000	-2.266330000000
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H	4.842925000000	3.044360000000	-3.536614000000
C	4.232248000000	1.199499000000	-2.618390000000
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H	4.421854000000	1.529157000000	-1.590573000000
C	3.772744000000	1.905674000000	-5.007255000000
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C	2.835825000000	3.767074000000	-1.710701000000
O	2.153598000000	3.367904000000	-0.753423000000
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H	5.122395000000	7.026599000000	-0.796549000000
H	5.567074000000	6.413762000000	0.796694000000
C	6.531802000000	5.396812000000	-0.859033000000
C	6.947071000000	5.682496000000	-2.168243000000
H	6.464462000000	6.489006000000	-2.717741000000
C	7.965554000000	4.957784000000	-2.787039000000
H	8.280095000000	5.180235000000	-3.801867000000
C	8.595339000000	3.919290000000	-2.094441000000

O	9.572781000000	3.223126000000	-2.748393000000
H	9.887448000000	2.501184000000	-2.181509000000
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C	7.192812000000	4.366973000000	-0.174805000000
H	6.902066000000	4.125925000000	0.845189000000
C	2.934494000000	5.935990000000	0.543854000000
O	2.906604000000	5.965551000000	1.767708000000
N	2.010091000000	6.524438000000	-0.261713000000
H	2.154813000000	6.497836000000	-1.263019000000
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H	-2.396270000000	3.684077000000	-6.078804000000
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H	-1.360965000000	2.547750000000	-0.506154000000
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H	-3.854871000000	1.591897000000	-0.049439000000
H	-2.475452000000	1.233650000000	0.998313000000
C	-3.845027000000	2.677746000000	1.776068000000
O	-4.940338000000	2.247017000000	2.131335000000
N	-3.223501000000	3.700268000000	2.419884000000
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H	-4.180537000000	3.596092000000	4.258021000000
C	-2.788568000000	5.242225000000	4.275539000000
H	-1.953772000000	4.635365000000	4.642782000000
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H	-3.264983000000	5.744248000000	5.120515000000
C	-5.091061000000	5.202469000000	3.250952000000
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H	-4.764686000000	5.058066000000	1.217785000000
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H	-7.176454000000	6.300544000000	2.420537000000
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O	-8.164863000000	6.011109000000	-0.266066000000
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O	-6.384544000000	2.044652000000	-4.771907000000
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O	-5.568177000000	-2.622498000000	0.029527000000
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H	-3.151008000000	-1.429852000000	6.171666000000
H	-4.042220000000	-1.555750000000	4.664137000000
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H	-4.470475000000	-3.991168000000	-3.713005000000
C	-3.066728000000	-2.458416000000	-4.313017000000
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O	-1.842818000000	-4.438983000000	-2.601423000000
N	-3.411652000000	-4.011516000000	-0.991101000000
H	-4.263453000000	-3.480252000000	-0.739423000000
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C	-1.676959000000	-3.702925000000	0.751262000000
H	-1.221997000000	-3.094346000000	-0.039373000000
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H	-1.625817000000	-2.036132000000	2.168889000000
H	-3.187771000000	-2.282796000000	1.359781000000
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O	-0.654213000000	-4.537033000000	1.340700000000
H	-0.024467000000	-3.949804000000	1.789894000000
C	5.379376000000	-4.954782000000	5.043081000000
H	4.531694000000	-5.626185000000	4.883986000000
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S	4.847027000000	-3.380474000000	5.778102000000
C	-7.881262000000	-5.186188000000	-0.643805000000
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H	-7.183391000000	-4.500296000000	-0.153984000000
C	-8.328812000000	-4.641777000000	-1.982936000000
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O	2.063720000000	-1.424599000000	3.163961000000
Fe	3.164214000000	-2.274055000000	4.255779000000
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N	1.573130000000	-2.747197000000	5.404242000000
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C	5.637674000000	0.127166000000	4.385495000000
C	3.640052000000	-4.406262000000	2.151577000000
C	0.740124000000	-3.824610000000	5.275447000000
C	2.768728000000	-0.202312000000	6.439136000000
C	5.747021000000	-0.846532000000	3.406291000000
C	3.093532000000	-5.633388000000	1.622464000000
C	-0.345523000000	-3.741001000000	6.225206000000
C	3.336313000000	0.999114000000	6.999335000000
C	6.787289000000	-0.907293000000	2.409189000000
C	2.026446000000	-5.957131000000	2.402803000000
C	-0.157084000000	-2.591465000000	6.928829000000
C	4.484635000000	1.249657000000	6.310381000000
C	6.526043000000	-1.987636000000	1.622106000000
C	1.915439000000	-4.921880000000	3.402645000000
C	1.045721000000	-1.981018000000	6.408411000000
C	4.612248000000	0.205943000000	5.324229000000
C	5.327803000000	-2.598843000000	2.145890000000
N	3.561591000000	-0.671385000000	5.420364000000
H	5.234838000000	-4.181586000000	0.753070000000
H	0.161703000000	-5.644789000000	4.345825000000
H	1.069410000000	-0.301153000000	7.699701000000
H	6.404111000000	0.895721000000	4.417431000000
C	2.745869000000	1.798376000000	2.577812000000
C	0.504462000000	-1.984611000000	-2.151110000000
C	1.253665000000	-2.459058000000	-1.071629000000
C	0.173023000000	-0.630080000000	-2.229654000000
C	1.657356000000	-1.590284000000	-0.053059000000
C	2.664619000000	0.567944000000	1.708491000000
C	0.569915000000	0.244502000000	-1.220374000000
C	1.298442000000	-0.244782000000	-0.120565000000
O	0.221139000000	1.573065000000	-1.294859000000
O	1.547223000000	0.685207000000	0.870948000000
H	0.142505000000	-2.677151000000	-2.904021000000
H	1.461148000000	-3.521438000000	-0.996317000000
H	-0.405473000000	-0.234147000000	-3.059394000000
H	2.182206000000	-1.959787000000	0.820988000000
H	2.483469000000	-0.444106000000	2.498571000000
H	3.565604000000	0.302257000000	1.141791000000
H	2.814137000000	2.706305000000	1.964771000000
H	1.844645000000	1.866754000000	3.196594000000
H	3.615967000000	1.741025000000	3.235599000000
H	0.950359000000	2.128595000000	-0.919831000000
O	0.374547000000	-5.657014000000	-1.174328000000
H	-0.352705000000	-5.251753000000	-1.695512000000
H	0.160460000000	-5.402240000000	-0.254180000000
O	-0.301395000000	0.153984000000	3.192796000000
H	0.385413000000	-0.516978000000	3.388727000000
H	-0.023717000000	0.485498000000	2.324264000000
H	5.852166000000	-4.763188000000	4.072244000000
H	2.900410000000	1.564901000000	7.812860000000
H	5.184541000000	2.065149000000	6.441240000000
H	-0.765990000000	-2.177954000000	7.722562000000
H	-1.142801000000	-4.467197000000	6.317882000000
H	1.346518000000	-6.792511000000	2.302649000000
H	3.477554000000	-6.159060000000	0.758734000000
H	7.606340000000	-0.202524000000	2.336072000000
H	7.062224000000	-2.366556000000	0.761833000000
H	4.554771000000	10.932468000000	-3.377832000000
H	-3.397492000000	-5.036263000000	0.814092000000
H	0.901127000000	8.277352000000	0.170426000000
H	-7.381010000000	-6.157756000000	-0.757501000000
H	-2.689964000000	-9.739101000000	-7.540733000000
H	-6.342899000000	7.085059000000	1.071264000000
H	7.857571000000	-4.269594000000	-4.223557000000
H	4.259047000000	-4.013285000000	-1.609724000000
H	-4.523786000000	-2.562858000000	-2.694261000000

H	-5.872476000000	-2.901448000000	5.595995000000
H	-6.716777000000	-2.394599000000	7.070100000000
H	2.574992000000	4.037333000000	-3.815647000000
H	-9.594286000000	-0.136049000000	1.259834000000

***TransitionState / HS_TS1**

C	-5.546083000000	9.646335000000	2.770257000000
H	-6.522506000000	9.210782000000	3.007851000000
H	-5.502779000000	9.812941000000	1.688210000000
C	-4.412045000000	8.764607000000	3.242974000000
C	-4.601643000000	7.829650000000	4.270713000000
H	-5.586566000000	7.726401000000	4.722523000000
C	-3.540849000000	7.048382000000	4.738307000000
H	-3.707261000000	6.341697000000	5.547859000000
C	-2.267423000000	7.188031000000	4.180883000000
H	-1.437369000000	6.593644000000	4.553426000000
C	-2.061882000000	8.113170000000	3.151249000000
H	-1.076658000000	8.232643000000	2.707203000000
C	-3.128882000000	8.887950000000	2.688721000000
H	-2.959037000000	9.608039000000	1.891148000000
C	-7.733694000000	-4.220175000000	3.081456000000
H	-8.401767000000	-4.813279000000	2.447037000000
C	-8.383752000000	-2.835448000000	3.346052000000
H	-9.334200000000	-3.052385000000	3.857947000000
C	-7.527186000000	-1.985618000000	4.298308000000
H	-7.302072000000	-2.532039000000	5.222721000000
H	-6.572757000000	-1.709364000000	3.833788000000
H	-8.039985000000	-1.061464000000	4.584920000000
C	-8.727461000000	-2.093077000000	2.038381000000
H	-7.800845000000	-1.787039000000	1.539661000000
H	-9.217276000000	-2.797085000000	1.353448000000
C	-9.644416000000	-0.877735000000	2.234714000000
H	-9.169825000000	-0.097493000000	2.841520000000
H	-9.906819000000	-0.438962000000	1.262889000000
H	-10.580737000000	-1.162435000000	2.732286000000
C	-6.386430000000	-4.165488000000	2.359927000000
O	-6.318778000000	-3.941900000000	1.147902000000
N	-5.295044000000	-4.365026000000	3.146815000000
H	-5.448416000000	-4.557808000000	4.126234000000
C	-3.913039000000	-4.361168000000	2.664553000000
H	-3.371864000000	-3.532041000000	3.139298000000
C	-3.155480000000	-5.680473000000	2.910189000000
H	-2.170430000000	-5.544116000000	2.442820000000
C	-2.925806000000	-5.934737000000	4.409417000000
H	-2.457543000000	-5.066844000000	4.889811000000
H	-3.867253000000	-6.149508000000	4.937152000000
H	-2.259635000000	-6.787552000000	4.570531000000
C	-3.843473000000	-6.870947000000	2.211118000000
H	-4.766208000000	-7.133398000000	2.749156000000
H	-4.166237000000	-6.551944000000	1.209836000000
C	-2.948983000000	-8.109389000000	2.073838000000
H	-2.670799000000	-8.521668000000	3.050120000000
H	-3.460092000000	-8.902765000000	1.514676000000
H	-2.021026000000	-7.857672000000	1.547733000000
C	1.933108000000	-9.302715000000	7.766480000000
H	1.395093000000	-10.219316000000	8.032282000000
H	1.720698000000	-8.553173000000	8.538942000000
C	1.541379000000	-8.810014000000	6.391009000000
C	1.954755000000	-7.547474000000	5.938815000000
H	2.552000000000	-6.916569000000	6.595187000000
C	1.615932000000	-7.089731000000	4.665330000000
H	1.940740000000	-6.109814000000	4.324347000000
C	0.850056000000	-7.893504000000	3.813158000000
H	0.589161000000	-7.529794000000	2.822479000000
C	0.429693000000	-9.150286000000	4.252485000000
H	-0.164577000000	-9.784813000000	3.598576000000
C	0.772326000000	-9.602261000000	5.530433000000
H	0.440305000000	-10.584099000000	5.863707000000
C	-2.932516000000	3.003641000000	3.186155000000
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C	-4.063828000000	2.060286000000	3.671217000000

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C	-4.197332000000	0.822113000000	2.773249000000
H	-3.270768000000	0.235769000000	2.768982000000
H	-5.004797000000	0.173168000000	3.131315000000
H	-4.424670000000	1.090622000000	1.735389000000
C	-3.810984000000	1.661441000000	5.132114000000
H	-4.620595000000	1.024738000000	5.506621000000
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C	-3.123935000000	3.504846000000	1.766350000000
O	-2.431972000000	3.132808000000	0.805056000000
N	-4.114537000000	4.413930000000	1.571238000000
H	-4.752549000000	4.599666000000	2.335545000000
C	-4.538636000000	4.785715000000	0.223030000000
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C	-5.835585000000	5.626228000000	0.288570000000
H	-5.629271000000	6.564403000000	0.818657000000
H	-6.093414000000	5.887642000000	-0.743370000000
C	-6.967147000000	4.879298000000	0.963636000000
C	-7.355105000000	5.174142000000	2.279171000000
H	-6.885471000000	6.006350000000	2.800990000000
C	-8.332510000000	4.427806000000	2.937434000000
H	-8.626906000000	4.657624000000	3.956645000000
C	-8.947590000000	3.358888000000	2.278922000000
O	-9.885873000000	2.644029000000	2.969164000000
H	-10.194561000000	1.906667000000	2.419077000000
C	-8.590627000000	3.062469000000	0.957517000000
H	-9.074686000000	2.239471000000	0.435345000000
C	-7.610988000000	3.815907000000	0.315422000000
H	-7.339615000000	3.566541000000	-0.707956000000
C	-3.444528000000	5.520539000000	-0.575381000000
O	-3.429546000000	5.448469000000	-1.798127000000
N	-2.561848000000	6.245854000000	0.162103000000
H	-2.689395000000	6.291623000000	1.165260000000
C	-1.431023000000	6.946455000000	-0.418413000000
H	-1.347296000000	6.608735000000	-1.456411000000
C	-0.120237000000	6.698497000000	0.347579000000
O	0.585846000000	7.644557000000	0.681403000000
N	0.180365000000	5.390718000000	0.607231000000
H	-0.519752000000	4.687685000000	0.395131000000
C	1.342825000000	5.021791000000	1.428610000000
H	1.851395000000	5.964989000000	1.634342000000
C	0.900085000000	4.384093000000	2.764290000000
H	0.111637000000	5.043824000000	3.153316000000
H	0.434032000000	3.406423000000	2.586397000000
C	2.000638000000	4.239299000000	3.840489000000
H	2.594194000000	5.165398000000	3.842947000000
C	1.351303000000	4.098588000000	5.227144000000
H	0.721769000000	4.964960000000	5.470583000000
H	0.721078000000	3.199999000000	5.276367000000
H	2.115705000000	4.008345000000	6.006720000000
C	2.953587000000	3.062358000000	3.582647000000
H	3.711053000000	2.987849000000	4.369760000000
H	2.396972000000	2.115514000000	3.548904000000
H	3.496292000000	3.169337000000	2.640021000000
C	2.367910000000	4.212935000000	0.605518000000
O	3.492943000000	4.673690000000	0.409956000000
N	1.963178000000	3.026908000000	0.066879000000
H	1.136860000000	2.564733000000	0.445092000000
C	2.925151000000	2.156596000000	-0.615141000000
H	3.690945000000	1.767327000000	0.064945000000
H	2.369209000000	1.303303000000	-1.019644000000
C	3.669113000000	2.819715000000	-1.778592000000
O	4.809619000000	2.471548000000	-2.078596000000
N	2.993739000000	3.772850000000	-2.471940000000
H	2.060662000000	4.018409000000	-2.169848000000
C	3.578261000000	4.451617000000	-3.621803000000
H	4.011028000000	3.690885000000	-4.279432000000
C	2.496321000000	5.221113000000	-4.385490000000
H	1.722188000000	4.540104000000	-4.755583000000
H	2.023543000000	5.977285000000	-3.745425000000

H	2.956672000000	5.733789000000	-5.232921000000
C	4.762738000000	5.392384000000	-3.296770000000
O	5.419576000000	5.851468000000	-4.228255000000
N	4.996760000000	5.663005000000	-1.987685000000
H	4.390251000000	5.274531000000	-1.270194000000
C	6.127875000000	6.459544000000	-1.553070000000
H	6.728950000000	6.676885000000	-2.441478000000
C	7.017918000000	5.800095000000	-0.486890000000
O	7.683025000000	6.510352000000	0.262024000000
N	7.027016000000	4.439708000000	-0.462402000000
H	6.412710000000	3.924099000000	-1.085306000000
C	7.747885000000	3.696122000000	0.571391000000
H	8.456393000000	4.404080000000	1.004767000000
C	6.768706000000	3.204356000000	1.659541000000
H	6.267955000000	4.085379000000	2.076624000000
H	5.983099000000	2.593114000000	1.199305000000
C	7.442124000000	2.408873000000	2.798034000000
H	8.010434000000	1.569209000000	2.383968000000
H	8.132931000000	3.054662000000	3.348682000000
C	6.408379000000	1.888167000000	3.794735000000
O	6.119723000000	2.499843000000	4.824079000000
N	5.822546000000	0.704133000000	3.452093000000
H	5.886132000000	0.299415000000	2.509212000000
H	5.040886000000	0.417729000000	4.026938000000
C	8.613299000000	2.587891000000	-0.076363000000
O	9.798932000000	2.784974000000	-0.334094000000
N	7.955110000000	1.430098000000	-0.344279000000
H	7.028731000000	1.259753000000	0.047968000000
C	8.630572000000	0.208494000000	-0.759099000000
H	8.776410000000	-0.434487000000	0.121728000000
C	7.842855000000	-0.568020000000	-1.827028000000
H	7.987935000000	-0.092072000000	-2.805780000000
H	8.276386000000	-1.574960000000	-1.891514000000
C	6.319613000000	-0.672597000000	-1.573427000000
H	5.857871000000	0.297297000000	-1.779393000000
H	5.905461000000	-1.407668000000	-2.272900000000
C	5.946131000000	-1.091203000000	-0.138274000000
O	5.794163000000	-2.326310000000	0.086586000000
O	5.833238000000	-0.157710000000	0.715705000000
C	5.950098000000	-2.252446000000	-6.322300000000
H	5.271473000000	-2.876605000000	-6.920703000000
C	5.395862000000	-0.827364000000	-6.173032000000
H	6.107689000000	-0.252927000000	-5.560967000000
C	5.297750000000	-0.143413000000	-7.545469000000
H	4.575174000000	-0.664524000000	-8.189809000000
H	4.978541000000	0.900669000000	-7.461607000000
H	6.266627000000	-0.152173000000	-8.060173000000
C	4.048669000000	-0.843081000000	-5.423035000000
H	3.309241000000	-1.390879000000	-6.028558000000
H	4.173861000000	-1.426752000000	-4.500615000000
C	3.490942000000	0.536467000000	-5.052343000000
H	3.280843000000	1.143281000000	-5.942160000000
H	2.557394000000	0.440459000000	-4.487146000000
H	4.203963000000	1.088497000000	-4.427741000000
C	4.047753000000	-2.997650000000	3.352801000000
H	4.684146000000	-3.719596000000	3.883195000000
C	3.188347000000	-2.232141000000	4.361850000000
H	3.817142000000	-1.766551000000	5.129180000000
H	2.613766000000	-1.439592000000	3.867248000000
H	2.478800000000	-2.904084000000	4.853379000000
C	3.216474000000	-3.787506000000	2.346368000000
O	2.153270000000	-4.351577000000	2.682448000000
N	3.736553000000	-3.850473000000	1.108411000000
H	4.555471000000	-3.265223000000	0.866196000000
C	3.081287000000	-4.574196000000	0.033706000000
H	2.600742000000	-5.464222000000	0.447916000000
C	2.016567000000	-3.714546000000	-0.669957000000
H	1.488228000000	-3.146327000000	0.104691000000
C	2.601304000000	-2.756656000000	-1.701908000000
H	1.850197000000	-2.051762000000	-2.080677000000
H	3.417315000000	-2.178231000000	-1.257036000000

H	3.011964000000	-3.322289000000	-2.547323000000
O	1.089721000000	-4.643208000000	-1.278080000000
H	0.424246000000	-4.120421000000	-1.754016000000
C	-5.002664000000	-5.126461000000	-5.092607000000
H	-4.171758000000	-5.788105000000	-4.835588000000
H	-5.694635000000	-5.633177000000	-5.771977000000
S	-4.411700000000	-3.608115000000	-5.901901000000
C	8.385265000000	-4.569520000000	0.860158000000
H	9.266184000000	-4.645753000000	0.208560000000
H	7.627253000000	-3.970003000000	0.347010000000
C	8.745187000000	-3.961506000000	2.198357000000
C	8.096865000000	-2.805285000000	2.654535000000
H	7.328242000000	-2.352259000000	2.033854000000
C	8.425549000000	-2.239128000000	3.889879000000
H	7.908377000000	-1.340027000000	4.216205000000
C	9.408395000000	-2.822663000000	4.690943000000
H	9.667094000000	-2.381925000000	5.650882000000
C	10.061035000000	-3.976625000000	4.247848000000
H	10.829889000000	-4.438833000000	4.863684000000
C	9.731228000000	-4.537625000000	3.013574000000
H	10.246454000000	-5.435485000000	2.675035000000
O	-1.939020000000	-1.419871000000	-3.335635000000
Fe	-2.904919000000	-2.412197000000	-4.403451000000
N	-2.584842000000	-4.066164000000	-3.316950000000
N	-1.263453000000	-2.797611000000	-5.486462000000
N	-4.629425000000	-2.065461000000	-3.363324000000
C	-4.448437000000	-3.878772000000	-1.718566000000
C	-0.492117000000	-4.826446000000	-4.357222000000
C	-1.406866000000	-0.942974000000	-7.081301000000
C	-5.502369000000	-0.148317000000	-4.614927000000
C	-3.304071000000	-4.488098000000	-2.223239000000
C	-0.369050000000	-3.818187000000	-5.304020000000
C	-2.623588000000	-0.410998000000	-6.668139000000
C	-5.559920000000	-1.077155000000	-3.584773000000
C	-2.696734000000	-5.666715000000	-1.655247000000
C	0.719548000000	-3.707586000000	-6.249146000000
C	-3.261372000000	0.730428000000	-7.276253000000
C	-6.599423000000	-1.143348000000	-2.583821000000
C	-1.596663000000	-5.946901000000	-2.407680000000
C	0.465368000000	-2.609088000000	-7.008387000000
C	-4.420277000000	0.944016000000	-6.593133000000
C	-6.290660000000	-2.180746000000	-1.756459000000
C	-1.525436000000	-4.933593000000	-3.432443000000
C	-0.779957000000	-2.051325000000	-6.528467000000
C	-4.488534000000	-0.062529000000	-5.562900000000
C	-5.064915000000	-2.755647000000	-2.261375000000
N	-3.388962000000	-0.884203000000	-5.633673000000
H	-4.907724000000	-4.304159000000	-0.831027000000
H	0.295240000000	-5.571789000000	-4.309875000000
H	-0.908245000000	-0.452717000000	-7.911848000000
H	-6.306469000000	0.578663000000	-4.679886000000
C	-2.868719000000	1.636349000000	-2.596565000000
C	-0.363727000000	-2.098425000000	2.039465000000
C	-1.078150000000	-2.590441000000	0.944146000000
C	-0.135168000000	-0.726131000000	2.165389000000
C	-1.549084000000	-1.719426000000	-0.042871000000
C	-2.704816000000	0.406898000000	-1.741407000000
C	-0.600693000000	0.150939000000	1.188434000000
C	-1.293352000000	-0.354205000000	0.073147000000
O	-0.352157000000	1.498343000000	1.307303000000
O	-1.614404000000	0.587844000000	-0.885924000000
H	0.050802000000	-2.787066000000	2.768504000000
H	-1.210492000000	-3.662228000000	0.838438000000
H	0.413807000000	-0.316956000000	3.008517000000
H	-2.051923000000	-2.097380000000	-0.925298000000
H	-2.425915000000	-0.594303000000	-2.600285000000
H	-3.589024000000	0.042573000000	-1.205226000000
H	-3.038624000000	2.530451000000	-1.982633000000
H	-1.959623000000	1.795200000000	-3.186670000000
H	-3.708738000000	1.509515000000	-3.283330000000
H	-1.127523000000	2.008685000000	0.961469000000

O	0.035671000000	-5.705961000000	1.236630000000
H	0.732977000000	-5.259959000000	1.765067000000
H	0.281024000000	-5.490175000000	0.314299000000
O	0.415226000000	0.195373000000	-3.048957000000
H	-0.212550000000	-0.494359000000	-3.343786000000
H	-0.003631000000	0.523912000000	-2.237956000000
H	-5.542291000000	-4.870721000000	-4.173736000000
H	-2.858460000000	1.287714000000	-8.112346000000
H	-5.164060000000	1.714521000000	-6.752163000000
H	1.052532000000	-2.198336000000	-7.819553000000
H	1.560066000000	-4.387219000000	-6.303855000000
H	-0.870691000000	-6.737414000000	-2.272317000000
H	-3.065139000000	-6.191764000000	-0.784197000000
H	-7.449860000000	-0.474109000000	-2.538499000000
H	-6.812095000000	-2.555046000000	-0.884819000000
H	-5.504456000000	10.633522000000	3.249372000000
H	3.845822000000	-4.895667000000	-0.680865000000
H	-1.582167000000	8.030440000000	-0.421435000000
H	7.990350000000	-5.587762000000	0.979876000000
H	3.007494000000	-9.523427000000	7.823366000000
H	5.804890000000	7.415185000000	-1.125839000000
H	-7.636575000000	-4.750735000000	4.037967000000
H	-3.966978000000	-4.139986000000	1.597180000000
H	4.724678000000	-2.323790000000	2.817466000000
H	6.073097000000	-2.735863000000	-5.345914000000
H	6.926784000000	-2.252473000000	-6.822403000000
H	-2.867017000000	3.869331000000	3.858419000000
H	9.620001000000	0.489695000000	-1.126951000000

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C	-4.458158000000	-10.288151000000	-1.327512000000
H	-5.434974000000	-9.902055000000	-1.638983000000
H	-4.342886000000	-10.099009000000	-0.253782000000
C	-3.334537000000	-9.667367000000	-2.126878000000
C	-3.577592000000	-9.059792000000	-3.366032000000
H	-4.595223000000	-9.017297000000	-3.749238000000
C	-2.530639000000	-8.522712000000	-4.121129000000
H	-2.739920000000	-8.066425000000	-5.085483000000
C	-1.219861000000	-8.576560000000	-3.642866000000
H	-0.405025000000	-8.160840000000	-4.228781000000
C	-0.960104000000	-9.175826000000	-2.406545000000
H	0.055656000000	-9.217957000000	-2.021854000000
C	-2.011479000000	-9.715003000000	-1.660111000000
H	-1.800893000000	-10.191126000000	-0.704361000000
C	-8.631730000000	2.729808000000	-2.713640000000
H	-9.401341000000	3.355830000000	-2.249459000000
C	-8.960290000000	1.237387000000	-2.439520000000
H	-9.962780000000	1.075948000000	-2.865471000000
C	-7.987370000000	0.301886000000	-3.176110000000
H	-7.960446000000	0.526058000000	-4.250007000000
H	-6.967068000000	0.403638000000	-2.787425000000
H	-8.282705000000	-0.747932000000	-3.073069000000
C	-9.046973000000	0.927295000000	-0.930823000000
H	-8.042960000000	0.963637000000	-0.492334000000
H	-9.616468000000	1.724615000000	-0.437193000000
C	-9.706712000000	-0.421678000000	-0.612239000000
H	-9.142790000000	-1.262200000000	-1.034827000000
H	-9.774555000000	-0.565184000000	0.474623000000
H	-10.725941000000	-0.472549000000	-1.016123000000
C	-7.291753000000	3.202156000000	-2.145975000000
O	-7.173632000000	3.494944000000	-0.953287000000
N	-6.268955000000	3.257820000000	-3.040094000000
H	-6.463045000000	2.986990000000	-3.993494000000
C	-4.897216000000	3.656330000000	-2.717912000000
H	-4.243518000000	2.775713000000	-2.774132000000
C	-4.337414000000	4.765340000000	-3.629118000000
H	-3.324321000000	4.955876000000	-3.249334000000
C	-4.209132000000	4.283851000000	-5.084521000000
H	-3.645827000000	3.344229000000	-5.137461000000
H	-5.190607000000	4.120481000000	-5.555149000000
H	-3.678031000000	5.015545000000	-5.701175000000

C	-5.148724000000	6.069812000000	-3.502247000000
H	-6.164254000000	5.915523000000	-3.896362000000
H	-5.272869000000	6.295556000000	-2.433662000000
C	-4.508280000000	7.281617000000	-4.190879000000
H	-4.453220000000	7.152981000000	-5.277953000000
H	-5.089854000000	8.191708000000	-4.000083000000
H	-3.489009000000	7.451185000000	-3.824951000000
C	1.658590000000	12.000351000000	-3.278710000000
H	1.051955000000	12.891258000000	-3.082836000000
H	2.000231000000	12.049534000000	-4.320031000000
C	0.880799000000	10.731486000000	-3.008439000000
C	1.393404000000	9.482507000000	-3.392238000000
H	2.354274000000	9.435432000000	-3.902085000000
C	0.693575000000	8.304617000000	-3.131396000000
H	1.099760000000	7.343059000000	-3.436000000000
C	-0.542908000000	8.351922000000	-2.476628000000
H	-1.071140000000	7.423261000000	-2.271947000000
C	-1.065482000000	9.589536000000	-2.096469000000
H	-2.031438000000	9.643922000000	-1.598036000000
C	-0.359440000000	10.767276000000	-2.360356000000
H	-0.776856000000	11.727041000000	-2.060483000000
C	-3.264026000000	-4.722107000000	-2.896613000000
H	-2.456729000000	-4.208658000000	-3.427365000000
C	-4.601554000000	-3.971292000000	-3.123223000000
H	-5.386760000000	-4.480665000000	-2.543753000000
C	-4.521284000000	-2.514591000000	-2.644402000000
H	-3.774164000000	-1.955282000000	-3.219839000000
H	-5.487088000000	-2.012406000000	-2.772275000000
H	-4.243281000000	-2.439312000000	-1.587343000000
C	-4.992807000000	-4.045390000000	-4.606045000000
H	-5.948313000000	-3.538252000000	-4.782115000000
H	-4.236314000000	-3.558354000000	-5.233729000000
H	-5.094394000000	-5.083280000000	-4.945826000000
C	-2.852728000000	-4.814445000000	-1.438212000000
O	-1.878499000000	-4.211845000000	-0.962378000000
N	-3.607683000000	-5.618366000000	-0.638506000000
H	-4.480864000000	-5.970889000000	-1.011830000000
C	-3.481469000000	-5.541646000000	0.817168000000
H	-3.491565000000	-4.489593000000	1.117675000000
C	-4.665906000000	-6.263459000000	1.500078000000
H	-4.636043000000	-7.330831000000	1.245937000000
H	-4.496122000000	-6.186613000000	2.579397000000
C	-6.004544000000	-5.670378000000	1.111069000000
C	-6.884146000000	-6.347947000000	0.254199000000
H	-6.634509000000	-7.352118000000	-0.084584000000
C	-8.083315000000	-5.772658000000	-0.166410000000
H	-8.760733000000	-6.301610000000	-0.829403000000
C	-8.427377000000	-4.490018000000	0.271063000000
O	-9.603720000000	-3.961892000000	-0.178484000000
H	-9.704055000000	-3.059366000000	0.164252000000
C	-7.571492000000	-3.804119000000	1.142702000000
H	-7.837551000000	-2.810138000000	1.496536000000
C	-6.377615000000	-4.392362000000	1.552126000000
H	-5.722943000000	-3.842664000000	2.224524000000
C	-2.138640000000	-6.076570000000	1.344249000000
O	-1.720444000000	-5.692878000000	2.431174000000
N	-1.507622000000	-6.989103000000	0.557467000000
H	-1.930353000000	-7.240006000000	-0.327418000000
C	-0.206888000000	-7.540984000000	0.878313000000
H	0.042433000000	-7.205092000000	1.889753000000
C	0.931741000000	-7.134561000000	-0.072279000000
O	1.847918000000	-7.920366000000	-0.286403000000
N	0.865321000000	-5.872079000000	-0.588609000000
H	0.009364000000	-5.335660000000	-0.480722000000
C	1.933035000000	-5.345189000000	-1.451968000000
H	2.733850000000	-6.084562000000	-1.390562000000
C	1.486352000000	-5.202800000000	-2.922120000000
H	0.866874000000	-6.083133000000	-3.139426000000
H	0.832931000000	-4.330452000000	-3.058535000000
C	2.643671000000	-5.156809000000	-3.944524000000
H	3.260451000000	-6.052114000000	-3.774909000000

C	2.081003000000	-5.239595000000	-5.371914000000
H	1.476603000000	-6.144590000000	-5.517845000000
H	1.444642000000	-4.372555000000	-5.593779000000
H	2.891143000000	-5.254031000000	-6.109786000000
C	3.552600000000	-3.928038000000	-3.793839000000
H	4.376826000000	-3.960173000000	-4.513864000000
H	2.987147000000	-3.000020000000	-3.953953000000
H	4.020249000000	-3.875663000000	-2.806820000000
C	2.501072000000	-4.086689000000	-0.763914000000
O	3.526640000000	-4.157532000000	-0.082884000000
N	1.770956000000	-2.941754000000	-0.848947000000
H	0.993215000000	-2.874518000000	-1.502232000000
C	2.251686000000	-1.688769000000	-0.275681000000
H	3.273438000000	-1.458793000000	-0.602527000000
H	1.613904000000	-0.882605000000	-0.647580000000
C	2.259824000000	-1.598479000000	1.253133000000
O	2.714698000000	-0.583781000000	1.792360000000
N	1.749970000000	-2.640004000000	1.954324000000
H	1.362080000000	-3.417286000000	1.435960000000
C	1.895197000000	-2.767885000000	3.401720000000
H	2.050256000000	-1.757395000000	3.786024000000
C	0.626429000000	-3.347005000000	4.036569000000
H	-0.195863000000	-2.632896000000	3.933706000000
H	0.325857000000	-4.292541000000	3.569440000000
H	0.812576000000	-3.527826000000	5.097715000000
C	3.146381000000	-3.567904000000	3.841812000000
O	3.379590000000	-3.692946000000	5.042955000000
N	3.937495000000	-4.076470000000	2.859778000000
H	3.653748000000	-4.009208000000	1.884776000000
C	5.100695000000	-4.899496000000	3.153151000000
H	5.350692000000	-4.751094000000	4.207535000000
C	6.331193000000	-4.600678000000	2.283645000000
O	7.164146000000	-5.477175000000	2.083280000000
N	6.422932000000	-3.329370000000	1.804565000000
H	5.644955000000	-2.703517000000	1.969514000000
C	7.414372000000	-2.935546000000	0.801619000000
H	8.234876000000	-3.649145000000	0.893943000000
C	6.789557000000	-3.018626000000	-0.609492000000
H	6.478185000000	-4.056788000000	-0.769694000000
H	5.870753000000	-2.421732000000	-0.634250000000
C	7.719252000000	-2.577707000000	-1.758369000000
H	8.108921000000	-1.572469000000	-1.564762000000
H	8.566577000000	-3.264792000000	-1.844169000000
C	6.982371000000	-2.593109000000	-3.099617000000
O	7.040066000000	-3.552238000000	-3.868711000000
N	6.258159000000	-1.468972000000	-3.373995000000
H	6.008189000000	-0.771875000000	-2.659112000000
H	5.668336000000	-1.519274000000	-4.194299000000
C	8.008324000000	-1.557845000000	1.184122000000
O	9.058934000000	-1.480274000000	1.820218000000
N	7.264145000000	-0.490534000000	0.794509000000
H	6.496792000000	-0.608968000000	0.126007000000
C	7.767635000000	0.878646000000	0.798158000000
H	8.110598000000	1.124943000000	-0.217277000000
C	6.708366000000	1.905070000000	1.233377000000
H	6.632973000000	1.909563000000	2.328623000000
H	7.072594000000	2.897387000000	0.935971000000
C	5.283059000000	1.687209000000	0.668096000000
H	4.808846000000	0.853063000000	1.194128000000
H	4.695744000000	2.586281000000	0.880191000000
C	5.224673000000	1.390131000000	-0.845118000000
O	4.992895000000	2.341203000000	-1.639949000000
O	5.435846000000	0.181052000000	-1.186261000000
C	8.017635000000	0.311792000000	4.907450000000
H	8.463398000000	0.293655000000	5.912271000000
C	6.645195000000	-0.378637000000	4.903384000000
H	6.271832000000	-0.359704000000	3.868066000000
C	6.789934000000	-1.849164000000	5.325671000000
H	7.202488000000	-1.918559000000	6.342320000000
H	5.831359000000	-2.379302000000	5.320640000000
H	7.473179000000	-2.375237000000	4.649480000000

C	5.628445000000	0.386395000000	5.774599000000
H	5.917666000000	0.288913000000	6.832843000000
H	5.701339000000	1.458129000000	5.537792000000
C	4.170945000000	-0.058596000000	5.592017000000
H	4.018051000000	-1.107604000000	5.867584000000
H	3.494601000000	0.548127000000	6.208770000000
H	3.858307000000	0.056643000000	4.546050000000
C	3.340804000000	3.666493000000	-4.250027000000
H	3.930300000000	4.512220000000	-4.632618000000
C	2.603206000000	2.992824000000	-5.410767000000
H	3.308791000000	2.682433000000	-6.189453000000
H	2.066679000000	2.100568000000	-5.067048000000
H	1.870871000000	3.677532000000	-5.848572000000
C	2.379162000000	4.227738000000	-3.206918000000
O	1.301254000000	4.756919000000	-3.541650000000
N	2.798159000000	4.137721000000	-1.927141000000
H	3.636993000000	3.577400000000	-1.721862000000
C	1.961679000000	4.592041000000	-0.828810000000
H	1.396199000000	5.465939000000	-1.160442000000
C	0.971604000000	3.506678000000	-0.363329000000
H	0.597026000000	3.005673000000	-1.266337000000
C	1.633983000000	2.468083000000	0.530015000000
H	0.928531000000	1.684053000000	0.816448000000
H	2.472453000000	1.994162000000	0.011709000000
H	2.012808000000	2.931378000000	1.449569000000
O	-0.107161000000	4.180688000000	0.287418000000
H	-0.583358000000	3.566048000000	0.903947000000
C	-4.641578000000	5.784384000000	4.610275000000
H	-4.093476000000	6.600600000000	4.131490000000
H	-5.267516000000	6.177177000000	5.417190000000
S	-3.502336000000	4.546140000000	5.304145000000
C	7.555940000000	4.631076000000	-2.518150000000
H	8.138138000000	5.168841000000	-1.758679000000
H	6.707965000000	4.143403000000	-2.028083000000
C	8.409427000000	3.621411000000	-3.254022000000
C	7.943037000000	2.316784000000	-3.470556000000
H	6.962631000000	2.036164000000	-3.093151000000
C	8.724426000000	1.383204000000	-4.157606000000
H	8.341484000000	0.376161000000	-4.303036000000
C	9.984479000000	1.740121000000	-4.641089000000
H	10.594613000000	1.012673000000	-5.171384000000
C	10.459745000000	3.037588000000	-4.431765000000
H	11.442490000000	3.324908000000	-4.800011000000
C	9.678240000000	3.966294000000	-3.743170000000
H	10.058375000000	4.973514000000	-3.578221000000
O	-1.442466000000	2.582567000000	2.132146000000
Fe	-2.225262000000	3.541861000000	3.480982000000
N	-2.615135000000	5.068959000000	2.222727000000
N	-0.501206000000	4.400183000000	4.038300000000
N	-4.039057000000	2.749937000000	3.044237000000
C	-4.777202000000	4.340229000000	1.326764000000
C	-0.581088000000	6.380559000000	2.590194000000
C	0.270794000000	2.770370000000	5.700430000000
C	-3.956193000000	0.764474000000	4.484760000000
C	-3.692068000000	5.211509000000	1.388669000000
C	0.025787000000	5.560244000000	3.536262000000
C	-0.812321000000	1.904074000000	5.648008000000
C	-4.565336000000	1.577693000000	3.540600000000
C	-3.560363000000	6.411918000000	0.596513000000
C	1.312490000000	5.824992000000	4.132249000000
C	-0.944195000000	0.704452000000	6.438183000000
C	-5.834284000000	1.300970000000	2.909706000000
C	-2.387138000000	6.995656000000	0.964754000000
C	1.556468000000	4.807386000000	5.004490000000
C	-2.131812000000	0.139290000000	6.090339000000
C	-6.062228000000	2.301662000000	2.014177000000
C	-1.804630000000	6.145727000000	1.976064000000
C	0.415716000000	3.927566000000	4.939463000000
C	-2.723287000000	0.997200000000	5.089397000000
C	-4.932329000000	3.196167000000	2.103283000000
N	-1.904910000000	2.065145000000	4.833500000000

H	-5.562991000000	4.547821000000	0.606507000000
H	-0.037220000000	7.269073000000	2.284363000000
H	1.079568000000	2.517331000000	6.379319000000
H	-4.492429000000	-0.130528000000	4.787603000000
C	-2.595210000000	-1.670808000000	1.826939000000
C	-0.813091000000	1.118048000000	-3.726330000000
C	-1.341519000000	1.780262000000	-2.616595000000
C	-0.614917000000	-0.263813000000	-3.690618000000
C	-1.678512000000	1.061831000000	-1.463744000000
C	-1.967239000000	-0.678453000000	0.912024000000
C	-0.941836000000	-0.986431000000	-2.545160000000
C	-1.476775000000	-0.318170000000	-1.426387000000
O	-0.695051000000	-2.339040000000	-2.523276000000
O	-1.785206000000	-1.146598000000	-0.364437000000
H	-0.536676000000	1.681504000000	-4.612431000000
H	-1.463932000000	2.860754000000	-2.621856000000
H	-0.194568000000	-0.801627000000	-4.535375000000
H	-2.063214000000	1.591874000000	-0.598917000000
H	-0.786838000000	1.976785000000	2.543067000000
H	-2.097834000000	0.390981000000	1.051880000000
H	-3.652806000000	-1.863119000000	1.565797000000
H	-2.070879000000	-2.633744000000	1.798082000000
H	-2.574559000000	-1.291286000000	2.852545000000
H	-1.210916000000	-2.794245000000	-1.815860000000
O	-1.231322000000	5.086358000000	-2.198009000000
H	-0.376034000000	5.002459000000	-2.674376000000
H	-1.007850000000	4.864006000000	-1.267662000000
O	0.235478000000	0.343732000000	2.961648000000
H	-0.248808000000	-0.179021000000	2.295632000000
H	1.171191000000	0.262172000000	2.687757000000
H	-5.290441000000	5.319737000000	3.858593000000
H	-0.210549000000	0.351662000000	7.151528000000
H	-2.580425000000	-0.772067000000	6.465344000000
H	2.422594000000	4.649683000000	5.634283000000
H	1.937485000000	6.677008000000	3.897041000000
H	-1.928052000000	7.895982000000	0.576846000000
H	-4.276164000000	6.743411000000	-0.144448000000
H	-6.453979000000	0.440831000000	3.132214000000
H	-6.890147000000	2.447968000000	1.332915000000
H	-4.483386000000	-11.378086000000	-1.458128000000
H	2.604390000000	4.900267000000	0.003727000000
H	-0.233651000000	-8.634151000000	0.881248000000
H	7.154197000000	5.388789000000	-3.205766000000
H	2.553912000000	12.065998000000	-2.645840000000
H	4.882327000000	-5.963583000000	3.009114000000
H	-8.675204000000	2.906221000000	-3.796746000000
H	-4.909375000000	3.983739000000	-1.677149000000
H	4.044795000000	2.980589000000	-3.767721000000
H	7.936194000000	1.362793000000	4.600400000000
H	8.704650000000	-0.189175000000	4.216619000000
H	-3.338691000000	-5.740285000000	-3.301269000000
H	8.638042000000	0.912433000000	1.456849000000

⁴Intermediate / HS_I1

C	-4.450539000000	-10.288653000000	-1.319121000000
H	-5.427721000000	-9.904192000000	-1.631443000000
H	-4.335979000000	-10.098102000000	-0.245559000000
C	-3.327397000000	-9.667304000000	-2.118719000000
C	-3.570960000000	-9.060046000000	-3.357926000000
H	-4.588658000000	-9.018270000000	-3.741029000000
C	-2.524458000000	-8.522266000000	-4.113166000000
H	-2.734136000000	-8.066164000000	-5.077518000000
C	-1.213620000000	-8.575197000000	-3.635005000000
H	-0.399014000000	-8.158950000000	-4.220854000000
C	-0.953345000000	-9.174207000000	-2.398663000000
H	0.062500000000	-9.215597000000	-2.014117000000
C	-2.004272000000	-9.713997000000	-1.652053000000
H	-1.793251000000	-10.189715000000	-0.696198000000
C	-8.638680000000	2.737456000000	-2.715086000000
H	-9.411004000000	3.362180000000	-2.253712000000
C	-8.962191000000	1.244612000000	-2.436983000000

H	-9.963656000000	1.078271000000	-2.863460000000
C	-7.985096000000	0.310508000000	-3.169813000000
H	-7.956976000000	0.532466000000	-4.244144000000
H	-6.965781000000	0.416132000000	-2.779591000000
H	-8.277454000000	-0.739967000000	-3.065092000000
C	-9.049149000000	0.938918000000	-0.927424000000
H	-8.046115000000	0.983569000000	-0.487434000000
H	-9.624893000000	1.734111000000	-0.437557000000
C	-9.700427000000	-0.413263000000	-0.605100000000
H	-9.129967000000	-1.251475000000	-1.023442000000
H	-9.769318000000	-0.553223000000	0.482159000000
H	-10.718508000000	-0.472587000000	-1.010758000000
C	-7.300896000000	3.215698000000	-2.147196000000
O	-7.185924000000	3.515833000000	-0.956054000000
N	-6.276250000000	3.268001000000	-3.039485000000
H	-6.467969000000	2.991104000000	-3.991605000000
C	-4.904996000000	3.667431000000	-2.716354000000
H	-4.251287000000	2.786618000000	-2.769944000000
C	-4.343849000000	4.774453000000	-3.629182000000
H	-3.330172000000	4.963747000000	-3.250357000000
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H	-3.655267000000	3.350204000000	-5.135980000000
H	-5.198608000000	4.129151000000	-5.554268000000
H	-3.684182000000	5.020914000000	-5.701505000000
C	-5.153133000000	6.080357000000	-3.503705000000
H	-6.168993000000	5.927053000000	-3.897344000000
H	-5.276716000000	6.307702000000	-2.435385000000
C	-4.511031000000	7.290326000000	-4.194035000000
H	-4.456607000000	7.160323000000	-5.280977000000
H	-5.091021000000	8.201591000000	-4.004056000000
H	-3.491305000000	7.458629000000	-3.828746000000
C	1.676542000000	11.997379000000	-3.254433000000
H	1.071532000000	12.888303000000	-3.053660000000
H	2.018855000000	12.051975000000	-4.295256000000
C	0.896109000000	10.728487000000	-2.992024000000
C	1.405325000000	9.480987000000	-3.385004000000
H	2.365532000000	9.435158000000	-3.896207000000
C	0.703016000000	8.302989000000	-3.131401000000
H	1.106659000000	7.342562000000	-3.442876000000
C	-0.532597000000	8.348716000000	-2.474900000000
H	-1.062834000000	7.419940000000	-2.276019000000
C	-1.051732000000	9.584887000000	-2.085432000000
H	-2.016762000000	9.638049000000	-1.585094000000
C	-0.343237000000	10.762735000000	-2.342133000000
H	-0.757968000000	11.721380000000	-2.035050000000
C	-3.259399000000	-4.722386000000	-2.892316000000
H	-2.453011000000	-4.208625000000	-3.424155000000
C	-4.597965000000	-3.973567000000	-3.119231000000
H	-5.382355000000	-4.483292000000	-2.538955000000
C	-4.519385000000	-2.516250000000	-2.641981000000
H	-3.773086000000	-1.956631000000	-3.218192000000
H	-5.485827000000	-2.015341000000	-2.770086000000
H	-4.241183000000	-2.439530000000	-1.585071000000
C	-4.989689000000	-4.049753000000	-4.601819000000
H	-5.945878000000	-3.543970000000	-4.778091000000
H	-4.234016000000	-3.562484000000	-5.230307000000
H	-5.090140000000	-5.088130000000	-4.940436000000
C	-2.846964000000	-4.812494000000	-1.434100000000
O	-1.872107000000	-4.209447000000	-0.960098000000
N	-3.601374000000	-5.614921000000	-0.632391000000
H	-4.475113000000	-5.967740000000	-1.004130000000
C	-3.473465000000	-5.536037000000	0.823013000000
H	-3.482335000000	-4.483510000000	1.121782000000
C	-4.657652000000	-6.255728000000	1.508549000000
H	-4.628931000000	-7.323574000000	1.256299000000
H	-4.486419000000	-6.177073000000	2.587515000000
C	-5.996259000000	-5.662262000000	1.120113000000
C	-6.877329000000	-6.340545000000	0.265294000000
H	-6.628726000000	-7.345374000000	-0.072290000000
C	-8.076664000000	-5.765143000000	-0.154684000000
H	-8.755248000000	-6.294668000000	-0.816025000000

C	-8.419425000000	-4.481669000000	0.281381000000
O	-9.596118000000	-3.953580000000	-0.167285000000
H	-9.695932000000	-3.050811000000	0.174948000000
C	-7.561969000000	-3.794955000000	1.150820000000
H	-7.826925000000	-2.800227000000	1.503390000000
C	-6.367951000000	-4.383324000000	1.559655000000
H	-5.712089000000	-3.833036000000	2.230404000000
C	-2.130560000000	-6.071161000000	1.349701000000
O	-1.711462000000	-5.686395000000	2.435891000000
N	-1.500414000000	-6.984793000000	0.563484000000
H	-1.923800000000	-7.236527000000	-0.320845000000
C	-0.199640000000	-7.536668000000	0.884131000000
H	0.050087000000	-7.200394000000	1.895338000000
C	0.938786000000	-7.130667000000	-0.066843000000
O	1.855319000000	-7.916270000000	-0.280081000000
N	0.871983000000	-5.868600000000	-0.584122000000
H	0.015748000000	-5.332472000000	-0.476936000000
C	1.939508000000	-5.342191000000	-1.448049000000
H	2.740626000000	-6.081161000000	-1.385726000000
C	1.493068000000	-5.201732000000	-2.918385000000
H	0.872506000000	-6.081618000000	-3.134378000000
H	0.840823000000	-4.328794000000	-3.056447000000
C	2.650656000000	-5.158993000000	-3.940671000000
H	3.265778000000	-6.055211000000	-3.769843000000
C	2.088150000000	-5.242399000000	-5.368080000000
H	1.482038000000	-6.146393000000	-5.513091000000
H	1.453502000000	-4.374407000000	-5.591133000000
H	2.898450000000	-5.259254000000	-6.105718000000
C	3.561730000000	-3.931761000000	-3.790984000000
H	4.386122000000	-3.966129000000	-4.510718000000
H	2.998139000000	-3.002803000000	-3.952212000000
H	4.029117000000	-3.879330000000	-2.803832000000
C	2.506915000000	-4.082600000000	-0.761311000000
O	3.532241000000	-4.152206000000	-0.079856000000
N	1.776211000000	-2.938103000000	-0.847733000000
H	0.998943000000	-2.871851000000	-1.501636000000
C	2.256163000000	-1.684214000000	-0.275749000000
H	3.277820000000	-1.453947000000	-0.602774000000
H	1.617907000000	-0.878847000000	-0.648561000000
C	2.264249000000	-1.592357000000	1.252945000000
O	2.718251000000	-0.576689000000	1.791152000000
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H	2.054168000000	-1.748719000000	3.785878000000
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H	0.332898000000	-4.286242000000	3.571715000000
H	0.819230000000	-3.520091000000	5.099409000000
C	3.152547000000	-3.557850000000	3.843761000000
O	3.386456000000	-3.680313000000	5.045025000000
N	3.943500000000	-4.067911000000	2.862351000000
H	3.659416000000	-4.002483000000	1.887332000000
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C	6.337313000000	-4.592373000000	2.286802000000
O	7.170540000000	-5.468945000000	2.087874000000
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H	5.650401000000	-2.695968000000	1.969357000000
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H	8.241371000000	-3.641919000000	0.896676000000
C	6.796374000000	-3.016249000000	-0.609058000000
H	6.485974000000	-4.055052000000	-0.766993000000
H	5.877119000000	-2.420141000000	-0.635892000000
C	7.726623000000	-2.577463000000	-1.758337000000
H	8.115473000000	-1.571501000000	-1.566911000000
H	8.574486000000	-3.264178000000	-1.841809000000
C	6.990790000000	-2.596690000000	-3.100112000000
O	7.049227000000	-3.557943000000	-3.866471000000
N	6.266788000000	-1.473311000000	-3.378355000000
H	6.015167000000	-0.774958000000	-2.665250000000

H	5.677367000000	-1.526341000000	-4.198790000000
C	8.012423000000	-1.550207000000	1.182258000000
O	9.062273000000	-1.470136000000	1.819308000000
N	7.267680000000	-0.484559000000	0.789257000000
H	6.500992000000	-0.605423000000	0.120451000000
C	7.769683000000	0.885149000000	0.790202000000
H	8.113212000000	1.129527000000	-0.225515000000
C	6.708955000000	1.911387000000	1.222320000000
H	6.632241000000	1.917685000000	2.317382000000
H	7.072700000000	2.903457000000	0.923453000000
C	5.284493000000	1.691185000000	0.655622000000
H	4.810127000000	0.858217000000	1.183357000000
H	4.696381000000	2.590463000000	0.864596000000
C	5.228241000000	1.389975000000	-0.856856000000
O	4.997261000000	2.338703000000	-1.654720000000
O	5.440239000000	0.180013000000	-1.194360000000
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H	8.468186000000	0.310119000000	5.906884000000
C	6.649493000000	-0.363467000000	4.899803000000
H	6.274970000000	-0.344503000000	3.864894000000
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H	7.209408000000	-1.903334000000	6.337773000000
H	5.837529000000	-2.364846000000	5.317444000000
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C	5.633250000000	0.400616000000	5.772434000000
H	5.923797000000	0.302963000000	6.830293000000
H	5.705137000000	1.472483000000	5.535923000000
C	4.175825000000	-0.045282000000	5.591491000000
H	4.023964000000	-1.094558000000	5.866616000000
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C	3.341590000000	3.659121000000	-4.267279000000
H	3.930497000000	4.504374000000	-4.651813000000
C	2.602409000000	2.983835000000	-5.426068000000
H	3.306857000000	2.672658000000	-6.205472000000
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C	2.381389000000	4.221727000000	-3.223534000000
O	1.303190000000	4.750877000000	-3.557397000000
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H	3.641433000000	3.573182000000	-1.739298000000
C	1.967327000000	4.589018000000	-0.845449000000
H	1.403123000000	5.463849000000	-1.176885000000
C	0.975539000000	3.505865000000	-0.378848000000
H	0.599042000000	3.005361000000	-1.281308000000
C	1.635961000000	2.466072000000	0.514570000000
H	0.929256000000	1.682976000000	0.800526000000
H	2.474013000000	1.991212000000	-0.003554000000
H	2.015039000000	2.928574000000	1.434411000000
O	-0.101193000000	4.182798000000	0.272173000000
H	-0.578878000000	3.569648000000	0.888570000000
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H	-4.059946000000	6.617763000000	4.126896000000
H	-5.237888000000	6.228191000000	5.419242000000
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C	7.560851000000	4.626454000000	-2.534722000000
H	8.143163000000	5.162276000000	-1.773946000000
H	6.712396000000	4.138383000000	-2.045897000000
C	8.413822000000	3.617500000000	-3.272177000000
C	7.948777000000	2.312026000000	-3.486396000000
H	6.969644000000	2.030397000000	-3.106435000000
C	8.729812000000	1.378918000000	-4.174495000000
H	8.348023000000	0.371149000000	-4.317878000000
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H	10.597955000000	1.010204000000	-5.192687000000
C	10.461972000000	3.035621000000	-4.454632000000
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C	9.680875000000	3.963807000000	-3.764901000000
H	10.059953000000	4.971734000000	-3.601842000000
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Fe	-2.260938000000	3.499741000000	3.478765000000

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C	-3.698350000000	5.204165000000	1.387240000000
C	0.015271000000	5.503939000000	3.551670000000
C	-0.870760000000	1.856432000000	5.652378000000
C	-4.618660000000	1.575638000000	3.537654000000
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C	-5.894584000000	1.324586000000	2.911782000000
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C	1.531669000000	4.736483000000	5.026922000000
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C	0.380498000000	3.870904000000	4.957496000000
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C	-4.965363000000	3.207928000000	2.107020000000
N	-1.957740000000	2.024562000000	4.827616000000
H	-5.581284000000	4.563010000000	0.609842000000
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H	1.018920000000	2.450166000000	6.400767000000
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C	-0.814351000000	1.117043000000	-3.731918000000
C	-1.344474000000	1.779996000000	-2.623413000000
C	-0.613543000000	-0.264352000000	-3.693998000000
C	-1.680309000000	1.062591000000	-1.469585000000
C	-1.961801000000	-0.674192000000	0.909549000000
C	-0.939246000000	-0.985955000000	-2.547450000000
C	-1.475742000000	-0.316963000000	-1.430000000000
O	-0.689685000000	-2.337919000000	-2.523283000000
O	-1.782889000000	-1.144108000000	-0.366580000000
H	-0.538765000000	1.679661000000	-4.618814000000
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H	-0.191912000000	-0.802705000000	-4.537769000000
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H	-1.205036000000	-2.793111000000	-1.815470000000
O	-1.229342000000	5.084402000000	-2.211263000000
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O	0.239500000000	0.353069000000	2.960082000000
H	-0.244201000000	-0.174321000000	2.297358000000
H	1.175137000000	0.271542000000	2.685652000000
H	-5.287613000000	5.363488000000	3.865514000000
H	-0.292996000000	0.301138000000	7.161885000000
H	-2.666790000000	-0.804599000000	6.460755000000
H	2.393779000000	4.569222000000	5.659734000000
H	1.938960000000	6.599443000000	3.916430000000
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H	-6.527867000000	0.474218000000	3.133547000000
H	-6.937663000000	2.494641000000	1.344173000000
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H	2.611381000000	4.896405000000	-0.013620000000
H	-0.226576000000	-8.629824000000	0.887510000000
H	7.160024000000	5.385831000000	-3.221016000000
H	2.571637000000	12.057620000000	-2.620693000000
H	4.888834000000	-5.954530000000	3.014280000000
H	-8.681409000000	2.910443000000	-3.798770000000
H	-4.918634000000	3.996997000000	-1.676281000000

H	4.046363000000	2.973938000000	-3.785064000000
H	7.939020000000	1.378814000000	4.595446000000
H	8.708132000000	-0.172751000000	4.211075000000
H	-3.332971000000	-5.741178000000	-3.295626000000
H	8.639514000000	0.921421000000	1.449524000000

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C	-7.704278000000	-6.995907000000	-3.829811000000
H	-8.371365000000	-6.140020000000	-3.977361000000
H	-7.647065000000	-7.201078000000	-2.754230000000
C	-6.336006000000	-6.742158000000	-4.421505000000
C	-6.119966000000	-5.695438000000	-5.327518000000
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C	-4.860223000000	-5.484555000000	-5.896978000000
H	-4.718046000000	-4.672827000000	-6.606082000000
C	-3.789919000000	-6.316053000000	-5.561889000000
H	-2.809818000000	-6.152362000000	-6.000973000000
C	-3.988158000000	-7.364925000000	-4.658203000000
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C	-5.250841000000	-7.571494000000	-4.096925000000
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⁴Product / HS_P1

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H	0.412183000000	8.113072000000	-2.966521000000
C	5.461302000000	11.370065000000	-2.244485000000
H	4.934365000000	12.326305000000	-2.151681000000
H	5.819617000000	11.281431000000	-3.276791000000
C	4.571473000000	10.207523000000	-1.864230000000
C	4.860398000000	8.908167000000	-2.306238000000
H	5.723746000000	8.744984000000	-2.949174000000
C	4.062101000000	7.824871000000	-1.936538000000
H	4.295603000000	6.821345000000	-2.282773000000
C	2.949464000000	8.024760000000	-1.112489000000
H	2.330456000000	7.175911000000	-0.831900000000
C	2.648546000000	9.314615000000	-0.669523000000
H	1.783560000000	9.484079000000	-0.031967000000
C	3.452225000000	10.394649000000	-1.043437000000
H	3.207705000000	11.396511000000	-0.694542000000
C	-4.014981000000	-2.449404000000	-3.417540000000
H	-3.030511000000	-2.176418000000	-3.808496000000
C	-4.934665000000	-1.201620000000	-3.383302000000
H	-5.918426000000	-1.505189000000	-2.994727000000
C	-4.381903000000	-0.108230000000	-2.458744000000
H	-3.386898000000	0.217007000000	-2.786289000000
H	-5.040972000000	0.766639000000	-2.461597000000
H	-4.301697000000	-0.455290000000	-1.422782000000
C	-5.134501000000	-0.672081000000	-4.810572000000
H	-5.808915000000	0.191805000000	-4.813255000000
H	-4.178966000000	-0.352292000000	-5.244679000000
H	-5.563132000000	-1.437267000000	-5.469359000000
C	-3.791905000000	-3.091643000000	-2.059582000000
O	-2.712591000000	-3.049731000000	-1.449552000000
N	-4.855355000000	-3.754054000000	-1.522827000000
H	-5.753585000000	-3.647413000000	-1.976862000000
C	-4.840665000000	-4.216175000000	-0.136797000000
H	-4.221123000000	-3.518474000000	0.435148000000
C	-6.264849000000	-4.205167000000	0.460796000000
H	-6.911799000000	-4.877087000000	-0.120087000000
H	-6.182479000000	-4.633275000000	1.465020000000
C	-6.847649000000	-2.808021000000	0.497249000000
C	-7.859437000000	-2.403052000000	-0.384162000000
H	-8.301612000000	-3.129666000000	-1.064625000000
C	-8.328347000000	-1.088818000000	-0.404525000000
H	-9.113785000000	-0.782242000000	-1.088516000000
C	-7.783118000000	-0.141333000000	0.469649000000
O	-8.260275000000	1.133681000000	0.406531000000
H	-7.784634000000	1.698810000000	1.044326000000
C	-6.785668000000	-0.533014000000	1.373804000000
H	-6.372491000000	0.187753000000	2.074048000000
C	-6.332322000000	-1.849413000000	1.381368000000
H	-5.558795000000	-2.131958000000	2.092441000000
C	-4.146778000000	-5.576782000000	0.064694000000
O	-3.917734000000	-5.977074000000	1.200260000000
N	-3.793103000000	-6.245392000000	-1.067810000000
H	-4.093149000000	-5.873644000000	-1.959500000000
C	-3.036493000000	-7.480570000000	-1.050317000000
H	-2.835502000000	-7.715134000000	-0.000066000000
C	-1.703636000000	-7.424461000000	-1.813685000000
O	-1.252001000000	-8.441200000000	-2.329648000000
N	-1.073357000000	-6.215411000000	-1.828450000000
H	-1.569671000000	-5.398762000000	-1.489159000000
C	0.237877000000	-6.036251000000	-2.470385000000
H	0.676325000000	-7.034468000000	-2.521766000000
C	0.098308000000	-5.472758000000	-3.900665000000
H	-0.719233000000	-6.041890000000	-4.362100000000
H	-0.235511000000	-4.425057000000	-3.879369000000
C	1.348461000000	-5.605238000000	-4.797152000000

H	1.663727000000	-6.659402000000	-4.758378000000
C	0.968056000000	-5.287829000000	-6.252881000000
H	0.158871000000	-5.937324000000	-6.611674000000
H	0.633536000000	-4.246513000000	-6.352172000000
H	1.827232000000	-5.422511000000	-6.920073000000
C	2.531428000000	-4.734020000000	-4.350228000000
H	3.367708000000	-4.835082000000	-5.051429000000
H	2.262003000000	-3.671471000000	-4.320428000000
H	2.920425000000	-4.997265000000	-3.363542000000
C	1.118627000000	-5.242369000000	-1.484947000000
O	1.940609000000	-5.809441000000	-0.766347000000
N	0.839588000000	-3.912283000000	-1.373564000000
H	0.300948000000	-3.441806000000	-2.095023000000
C	1.666294000000	-3.037561000000	-0.551669000000
H	2.717938000000	-3.104781000000	-0.846842000000
H	1.335641000000	-2.011301000000	-0.730423000000
C	1.580945000000	-3.281158000000	0.953396000000
O	2.418130000000	-2.761707000000	1.704066000000
N	0.563296000000	-4.052103000000	1.395432000000
H	-0.068761000000	-4.428412000000	0.701806000000
C	0.393572000000	-4.448211000000	2.791427000000
H	0.498833000000	-3.553462000000	3.409912000000
C	-1.005716000000	-5.035519000000	3.002280000000
H	-1.779479000000	-4.292224000000	2.785511000000
H	-1.182179000000	-5.906996000000	2.360704000000
H	-1.103128000000	-5.353231000000	4.042818000000
C	1.465217000000	-5.435772000000	3.305299000000
O	1.537836000000	-5.651382000000	4.513857000000
N	2.266504000000	-6.019452000000	2.376499000000
H	2.110799000000	-5.838798000000	1.388125000000
C	3.376530000000	-6.888309000000	2.731266000000
H	3.422085000000	-6.924766000000	3.823640000000
C	4.730579000000	-6.426349000000	2.163124000000
O	5.570199000000	-7.252287000000	1.820159000000
N	4.896177000000	-5.079809000000	2.081563000000
H	4.122056000000	-4.477489000000	2.337245000000
C	6.010768000000	-4.469580000000	1.371559000000
H	6.610592000000	-5.313434000000	1.009594000000
C	5.451034000000	-3.667511000000	0.172111000000
H	4.563428000000	-4.201279000000	-0.176948000000
H	5.102655000000	-2.686586000000	0.520702000000
C	6.368737000000	-3.498562000000	-1.055413000000
H	7.346947000000	-3.082873000000	-0.803091000000
H	6.532289000000	-4.479897000000	-1.516419000000
C	5.654599000000	-2.612529000000	-2.076579000000
O	4.614766000000	-2.977488000000	-2.632452000000
N	6.235693000000	-1.404959000000	-2.299754000000
H	6.902064000000	-1.015282000000	-1.618177000000
H	5.703066000000	-0.752209000000	-2.861319000000
C	6.922857000000	-3.699302000000	2.369245000000
O	7.107738000000	-4.128423000000	3.508066000000
N	7.530315000000	-2.595823000000	1.873354000000
H	7.315032000000	-2.198486000000	0.962120000000
C	8.514371000000	-1.796416000000	2.585150000000
H	9.363306000000	-1.654180000000	1.907821000000
C	7.985056000000	-0.417233000000	3.034152000000
H	7.459514000000	-0.532739000000	3.990959000000
H	8.852966000000	0.227674000000	3.229646000000
C	7.014628000000	0.293661000000	2.065267000000
H	6.077341000000	-0.278780000000	2.051048000000
H	6.779170000000	1.283305000000	2.470469000000
C	7.452863000000	0.464913000000	0.591965000000
O	7.433072000000	1.626999000000	0.105366000000
O	7.763234000000	-0.592754000000	-0.044261000000
C	5.872539000000	-2.213150000000	6.390570000000
H	6.190792000000	-2.525317000000	7.395628000000
C	4.484402000000	-2.779654000000	6.055894000000
H	4.211547000000	-2.416016000000	5.052374000000
C	4.541126000000	-4.314754000000	6.000028000000
H	4.830351000000	-4.721738000000	6.980146000000
H	3.576848000000	-4.754698000000	5.725488000000

H	5.287553000000	-4.637470000000	5.266070000000
C	3.417550000000	-2.264392000000	7.043834000000
H	3.585753000000	-2.739643000000	8.022818000000
H	3.570206000000	-1.185892000000	7.203003000000
C	1.966861000000	-2.495957000000	6.598385000000
H	1.761342000000	-3.551609000000	6.390939000000
H	1.262045000000	-2.164922000000	7.373748000000
H	1.741277000000	-1.935718000000	5.681807000000
C	6.309754000000	3.550601000000	-2.575235000000
H	6.865863000000	4.498493000000	-2.598792000000
C	5.904559000000	3.163671000000	-4.001457000000
H	6.790190000000	3.074356000000	-4.638827000000
H	5.384671000000	2.198062000000	-4.014395000000
H	5.229238000000	3.911975000000	-4.426832000000
C	5.102078000000	3.763175000000	-1.671321000000
O	4.100281000000	4.393511000000	-2.063504000000
N	5.207310000000	3.238008000000	-0.433291000000
H	6.042729000000	2.688070000000	-0.180244000000
C	4.132511000000	3.360247000000	0.531067000000
H	3.676641000000	4.349480000000	0.433158000000
C	3.038080000000	2.297772000000	0.329106000000
H	2.832747000000	2.228582000000	-0.747654000000
C	3.428649000000	0.924874000000	0.862740000000
H	2.637072000000	0.185362000000	0.696229000000
H	4.330421000000	0.563625000000	0.357437000000
H	3.627770000000	0.970766000000	1.939719000000
O	1.870756000000	2.813928000000	0.996271000000
H	1.196721000000	2.108795000000	1.034390000000
C	-3.944010000000	6.053617000000	4.986460000000
H	-3.219740000000	6.480724000000	4.287477000000
H	-4.090654000000	6.754772000000	5.813982000000
S	-3.333856000000	4.470866000000	5.686301000000
C	10.438769000000	2.635318000000	-1.390443000000
H	11.296356000000	2.164861000000	-0.888672000000
H	9.567675000000	2.504193000000	-0.739735000000
C	10.195629000000	2.010669000000	-2.745810000000
C	9.443708000000	0.829722000000	-2.853874000000
H	9.017844000000	0.385520000000	-1.956785000000
C	9.225832000000	0.236515000000	-4.099081000000
H	8.631515000000	-0.672339000000	-4.157816000000
C	9.753097000000	0.811473000000	-5.258874000000
H	9.579216000000	0.350064000000	-6.228338000000
C	10.500267000000	1.987122000000	-5.163306000000
H	10.911795000000	2.447586000000	-6.059151000000
C	10.716098000000	2.579270000000	-3.916337000000
H	11.294342000000	3.499564000000	-3.850090000000
O	-0.368197000000	0.935106000000	1.341494000000
Fe	-3.137712000000	2.981403000000	3.809593000000
N	-2.605884000000	4.300840000000	2.400329000000
N	-1.190261000000	2.499372000000	4.031168000000
N	-5.045996000000	3.096297000000	3.153728000000
C	-4.804019000000	4.831993000000	1.427853000000
C	-0.177436000000	4.360935000000	2.789170000000
C	-1.386001000000	0.517728000000	5.471655000000
C	-6.071793000000	1.448414000000	4.661511000000
C	-3.433136000000	4.994115000000	1.538670000000
C	-0.110821000000	3.279987000000	3.651378000000
C	-2.772370000000	0.446790000000	5.479964000000
C	-6.132931000000	2.456353000000	3.707534000000
C	-2.672936000000	5.937762000000	0.761450000000
C	1.108766000000	2.747876000000	4.197873000000
C	-3.525300000000	-0.531526000000	6.219207000000
C	-7.349433000000	2.927293000000	3.098700000000
C	-1.374202000000	5.821336000000	1.158241000000
C	0.773832000000	1.637427000000	4.911144000000
C	-4.843283000000	-0.243617000000	6.027015000000
C	-6.987032000000	3.849460000000	2.153254000000
C	-1.340064000000	4.802052000000	2.174047000000
C	-0.656259000000	1.500612000000	4.825898000000
C	-4.898251000000	0.895931000000	5.149888000000
C	-5.553618000000	3.957526000000	2.205166000000

N	-3.623150000000	1.309686000000	4.823260000000
H	-5.313836000000	5.434962000000	0.684071000000
H	0.753641000000	4.841911000000	2.514727000000
H	-0.832610000000	-0.236100000000	6.020396000000
H	-7.009526000000	1.025782000000	5.008609000000
C	-2.224517000000	-0.626758000000	1.394483000000
C	0.569836000000	1.390448000000	-4.017281000000
C	0.472137000000	2.181005000000	-2.872443000000
C	0.159113000000	0.056344000000	-3.981948000000
C	-0.020752000000	1.631502000000	-1.683882000000
C	-1.417968000000	0.347733000000	0.553644000000
C	-0.334834000000	-0.498334000000	-2.801976000000
C	-0.405126000000	0.291894000000	-1.637817000000
O	-0.716007000000	-1.818065000000	-2.805040000000
O	-0.830651000000	-0.374301000000	-0.499723000000
H	0.973989000000	1.804963000000	-4.936414000000
H	0.809015000000	3.212286000000	-2.858139000000
H	0.218219000000	-0.579751000000	-4.860199000000
H	-0.053240000000	2.241245000000	-0.790408000000
H	-0.785291000000	1.414237000000	2.086062000000
H	-2.039564000000	1.153444000000	0.137208000000
H	-2.971947000000	-1.130795000000	0.775899000000
H	-1.550884000000	-1.368263000000	1.834402000000
H	-2.734008000000	-0.093270000000	2.204415000000
H	-1.380984000000	-2.012285000000	-2.101747000000
O	1.438336000000	4.874651000000	-1.035950000000
H	2.332290000000	4.752365000000	-1.425176000000
H	1.434434000000	4.252555000000	-0.281757000000
O	0.761145000000	-1.112467000000	3.317273000000
H	0.552511000000	-0.446834000000	2.639237000000
H	1.508190000000	-1.615157000000	2.936920000000
H	-4.899557000000	5.916188000000	4.471864000000
H	-3.085278000000	-1.325510000000	6.808714000000
H	-5.710065000000	-0.756432000000	6.424363000000
H	1.420158000000	0.945468000000	5.432376000000
H	2.089994000000	3.158628000000	4.005574000000
H	-0.498205000000	6.326637000000	0.772293000000
H	-3.106817000000	6.567336000000	-0.003292000000
H	-8.344717000000	2.599771000000	3.374284000000
H	-7.623967000000	4.430377000000	1.497760000000
H	-8.275816000000	-7.847574000000	-4.254274000000
H	4.555486000000	3.276910000000	1.538117000000
H	-3.608971000000	-8.309233000000	-1.477295000000
H	10.661333000000	3.705560000000	-1.477013000000
H	6.349659000000	11.423811000000	-1.599986000000
H	3.219562000000	-7.905333000000	2.358654000000
H	-5.823457000000	5.555767000000	-4.860532000000
H	-2.584043000000	5.166298000000	-1.832333000000
H	6.975157000000	2.800852000000	-2.136032000000
H	5.875718000000	-1.114926000000	6.369408000000
H	6.615810000000	-2.578409000000	5.673478000000
H	-4.445651000000	-3.201292000000	-4.092083000000
H	8.850831000000	-2.372279000000	3.450391000000

Part 3.2 Wildtype CYP199A4 system

Part 3.2.1 QM cluster energies, charges, and spin densities

Table S5: Absolute (free) energies (in au) of UB3LYP/BS1 optimized geometries of WT CYP199A4 cluster model as obtained in Gaussian-09. Also shown are the degree of spin contamination in the structures (S^2 values).

	E [BS1, au]	ZPE	G [au]	E [BS2, au]	S^2
² RC _{WT}	-6054.99	2.17	-6053.05	-6056.58	1.7957
⁴ RC _{WT}	-6054.99	2.17	-6053.05	-6056.57	3.7974
² TS1 _{WT}	-6054.94	2.16	-6053.00	-6056.53	1.2500
⁴ TS1 _{WT}	-6054.94	2.16	-6053.01	-6056.53	3.8276
² IM1 _{WT}	-6054.97	2.16	-6053.03	-6056.60	1.3818
⁴ IM1 _{WT}	-6054.96	2.16	-6053.03	-6056.59	3.8084
² PR1 _{WT}	-6055.06	2.17	-6053.11	-6056.70	0.8259
⁴ PR1 _{WT}	-6055.06	2.17	-6053.13	-6056.69	3.7907
² TS2 _{WT}	-6054.94	2.16	-6053.00	-6056.54	1.5718
⁴ TS2 _{WT}	-6054.94	2.16	-6053.00	-6056.54	3.7940
² IM2 _{WT}	-6054.95	2.16	-6053.01	-6056.58	1.3385
⁴ IM2 _{WT}	-6054.95	2.16	-6053.00	-6056.58	3.8366

Table S6: Relative (free) energies (in au) of UB3LYP/BS1 optimized geometries of WT CYP199A4 cluster model as obtained in Gaussian-09.

	ΔE	$\Delta E + ZPE$	ΔG	ΔE [BS2]	ΔE [BS2] + ZPE	ΔG [BS2]
² RC _{WT}	0.00	0.00	0.00	0.00	0.00	0.00
⁴ RC _{WT}	0.17	0.21	-0.30	0.20	0.24	-0.28
² TS1 _{WT}	30.10	26.44	28.01	25.54	21.88	23.45
⁴ TS1 _{WT}	30.48	25.67	26.77	28.67	23.86	24.96
² IM1 _{WT}	11.90	9.92	13.19	-17.12	-19.10	-15.83
⁴ IM1 _{WT}	15.51	13.17	13.99	-12.06	-14.40	-13.59
² PR1 _{WT}	-43.81	-42.12	-40.31	-75.48	-73.79	-71.98
⁴ PR1 _{WT}	-45.20	-44.29	-49.12	-69.32	-68.41	-73.24
² TS2 _{WT}	29.16	28.50	32.76	23.86	23.19	27.46
⁴ TS2 _{WT}	30.29	29.62	32.76	22.68	22.01	25.15
² IM2 _{WT}	20.37	20.00	23.73	-5.96	-6.33	-2.59
⁴ IM2 _{WT}	22.85	22.32	27.69	-5.97	-6.50	-1.12

Table S7: Group charges and spin densities (in au) of UB3LYP/BS1 optimized geometries of WT CYP199A4 cluster model as obtained in Gaussian-09.

(c) Charges

	Fe	O	Por	Axial	SubH	Prot	Total
² RC _{WT}	0.49	-0.54	0.07	-0.03	-0.59	0.61	0.00
⁴ RC _{WT}	0.47	-0.54	0.07	-0.03	-0.59	0.61	0.00
² TS1 _{WT}	0.38	-0.64	-0.12	-0.01	-0.22	0.60	0.00
⁴ TS1 _{WT}	0.38	-0.67	0.01	-0.03	-0.31	0.61	0.00
² IM1 _{WT}	0.26	-0.78	-0.12	-0.06	0.12	0.58	0.00
⁴ IM1 _{WT}	0.29	-0.77	0.10	-0.02	-0.18	0.58	0.00
² PR1 _{WT}	0.25	-0.59	-0.42	0.04	0.11	0.61	0.00
⁴ PR1 _{WT}	0.49	-0.64	-0.34	-0.16	0.03	0.62	0.00
² TS2 _{WT}	0.38	-0.53	-0.11	-0.01	-0.34	0.61	0.00
⁴ TS2 _{WT}	0.39	-0.55	-0.11	-0.00	-0.33	0.62	0.00
² IM2 _{WT}	0.24	-0.60	-0.10	-0.02	-0.13	0.60	0.00
⁴ IM2 _{WT}	0.33	-0.60	-0.01	0.01	-0.33	0.60	0.00

(d) Spin densities

	Fe	O	Por	Axial	SubH	Prot	Total
² RC _{WT}	1.40	0.72	-0.64	-0.48	0.00	0.01	1.00
⁴ RC _{WT}	1.25	0.77	0.55	0.42	0.00	0.01	3.00
² TS1 _{WT}	1.42	0.23	-0.38	-0.13	-0.15	0.00	1.00
⁴ TS1 _{WT}	0.96	0.58	0.65	0.31	0.50	0.01	3.00
² IM1 _{WT}	1.01	0.01	-0.61	-0.01	0.59	0.00	1.00
⁴ IM1 _{WT}	0.93	0.10	0.75	0.23	0.98	0.01	3.00
² PR1 _{WT}	1.08	0.00	-0.09	0.00	0.00	0.00	1.00
⁴ PR1 _{WT}	2.47	0.00	0.05	0.47	0.00	0.00	3.00
² TS2 _{WT}	1.04	0.51	-0.51	-0.41	0.36	0.00	1.00
⁴ TS2 _{WT}	2.32	0.60	-0.37	-0.12	0.57	0.00	3.00
² IM2 _{WT}	0.95	0.06	0.45	0.13	-0.59	0.00	1.00
⁴ IM2 _{WT}	0.92	0.18	0.60	0.35	0.94	0.01	3.00

Part 3.2.2: Cartesian coordinates of optimized geometries

²Reactant / LS_React

C	23.754996000000	43.178119000000	38.277338000000
H	24.252777000000	43.982843000000	38.832594000000
H	24.247542000000	42.231024000000	38.533751000000
N	23.757251000000	43.429601000000	36.847028000000
H	22.872696000000	43.322200000000	36.301613000000
C	24.878370000000	43.597671000000	36.136323000000
N	26.087962000000	43.683313000000	36.705909000000
H	26.311627000000	43.481039000000	37.679654000000
H	26.873065000000	43.853233000000	36.072766000000
N	24.793249000000	43.698726000000	34.796540000000
H	23.889473000000	43.959150000000	34.369497000000
H	25.659117000000	43.906980000000	34.306049000000
C	32.231508000000	45.840947000000	30.821105000000
H	31.321700000000	46.313319000000	31.208180000000
C	32.289060000000	44.367577000000	31.224685000000
H	31.447001000000	43.828029000000	30.766844000000
H	33.217541000000	43.936316000000	30.838829000000
O	32.303218000000	44.191494000000	32.634203000000
H	31.377925000000	44.251049000000	32.959931000000
C	33.469823000000	46.611703000000	31.281666000000
O	34.592525000000	46.100300000000	31.281004000000
N	33.241790000000	47.895177000000	31.647112000000
H	32.302371000000	48.302851000000	31.675580000000
C	30.898016000000	34.042078000000	30.522087000000
H	31.981996000000	34.102534000000	30.670039000000
C	30.184599000000	35.328598000000	30.954808000000
H	30.576513000000	36.178540000000	30.375962000000
H	29.120725000000	35.248384000000	30.690781000000
C	30.288910000000	35.660146000000	32.457110000000
H	29.922045000000	34.784837000000	33.016349000000
C	31.737206000000	35.924642000000	32.898104000000
H	31.781880000000	36.157716000000	33.969053000000
H	32.388483000000	35.061624000000	32.721765000000
H	32.159706000000	36.779410000000	32.352152000000
C	29.391287000000	36.855411000000	32.811295000000
H	29.428150000000	37.084619000000	33.882530000000
H	29.708280000000	37.756544000000	32.269618000000
H	28.345462000000	36.660401000000	32.544334000000
C	19.861967000000	44.636025000000	32.328901000000
H	20.718497000000	44.994076000000	31.751195000000
H	19.477590000000	45.481855000000	32.911569000000
C	20.275360000000	43.476995000000	33.238968000000
H	19.434157000000	43.108626000000	33.834907000000
H	20.611147000000	42.628287000000	32.624902000000
C	21.425428000000	43.803679000000	34.196837000000
O	22.311289000000	44.647252000000	33.787908000000
O	21.458053000000	43.217902000000	35.303160000000
C	27.576548000000	44.611136000000	43.097063000000
H	27.474749000000	45.699798000000	43.014648000000
C	26.166016000000	43.968537000000	43.152051000000
H	26.304190000000	42.890460000000	43.321755000000
C	25.312002000000	44.532190000000	44.296218000000
H	25.113049000000	45.600583000000	44.139180000000
H	24.345681000000	44.015697000000	44.345345000000
H	25.812184000000	44.432500000000	45.262816000000
C	25.463050000000	44.144682000000	41.797606000000
H	25.296375000000	45.211161000000	41.588538000000
H	26.059650000000	43.727261000000	40.978739000000
H	24.482495000000	43.652496000000	41.802513000000
C	28.404974000000	44.333191000000	44.346590000000
O	28.281680000000	44.987118000000	45.379403000000
N	29.254581000000	43.260470000000	44.261721000000
H	29.419886000000	42.838744000000	43.358483000000
C	30.109924000000	42.870285000000	45.373081000000
H	30.234464000000	41.782015000000	45.343195000000
C	31.489861000000	43.563277000000	45.377960000000
H	31.327809000000	44.643901000000	45.454877000000

H	32.013284000000	43.251246000000	46.292357000000
C	32.333522000000	43.242195000000	44.162431000000
C	32.541924000000	44.190891000000	43.153591000000
H	32.113539000000	45.184896000000	43.262381000000
C	33.291038000000	43.880052000000	42.012980000000
H	33.423547000000	44.628744000000	41.235031000000
C	33.842158000000	42.603170000000	41.864209000000
H	34.413322000000	42.340356000000	40.978074000000
C	33.644827000000	41.646977000000	42.867595000000
H	34.066512000000	40.652364000000	42.751205000000
C	32.900909000000	41.966451000000	44.002838000000
H	32.759720000000	41.217699000000	44.780388000000
C	28.374467000000	39.222198000000	44.010099000000
H	28.196955000000	40.274335000000	44.270885000000
H	29.319523000000	38.927732000000	44.483347000000
C	28.422060000000	39.025564000000	42.511239000000
C	29.461060000000	39.579912000000	41.748558000000
H	30.256523000000	40.133776000000	42.245767000000
C	29.503777000000	39.421541000000	40.361370000000
H	30.306267000000	39.883152000000	39.790915000000
C	28.503791000000	38.689587000000	39.710826000000
H	28.541020000000	38.560831000000	38.631830000000
C	27.468247000000	38.126590000000	40.458104000000
H	26.688030000000	37.552189000000	39.964360000000
C	27.428820000000	38.296854000000	41.844676000000
H	26.616541000000	37.855574000000	42.418640000000
C	28.444067000000	48.289759000000	38.628311000000
H	28.316901000000	48.002439000000	39.677784000000
C	27.066570000000	48.556104000000	37.981417000000
H	26.656266000000	49.483509000000	38.401705000000
H	27.215735000000	48.739351000000	36.909741000000
C	26.067610000000	47.411420000000	38.200534000000
H	26.512941000000	46.459047000000	37.897062000000
H	25.847173000000	47.329323000000	39.272748000000
C	24.738955000000	47.583724000000	37.458394000000
H	24.058315000000	46.790020000000	37.792691000000
H	24.271672000000	48.546170000000	37.710163000000
N	24.937245000000	47.481888000000	36.013902000000
H	25.899970000000	47.480957000000	35.645204000000
C	24.029339000000	47.011278000000	35.150317000000
N	24.378755000000	46.861604000000	33.858511000000
H	25.371465000000	46.927709000000	33.633524000000
H	23.772235000000	46.281788000000	33.286797000000
N	22.761949000000	46.729548000000	35.499479000000
H	22.543703000000	46.683251000000	36.483840000000
H	22.328018000000	45.996083000000	34.904480000000
C	29.195377000000	47.160530000000	37.930986000000
O	28.937404000000	45.968316000000	38.146891000000
N	30.123842000000	47.549931000000	37.026556000000
H	30.341516000000	48.535476000000	36.965890000000
C	30.965142000000	46.629699000000	36.265601000000
H	30.476193000000	45.654068000000	36.283247000000
C	31.179007000000	47.095672000000	34.827107000000
H	31.579739000000	48.116685000000	34.808709000000
H	31.919753000000	46.441416000000	34.351691000000
O	29.976641000000	47.110770000000	34.048047000000
H	29.786722000000	46.154084000000	33.794751000000
C	30.085942000000	43.060368000000	39.569452000000
H	29.936192000000	42.468610000000	40.478345000000
C	28.899092000000	42.850063000000	38.613470000000
H	29.180802000000	43.154674000000	37.597603000000
H	28.607533000000	41.798479000000	38.585560000000
O	27.748889000000	43.590313000000	39.045957000000
H	27.991275000000	44.532464000000	38.929911000000
C	31.408788000000	42.645699000000	38.930457000000
O	31.694918000000	41.462916000000	38.709911000000
N	32.205427000000	43.684652000000	38.589727000000
H	31.966594000000	44.630426000000	38.871035000000
C	33.544497000000	43.571659000000	38.033283000000
H	34.118199000000	42.824409000000	38.596498000000
C	33.534807000000	43.153751000000	36.555774000000

H	34.553440000000	42.996554000000	36.194834000000
H	32.985428000000	42.214944000000	36.461893000000
H	33.052732000000	43.910714000000	35.927649000000
C	34.204040000000	44.949404000000	38.252162000000
O	33.555677000000	45.897303000000	38.727902000000
N	35.495885000000	45.049285000000	37.896360000000
H	35.996261000000	44.232660000000	37.545213000000
C	36.271523000000	46.251691000000	38.157075000000
H	36.668937000000	46.244426000000	39.179552000000
H	37.101542000000	46.297584000000	37.447513000000
C	37.782852000000	42.527542000000	42.654076000000
H	37.668427000000	41.769489000000	41.871811000000
C	37.949741000000	43.910145000000	42.022969000000
H	38.039794000000	44.667797000000	42.817158000000
C	39.168734000000	43.996100000000	41.112061000000
H	40.086516000000	43.813144000000	41.681560000000
H	39.097858000000	43.248356000000	40.314156000000
H	39.237113000000	44.987105000000	40.651697000000
O	36.810428000000	44.244737000000	41.204058000000
H	36.005046000000	44.140170000000	41.740781000000
C	32.950441000000	35.205357000000	40.704581000000
H	32.863112000000	34.604242000000	39.788700000000
H	31.932912000000	35.424068000000	41.045877000000
C	33.736441000000	36.474706000000	40.461827000000
C	33.087263000000	37.672079000000	40.130181000000
H	32.000388000000	37.693429000000	40.079700000000
C	33.810902000000	38.842078000000	39.881445000000
H	33.285968000000	39.758307000000	39.621916000000
C	35.206853000000	38.836087000000	39.968241000000
H	35.765727000000	39.751580000000	39.791160000000
C	35.863461000000	37.648080000000	40.303034000000
H	36.948215000000	37.632920000000	40.382033000000
C	35.135950000000	36.481138000000	40.545527000000
H	35.658338000000	35.563387000000	40.810711000000
S	39.615583000000	41.442748000000	33.824437000000
O	37.161570000000	42.882532000000	36.858647000000
Fe	38.038074000000	42.346031000000	35.576242000000
C	36.352224000000	39.379027000000	35.430820000000
C	40.340619000000	40.929824000000	37.680332000000
C	39.921872000000	45.206249000000	35.464395000000
C	35.848798000000	43.704157000000	33.325829000000
C	37.490530000000	39.420253000000	36.222935000000
C	37.962687000000	38.325127000000	37.032557000000
C	39.079216000000	38.766678000000	37.673091000000
C	39.290505000000	40.128408000000	37.250425000000
C	40.588731000000	42.225574000000	37.255979000000
C	41.705521000000	43.029221000000	37.686071000000
C	41.592433000000	44.230923000000	37.057679000000
C	40.402941000000	44.166809000000	36.245998000000
C	38.773524000000	45.162788000000	34.680563000000
C	38.299987000000	46.254292000000	33.864798000000
C	37.155461000000	45.829687000000	33.260894000000
C	36.935924000000	44.477788000000	33.713169000000
C	35.624730000000	42.392906000000	33.729863000000
C	34.498964000000	41.597783000000	33.304411000000
C	34.651728000000	40.373408000000	33.881152000000
C	35.858886000000	40.433078000000	34.669164000000
N	38.316402000000	40.508757000000	36.362551000000
N	39.809861000000	42.930675000000	36.366028000000
N	37.934458000000	44.083230000000	34.568679000000
N	36.436566000000	41.669281000000	34.564561000000
H	35.789805000000	38.450599000000	35.419051000000
H	41.036068000000	40.497272000000	38.393028000000
H	40.490998000000	46.131070000000	35.460743000000
H	35.125463000000	44.170371000000	32.663471000000
C	31.120222000000	38.323669000000	36.599507000000
O	29.810360000000	38.659966000000	36.138745000000
C	29.636976000000	39.875532000000	35.551103000000
C	28.307562000000	40.270167000000	35.325126000000
C	28.035195000000	41.530487000000	34.814540000000
C	29.074845000000	42.421858000000	34.490051000000

C	30.395724000000	41.982005000000	34.643361000000
C	30.684112000000	40.726265000000	35.173975000000
C	28.790795000000	43.843454000000	34.111852000000
O	27.638344000000	44.316840000000	34.394584000000
O	29.716343000000	44.536540000000	33.586837000000
H	27.508501000000	39.583810000000	35.587589000000
H	27.004509000000	41.835501000000	34.671900000000
H	31.214942000000	42.635275000000	34.367930000000
H	31.718278000000	40.434941000000	35.311360000000
H	31.519383000000	39.107587000000	37.252212000000
H	31.008030000000	37.395667000000	37.161797000000
H	31.804239000000	38.155218000000	35.757842000000
O	27.198639000000	46.992524000000	34.469597000000
H	28.097103000000	47.376827000000	34.410168000000
H	27.376643000000	46.010646000000	34.452684000000
O	30.515966000000	48.805176000000	31.932916000000
H	30.231966000000	48.195510000000	32.655760000000
H	29.925461000000	48.610586000000	31.190186000000
O	36.370768000000	42.014719000000	39.461188000000
H	36.698011000000	42.157131000000	38.551078000000
H	36.572048000000	42.844489000000	39.939567000000
H	38.796921000000	47.212119000000	33.774836000000
H	36.496360000000	46.337018000000	32.566904000000
H	42.243750000000	45.092728000000	37.127195000000
H	42.470024000000	42.698642000000	38.377315000000
H	39.713337000000	38.233552000000	38.369566000000
H	37.480556000000	37.359155000000	37.102600000000
H	34.015402000000	39.501734000000	33.794556000000
H	33.698502000000	41.968329000000	32.678734000000
H	33.431605000000	34.572196000000	41.458770000000
H	27.574556000000	38.630749000000	44.467378000000
H	22.715828000000	43.123569000000	38.607383000000
H	34.039330000000	48.457047000000	31.912015000000
H	30.724454000000	33.836543000000	29.459411000000
H	19.074748000000	44.326477000000	31.631951000000
H	30.532902000000	33.177223000000	31.090559000000
H	31.937900000000	46.523784000000	36.764818000000
H	40.079581000000	42.628316000000	33.368221000000
H	36.894727000000	42.491309000000	43.296542000000
H	38.653191000000	42.274570000000	43.270991000000
H	35.632890000000	47.128554000000	38.032898000000
H	30.114369000000	44.118280000000	39.851386000000
H	29.036269000000	49.212540000000	38.612115000000
H	32.190700000000	45.911357000000	29.724087000000
H	28.092277000000	44.254947000000	42.195854000000
H	29.574350000000	43.129506000000	46.289493000000

⁴Reactant / HS_React

C	23.746847000000	43.178290000000	38.278020000000
H	24.242366000000	43.984077000000	38.833821000000
H	24.241558000000	42.232299000000	38.534342000000
N	23.749156000000	43.429976000000	36.847723000000
H	22.864810000000	43.321388000000	36.302161000000
C	24.870422000000	43.597412000000	36.137091000000
N	26.079755000000	43.684057000000	36.706975000000
H	26.302813000000	43.485030000000	37.681536000000
H	26.865171000000	43.853154000000	36.073980000000
N	24.785776000000	43.696583000000	34.797144000000
H	23.881915000000	43.955241000000	34.369142000000
H	25.651722000000	43.904331000000	34.306609000000
C	32.246147000000	45.824645000000	30.835482000000
H	31.332679000000	46.299151000000	31.211105000000
C	32.304134000000	44.355976000000	31.255873000000
H	31.466256000000	43.809363000000	30.798871000000
H	33.236047000000	43.922468000000	30.880934000000
O	32.309195000000	44.196056000000	32.667552000000
H	31.381021000000	44.253845000000	32.985339000000
C	33.479645000000	46.602967000000	31.296338000000
O	34.603935000000	46.095262000000	31.305398000000
N	33.245566000000	47.888542000000	31.650402000000
H	32.304456000000	48.292592000000	31.673345000000

C	30.890401000000	34.031363000000	30.527036000000
H	31.974200000000	34.094608000000	30.675110000000
C	30.173862000000	35.316825000000	30.957712000000
H	30.563977000000	36.166883000000	30.377827000000
H	29.110271000000	35.233749000000	30.693442000000
C	30.276809000000	35.650655000000	32.459636000000
H	29.911711000000	34.775255000000	33.019897000000
C	31.724289000000	35.919120000000	32.900945000000
H	31.767618000000	36.154854000000	33.971359000000
H	32.377444000000	35.057002000000	32.727127000000
H	32.145395000000	36.773444000000	32.353269000000
C	29.376275000000	36.844315000000	32.811843000000
H	29.411296000000	37.074405000000	33.882960000000
H	29.692011000000	37.745707000000	32.269873000000
H	28.331186000000	36.646854000000	32.543767000000
C	19.852101000000	44.628272000000	32.329427000000
H	20.707947000000	44.987035000000	31.751153000000
H	19.467236000000	45.473809000000	32.912208000000
C	20.267224000000	43.469780000000	33.239431000000
H	19.426802000000	43.100754000000	33.836049000000
H	20.603437000000	42.621357000000	32.625205000000
C	21.417659000000	43.797937000000	34.196332000000
O	22.303415000000	44.640731000000	33.785512000000
O	21.450659000000	43.214102000000	35.303666000000
C	27.580338000000	44.622324000000	43.107544000000
H	27.480804000000	45.711345000000	43.027172000000
C	26.168441000000	43.982707000000	43.162421000000
H	26.304383000000	42.904045000000	43.330202000000
C	25.316614000000	44.546316000000	44.308251000000
H	25.119550000000	45.615316000000	44.152936000000
H	24.349349000000	44.031613000000	44.357538000000
H	25.817562000000	44.444230000000	45.274204000000
C	25.464672000000	44.162728000000	41.808868000000
H	25.300876000000	45.229958000000	41.601389000000
H	26.059040000000	43.744573000000	40.988735000000
H	24.482678000000	43.673423000000	41.814293000000
C	28.409085000000	44.340243000000	44.355940000000
O	28.286566000000	44.991185000000	45.390716000000
N	29.257849000000	43.267082000000	44.267597000000
H	29.422957000000	42.848418000000	43.362897000000
C	30.114410000000	42.873722000000	45.376952000000
H	30.236298000000	41.785175000000	45.345883000000
C	31.495875000000	43.563642000000	45.379543000000
H	31.336300000000	44.644535000000	45.457962000000
H	32.020828000000	43.249553000000	46.292349000000
C	32.336028000000	43.242144000000	44.161677000000
C	32.543187000000	44.191244000000	43.152977000000
H	32.116486000000	45.185778000000	43.263562000000
C	33.288978000000	43.880214000000	42.010230000000
H	33.420448000000	44.629224000000	41.232424000000
C	33.837946000000	42.602682000000	41.859220000000
H	34.406680000000	42.339766000000	40.971575000000
C	33.641782000000	41.646001000000	42.862397000000
H	34.061936000000	40.650928000000	42.744270000000
C	32.901205000000	41.965689000000	43.999766000000
H	32.760881000000	41.216580000000	44.777124000000
C	28.375518000000	39.228263000000	44.008615000000
H	28.197601000000	40.280719000000	44.267826000000
H	29.322107000000	38.935661000000	44.479986000000
C	28.419473000000	39.028716000000	42.510027000000
C	29.453974000000	39.585676000000	41.743182000000
H	30.248529000000	40.143928000000	42.236931000000
C	29.493463000000	39.424544000000	40.356219000000
H	30.292618000000	39.888309000000	39.782816000000
C	28.494705000000	38.687019000000	39.710072000000
H	28.529279000000	38.556134000000	38.631236000000
C	27.463658000000	38.121338000000	40.461545000000
H	26.684417000000	37.542648000000	39.971273000000
C	27.427418000000	38.294424000000	41.847853000000
H	26.618586000000	37.851035000000	42.425053000000
C	28.431678000000	48.295978000000	38.624131000000

H	28.303776000000	48.010066000000	39.673905000000
C	27.054548000000	48.559705000000	37.975455000000
H	26.642541000000	49.487015000000	38.394292000000
H	27.204592000000	48.742017000000	36.903746000000
C	26.056884000000	47.413928000000	38.194752000000
H	26.503740000000	46.461870000000	37.892552000000
H	25.835642000000	47.332497000000	39.266850000000
C	24.728635000000	47.583704000000	37.451342000000
H	24.048939000000	46.789125000000	37.785532000000
H	24.259628000000	48.545590000000	37.702067000000
N	24.928304000000	47.481220000000	36.007086000000
H	25.891399000000	47.479674000000	35.639296000000
C	24.021482000000	47.008783000000	35.143305000000
N	24.372466000000	46.857165000000	33.852138000000
H	25.365522000000	46.922625000000	33.628362000000
H	23.766520000000	46.276926000000	33.280333000000
N	22.753973000000	46.726772000000	35.491598000000
H	22.534598000000	46.682812000000	36.475813000000
H	22.321305000000	45.991447000000	34.897762000000
C	29.185240000000	47.166610000000	37.929397000000
O	28.928479000000	45.974391000000	38.146888000000
N	30.114552000000	47.555763000000	37.025792000000
H	30.330742000000	48.541542000000	36.963638000000
C	30.957929000000	46.635626000000	36.267011000000
H	30.470769000000	45.659131000000	36.286257000000
C	31.172082000000	47.099249000000	34.827821000000
H	31.570273000000	48.121251000000	34.807954000000
H	31.915101000000	46.445929000000	34.354683000000
O	29.970638000000	47.109908000000	34.047327000000
H	29.781798000000	46.152091000000	33.797631000000
C	30.076581000000	43.069403000000	39.569297000000
H	29.928096000000	42.479631000000	40.479717000000
C	28.888382000000	42.856883000000	38.615529000000
H	29.168669000000	43.159321000000	37.598603000000
H	28.596962000000	41.805189000000	38.590248000000
O	27.738707000000	43.597684000000	39.048138000000
H	27.980627000000	44.539775000000	38.930472000000
C	31.398576000000	42.653390000000	38.929533000000
O	31.683876000000	41.470353000000	38.709686000000
N	32.195688000000	43.691540000000	38.587118000000
H	31.958164000000	44.637577000000	38.868557000000
C	33.534938000000	43.576160000000	38.031601000000
H	34.106716000000	42.828041000000	38.595526000000
C	33.526408000000	43.157662000000	36.554196000000
H	34.545279000000	42.998945000000	36.194531000000
H	32.976268000000	42.219346000000	36.459912000000
H	33.046303000000	43.914668000000	35.924654000000
C	34.196903000000	44.952595000000	38.250451000000
O	33.550424000000	45.901759000000	38.726066000000
N	35.488953000000	45.049717000000	37.894460000000
H	35.987311000000	44.232073000000	37.543540000000
C	36.267495000000	46.250207000000	38.155345000000
H	36.667139000000	46.240472000000	39.176942000000
H	37.095928000000	46.295907000000	37.443971000000
C	37.778920000000	42.518186000000	42.645525000000
H	37.660806000000	41.761483000000	41.862493000000
C	37.947737000000	43.901240000000	42.015961000000
H	38.041060000000	44.657678000000	42.810910000000
C	39.165092000000	43.985732000000	41.102733000000
H	40.083612000000	43.800399000000	41.670269000000
H	39.091386000000	43.238932000000	40.304187000000
H	39.234509000000	44.977110000000	40.643334000000
O	36.807361000000	44.239505000000	41.199859000000
H	36.002858000000	44.135708000000	41.738093000000
C	32.941947000000	35.199970000000	40.659111000000
H	32.844666000000	34.608038000000	39.738260000000
H	31.928144000000	35.416735000000	41.012558000000
C	33.727368000000	36.470576000000	40.421109000000
C	33.076799000000	37.671120000000	40.103895000000
H	31.989604000000	37.693750000000	40.061333000000
C	33.799573000000	38.842575000000	39.859562000000

H	33.273538000000	39.761220000000	39.611051000000
C	35.196074000000	38.834828000000	39.936522000000
H	35.754377000000	39.751430000000	39.763534000000
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H	35.650954000000	35.554986000000	40.748777000000
S	39.613838000000	41.457380000000	33.826377000000
O	37.170390000000	42.888826000000	36.854809000000
Fe	38.073851000000	42.350556000000	35.590235000000
C	36.383507000000	39.384132000000	35.451474000000
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C	37.527215000000	39.425841000000	36.235807000000
C	38.007623000000	38.328134000000	37.036933000000
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C	40.431420000000	44.175991000000	36.252042000000
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C	37.170251000000	45.837525000000	33.281959000000
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C	34.672759000000	40.377826000000	33.910387000000
C	35.883728000000	40.438093000000	34.693095000000
N	38.352027000000	40.515997000000	36.375431000000
N	39.838214000000	42.939547000000	36.376710000000
N	37.958988000000	44.092300000000	34.585198000000
N	36.461693000000	41.672741000000	34.584175000000
H	35.822677000000	38.454725000000	35.442534000000
H	41.089488000000	40.500221000000	38.381436000000
H	40.511625000000	46.143811000000	35.475840000000
H	35.148964000000	44.170905000000	32.681202000000
C	31.109366000000	38.313585000000	36.596023000000
O	29.799246000000	38.653919000000	36.139307000000
C	29.627294000000	39.870556000000	35.553384000000
C	28.298309000000	40.267339000000	35.328686000000
C	28.027417000000	41.528411000000	34.819176000000
C	29.068112000000	42.418541000000	34.494590000000
C	30.388459000000	41.976763000000	34.647059000000
C	30.675380000000	40.720239000000	35.176590000000
C	28.785523000000	43.840521000000	34.116604000000
O	27.632382000000	44.314017000000	34.396434000000
O	29.712499000000	44.533675000000	33.594223000000
H	27.498437000000	39.581850000000	35.590944000000
H	26.997072000000	41.834868000000	34.677235000000
H	31.208524000000	42.628746000000	34.371195000000
H	31.709242000000	40.427557000000	35.313475000000
H	31.511542000000	39.094312000000	37.250709000000
H	30.996707000000	37.383861000000	37.155333000000
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O	27.190989000000	46.989139000000	34.465995000000
H	28.088739000000	47.374930000000	34.405161000000
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O	30.515234000000	48.790868000000	31.922345000000
H	30.229824000000	48.186207000000	32.648820000000
H	29.927542000000	48.589722000000	31.179146000000
O	36.359136000000	42.016952000000	39.452398000000
H	36.689011000000	42.160056000000	38.543541000000
H	36.564352000000	42.844142000000	39.933715000000
H	38.804253000000	47.227699000000	33.799399000000
H	36.508201000000	46.343511000000	32.589838000000
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H	42.524699000000	42.699730000000	38.352192000000
H	39.768768000000	38.233080000000	38.360022000000
H	37.528220000000	37.360632000000	37.104922000000

H	34.034623000000	39.506984000000	33.828904000000
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H	33.429564000000	34.558725000000	41.402233000000
H	27.577442000000	38.636850000000	44.469143000000
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H	30.717559000000	33.823807000000	29.464635000000
H	19.064755000000	44.317846000000	31.633014000000
H	30.527199000000	33.166516000000	31.096745000000
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H	40.067873000000	42.642509000000	33.359420000000
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H	29.022756000000	49.219467000000	38.607188000000
H	32.213005000000	45.882836000000	29.737511000000
H	28.094686000000	44.266668000000	42.205337000000
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C	-5.418823000000	3.392485000000	1.481887000000
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H	-4.344595000000	3.596456000000	1.572584000000
N	-5.822589000000	2.216193000000	2.239816000000
H	-6.308677000000	2.345584000000	3.155554000000
C	-5.323542000000	0.996619000000	2.004826000000
N	-4.580384000000	0.720779000000	0.926072000000
H	-4.376269000000	1.366817000000	0.164878000000
H	-4.331018000000	-0.259739000000	0.786996000000
N	-5.565790000000	0.004265000000	2.883537000000
H	-6.335522000000	0.108975000000	3.564983000000
H	-5.284274000000	-0.928068000000	2.595038000000
C	-2.006668000000	-7.349421000000	-0.646975000000
H	-2.865775000000	-6.942346000000	-0.100542000000
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H	-0.298846000000	-6.632155000000	-1.728296000000
O	-1.696512000000	-5.160326000000	-1.731487000000
H	-2.252921000000	-4.685587000000	-1.077311000000
C	-2.443642000000	-8.173513000000	-1.861813000000
O	-1.626517000000	-8.584737000000	-2.679508000000
N	-3.776928000000	-8.426345000000	-1.943215000000
H	-4.457184000000	-8.075287000000	-1.265128000000
C	2.211111000000	2.765908000000	8.775931000000
H	1.561913000000	2.036212000000	9.272620000000
C	1.787605000000	3.020026000000	7.324183000000
H	0.751253000000	3.389637000000	7.303249000000
H	2.405792000000	3.828865000000	6.910902000000
C	1.898129000000	1.799625000000	6.388428000000
H	2.934817000000	1.430653000000	6.449348000000
C	0.964268000000	0.653112000000	6.806370000000
H	1.054870000000	-0.196768000000	6.118237000000
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H	-0.084327000000	0.980257000000	6.791386000000
C	1.633662000000	2.208891000000	4.931769000000
H	1.744909000000	1.357628000000	4.249790000000
H	0.612890000000	2.599504000000	4.817381000000
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C	-9.214420000000	0.523734000000	7.026787000000
H	-8.940183000000	-0.506783000000	6.784830000000
H	-10.134374000000	0.757736000000	6.478201000000
C	-8.084812000000	1.484667000000	6.651359000000
H	-8.341298000000	2.523519000000	6.884611000000
H	-7.188201000000	1.255766000000	7.246136000000
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O	-7.848988000000	0.320051000000	4.549553000000
O	-7.123799000000	2.445861000000	4.683879000000
C	-3.011600000000	4.674775000000	-4.087008000000
H	-2.607612000000	4.018703000000	-4.871534000000
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H	-4.826836000000	5.659517000000	-3.568520000000
C	-4.736443000000	5.609418000000	-5.709182000000
H	-4.395615000000	4.956359000000	-6.524352000000
H	-5.802463000000	5.810761000000	-5.869951000000
H	-4.201233000000	6.561089000000	-5.782941000000
C	-5.318231000000	3.657970000000	-4.199502000000
H	-5.047309000000	2.936233000000	-4.982847000000
H	-5.135507000000	3.177400000000	-3.231430000000
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C	0.098049000000	6.894011000000	-4.181962000000
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C	1.476793000000	6.494014000000	-4.740067000000
H	1.398529000000	6.349644000000	-5.824705000000
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C	2.023072000000	5.239285000000	-4.087818000000
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H	1.610309000000	3.960873000000	-5.774565000000
C	2.364882000000	2.822118000000	-4.108305000000
H	2.299702000000	1.868218000000	-4.625834000000
C	2.833346000000	2.869905000000	-2.791292000000
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C	2.925732000000	4.103578000000	-2.134375000000
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H	2.583106000000	6.226694000000	-2.251916000000
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C	-1.488588000000	5.832419000000	0.508820000000
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H	-0.535620000000	5.251656000000	-1.335913000000
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C	-0.605868000000	3.327759000000	1.468747000000
H	-0.269682000000	2.361490000000	1.834316000000
C	-1.331731000000	4.184832000000	2.300216000000
H	-1.559985000000	3.890621000000	3.322023000000
C	-1.767897000000	5.423546000000	1.821343000000
H	-2.330456000000	6.085882000000	2.476412000000
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C	-7.893097000000	-0.428002000000	-2.872219000000
H	-8.841187000000	-0.103001000000	-3.319851000000
H	-8.096127000000	-1.384492000000	-2.373927000000
C	-7.425361000000	0.622969000000	-1.856829000000
H	-6.431694000000	0.365474000000	-1.477252000000
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C	-8.368212000000	0.812558000000	-0.665213000000
H	-8.011872000000	1.671529000000	-0.081493000000
H	-9.386517000000	1.044368000000	-1.008022000000
N	-8.379365000000	-0.380338000000	0.179096000000
H	-7.878544000000	-1.221460000000	-0.144471000000
C	-8.628642000000	-0.373261000000	1.494503000000
N	-8.465932000000	-1.512898000000	2.192542000000
H	-7.971639000000	-2.276580000000	1.729926000000
H	-8.426810000000	-1.428201000000	3.203137000000
N	-9.087015000000	0.709642000000	2.145351000000
H	-9.051239000000	1.597211000000	1.665559000000
H	-8.809373000000	0.729823000000	3.147009000000
C	-5.621310000000	-1.392141000000	-3.524809000000
O	-4.706148000000	-0.807225000000	-2.929643000000
N	-5.594061000000	-2.725286000000	-3.764620000000
H	-6.362021000000	-3.127844000000	-4.284680000000
C	-4.502155000000	-3.615196000000	-3.382540000000
H	-3.830561000000	-3.046654000000	-2.736945000000
C	-4.978871000000	-4.882175000000	-2.672911000000
H	-5.770587000000	-5.376305000000	-3.249079000000

H	-4.129041000000	-5.570154000000	-2.608483000000
O	-5.515988000000	-4.634885000000	-1.369063000000
H	-4.760974000000	-4.291980000000	-0.799526000000
C	-1.560575000000	0.784638000000	-2.778757000000
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H	-1.843697000000	1.602806000000	-0.795337000000
O	-3.663774000000	1.485458000000	-1.696281000000
H	-4.159524000000	0.824245000000	-2.225213000000
C	-0.214999000000	0.134187000000	-2.479973000000
O	0.557597000000	0.608449000000	-1.643863000000
N	0.034670000000	-1.031016000000	-3.134918000000
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H	0.901241000000	-3.162797000000	-4.611354000000
C	2.417488000000	-1.052418000000	-3.781018000000
O	2.203671000000	-0.569216000000	-4.894260000000
N	3.630211000000	-1.083282000000	-3.176719000000
H	3.696802000000	-1.388783000000	-2.207702000000
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H	5.612729000000	-1.327517000000	-3.831129000000
C	6.860449000000	4.794637000000	-1.974433000000
H	6.743622000000	4.618434000000	-0.899105000000
C	7.156550000000	3.485586000000	-2.706222000000
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C	8.429410000000	2.808459000000	-2.214022000000
H	9.301170000000	3.444429000000	-2.402175000000
H	8.365290000000	2.616322000000	-1.136663000000
H	8.576236000000	1.851218000000	-2.724203000000
O	6.090802000000	2.537963000000	-2.522893000000
H	5.248936000000	2.953004000000	-2.783275000000
C	2.370823000000	6.313302000000	2.931860000000
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H	1.508440000000	5.656465000000	2.781347000000
C	3.675817000000	5.573682000000	2.740948000000
C	3.732319000000	4.390646000000	1.990056000000
H	2.814956000000	3.989145000000	1.564182000000
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C	6.119611000000	4.229539000000	2.336079000000
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Fe	4.982774000000	-2.788088000000	0.875522000000
C	3.442404000000	-2.394494000000	3.912499000000
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C	8.473243000000	-0.697822000000	-0.466863000000
C	8.334992000000	-1.557478000000	-1.513548000000
C	7.168338000000	-2.361686000000	-1.238762000000
C	5.574592000000	-4.155526000000	-1.810860000000
C	5.077420000000	-5.186924000000	-2.690369000000
C	4.003568000000	-5.747517000000	-2.069247000000
C	3.848499000000	-5.059904000000	-0.808016000000
C	2.721313000000	-4.746884000000	1.368681000000

C	1.744243000000	-5.142041000000	2.355065000000
C	1.899885000000	-4.308687000000	3.418831000000
C	2.970692000000	-3.402722000000	3.082027000000
N	5.227394000000	-1.579701000000	2.442771000000
N	6.612420000000	-1.992739000000	-0.040319000000
N	4.806874000000	-4.092589000000	-0.673992000000
N	3.455267000000	-3.680757000000	1.831113000000
H	2.960044000000	-2.268663000000	4.876563000000
H	7.878154000000	0.478200000000	1.905730000000
H	7.222083000000	-3.545916000000	-2.997597000000
H	2.202549000000	-6.185562000000	-0.093244000000
C	2.425794000000	-0.012395000000	1.031762000000
O	1.583859000000	-0.379106000000	2.061763000000
C	0.418384000000	-1.043683000000	1.755928000000
C	-0.695960000000	-0.764775000000	2.554844000000
C	-1.921677000000	-1.339099000000	2.236343000000
C	-2.042114000000	-2.222064000000	1.150422000000
C	-0.894051000000	-2.544892000000	0.411884000000
C	0.333295000000	-1.957417000000	0.703341000000
C	-3.384252000000	-2.764330000000	0.740401000000
O	-4.423161000000	-2.139962000000	1.134935000000
O	-3.416912000000	-3.789400000000	-0.004617000000
H	-0.594391000000	-0.072829000000	3.384783000000
H	-2.798563000000	-1.090895000000	2.824327000000
H	-0.966229000000	-3.238989000000	-0.417268000000
H	1.219879000000	-2.212068000000	0.135693000000
H	1.906898000000	0.263751000000	0.109817000000
H	3.148444000000	0.710734000000	1.401150000000
H	3.182636000000	-0.968659000000	0.617811000000
O	-6.885354000000	-2.713363000000	0.108276000000
H	-6.724484000000	-3.424330000000	-0.547191000000
H	-5.972801000000	-2.509832000000	0.452163000000
O	-5.688903000000	-7.152874000000	-0.153267000000
H	-5.734123000000	-6.252502000000	-0.550074000000
H	-5.383906000000	-7.007669000000	0.754580000000
O	4.741479000000	1.156493000000	-0.453350000000
H	4.793225000000	0.184434000000	-0.495196000000
H	5.408533000000	1.509922000000	-1.073691000000
H	5.507557000000	-5.437161000000	-3.651709000000
H	3.370779000000	-6.556128000000	-2.412240000000
H	8.955078000000	-1.653084000000	-2.395793000000
H	9.231365000000	0.058473000000	-0.310454000000
H	6.658422000000	0.899006000000	4.167730000000
H	4.581340000000	-0.277395000000	5.451229000000
H	1.351445000000	-4.293457000000	4.351829000000
H	1.042849000000	-5.957268000000	2.232147000000
H	2.276674000000	7.141999000000	2.216822000000
H	-2.782593000000	7.567290000000	0.584967000000
H	-5.968423000000	4.248557000000	1.877841000000
H	-4.089824000000	-9.015524000000	-2.702815000000
H	2.172046000000	3.690829000000	9.362858000000
H	-9.439454000000	0.583116000000	8.097883000000
H	3.239151000000	2.384974000000	8.826708000000
H	-3.934307000000	-3.910409000000	-4.275553000000
H	7.028493000000	-4.837267000000	0.801950000000
H	5.935169000000	5.250508000000	-2.346506000000
H	7.672868000000	5.515551000000	-2.124070000000
H	4.562664000000	-0.302523000000	-4.846825000000
H	-2.142369000000	0.197023000000	-3.498255000000
H	-7.355246000000	-1.237014000000	-4.812398000000
H	-1.482778000000	-8.037912000000	0.030877000000
H	-2.903151000000	4.128419000000	-3.138854000000
H	-0.274461000000	7.790214000000	-4.689117000000

***TransitionState1 / HS_TS1**

C	-6.011001000000	3.434219000000	1.456665000000
H	-6.227454000000	3.392513000000	0.381839000000
H	-4.953846000000	3.700429000000	1.583310000000
N	-6.345898000000	2.185479000000	2.123522000000
H	-6.875742000000	2.214988000000	3.023200000000
C	-5.748435000000	1.023932000000	1.827639000000

N	-4.955973000000	0.876716000000	0.758604000000
H	-4.718162000000	1.609337000000	0.090366000000
H	-4.596693000000	-0.065072000000	0.586232000000
N	-5.947766000000	-0.040641000000	2.626902000000
H	-6.735666000000	-0.038540000000	3.294748000000
H	-5.580927000000	-0.928007000000	2.294079000000
C	-2.686562000000	-7.538084000000	-0.096477000000
H	-3.582515000000	-6.954969000000	-0.340278000000
C	-2.048703000000	-7.037307000000	1.198801000000
H	-2.770983000000	-7.160747000000	2.022818000000
H	-1.173897000000	-7.653151000000	1.424907000000
O	-1.581011000000	-5.705091000000	1.116946000000
H	-2.320713000000	-5.104561000000	0.879892000000
C	-1.719106000000	-7.528737000000	-1.282101000000
O	-0.507523000000	-7.686925000000	-1.146966000000
N	-2.316099000000	-7.352763000000	-2.492780000000
H	-3.334293000000	-7.349655000000	-2.591437000000
C	2.719897000000	4.475672000000	7.473382000000
H	3.808392000000	4.386999000000	7.559728000000
C	2.051252000000	3.116829000000	7.233543000000
H	2.293331000000	2.438025000000	8.065440000000
H	0.960184000000	3.250000000000	7.261001000000
C	2.427301000000	2.430881000000	5.904239000000
H	2.200860000000	3.134995000000	5.088409000000
C	3.923390000000	2.093690000000	5.819716000000
H	4.160890000000	1.609728000000	4.865918000000
H	4.552332000000	2.986875000000	5.890074000000
H	4.213356000000	1.410628000000	6.631210000000
C	1.575575000000	1.170275000000	5.688235000000
H	1.782539000000	0.705524000000	4.716873000000
H	1.778147000000	0.423681000000	6.468780000000
H	0.503271000000	1.401598000000	5.728423000000
C	-9.633419000000	-0.108042000000	6.748010000000
H	-9.240398000000	-1.088339000000	6.464679000000
H	-10.572628000000	0.040764000000	6.202459000000
C	-8.622703000000	0.993168000000	6.423136000000
H	-8.997800000000	1.983671000000	6.702121000000
H	-7.705869000000	0.843964000000	7.012276000000
C	-8.189727000000	1.055253000000	4.955298000000
O	-8.274577000000	-0.029776000000	4.263514000000
O	-7.753196000000	2.144678000000	4.517018000000
C	-2.567619000000	5.972863000000	-4.329979000000
H	-2.888426000000	5.884115000000	-5.375683000000
C	-3.783556000000	6.387296000000	-3.461233000000
H	-3.403890000000	6.632115000000	-2.457731000000
C	-4.500076000000	7.624821000000	-4.020089000000
H	-4.945978000000	7.400823000000	-4.998590000000
H	-5.309575000000	7.937201000000	-3.348761000000
H	-3.808252000000	8.459110000000	-4.154974000000
C	-4.754962000000	5.205098000000	-3.319995000000
H	-5.129243000000	4.892315000000	-4.304519000000
H	-4.283369000000	4.338143000000	-2.842815000000
H	-5.624417000000	5.492374000000	-2.715050000000
C	-1.423196000000	6.981870000000	-4.288154000000
O	-1.510064000000	8.098424000000	-4.792709000000
N	-0.305713000000	6.564917000000	-3.611800000000
H	-0.246741000000	5.601122000000	-3.312836000000
C	0.900810000000	7.371540000000	-3.507637000000
H	1.139479000000	7.534795000000	-2.448598000000
C	2.112672000000	6.730970000000	-4.216744000000
H	1.894978000000	6.654981000000	-5.288412000000
H	2.962852000000	7.417617000000	-4.107761000000
C	2.467825000000	5.367625000000	-3.658279000000
C	2.145904000000	4.192349000000	-4.353886000000
H	1.684060000000	4.267204000000	-5.336457000000
C	2.416394000000	2.932403000000	-3.811309000000
H	2.164260000000	2.033082000000	-4.367913000000
C	3.010507000000	2.830720000000	-2.548905000000
H	3.203934000000	1.862571000000	-2.095608000000
C	3.348829000000	3.995727000000	-1.849513000000
H	3.810311000000	3.922088000000	-0.868682000000

C	3.081305000000	5.249741000000	-2.401587000000
H	3.344220000000	6.147862000000	-1.845933000000
C	-1.199461000000	7.381214000000	0.770124000000
H	-1.227433000000	7.474990000000	-0.320541000000
H	-0.543401000000	8.171199000000	1.156719000000
C	-0.724404000000	6.009310000000	1.193984000000
C	-0.445050000000	5.015738000000	0.247889000000
H	-0.569338000000	5.245761000000	-0.808418000000
C	-0.007820000000	3.744839000000	0.634238000000
H	0.203688000000	2.985253000000	-0.114052000000
C	0.155239000000	3.450958000000	1.990064000000
H	0.496595000000	2.465151000000	2.294185000000
C	-0.118201000000	4.432876000000	2.947818000000
H	0.004607000000	4.210752000000	4.005143000000
C	-0.553458000000	5.698087000000	2.551798000000
H	-0.764313000000	6.455746000000	3.304355000000
C	-6.999396000000	-0.378835000000	-4.292556000000
H	-6.902857000000	0.610875000000	-4.749335000000
C	-8.074585000000	-0.355471000000	-3.183757000000
H	-9.052594000000	-0.172141000000	-3.646924000000
H	-8.127828000000	-1.351417000000	-2.726412000000
C	-7.805647000000	0.711866000000	-2.113812000000
H	-6.792248000000	0.604276000000	-1.711932000000
H	-7.851575000000	1.704633000000	-2.579030000000
C	-8.793329000000	0.696437000000	-0.943399000000
H	-8.574139000000	1.562552000000	-0.305962000000
H	-9.825766000000	0.803694000000	-1.304686000000
N	-8.657968000000	-0.530349000000	-0.160316000000
H	-8.085622000000	-1.300151000000	-0.532846000000
C	-8.917453000000	-0.627525000000	1.150269000000
N	-8.647660000000	-1.785587000000	1.781876000000
H	-8.081180000000	-2.472297000000	1.283701000000
H	-8.627990000000	-1.759863000000	2.796275000000
N	-9.486388000000	0.362143000000	1.857824000000
H	-9.539429000000	1.276341000000	1.433204000000
H	-9.223937000000	0.348719000000	2.865807000000
C	-5.628722000000	-0.760501000000	-3.746568000000
O	-4.804497000000	0.083199000000	-3.373046000000
N	-5.377742000000	-2.086618000000	-3.649955000000
H	-6.075962000000	-2.744454000000	-3.968437000000
C	-4.145379000000	-2.613663000000	-3.070652000000
H	-3.941753000000	-2.084702000000	-2.135192000000
C	-4.243575000000	-4.114519000000	-2.823638000000
H	-4.584633000000	-4.629092000000	-3.730497000000
H	-3.247767000000	-4.502776000000	-2.582818000000
O	-5.164177000000	-4.457911000000	-1.780129000000
H	-4.670871000000	-4.288416000000	-0.916657000000
C	-1.683669000000	1.424187000000	-2.654566000000
H	-1.398341000000	2.456285000000	-2.887337000000
C	-2.590856000000	1.404997000000	-1.414374000000
H	-2.753272000000	0.361661000000	-1.107692000000
H	-2.099996000000	1.922315000000	-0.588388000000
O	-3.842900000000	2.060861000000	-1.628890000000
H	-4.311030000000	1.544551000000	-2.316995000000
C	-0.429958000000	0.614389000000	-2.344634000000
O	0.283922000000	0.892345000000	-1.381095000000
N	-0.232520000000	-0.486513000000	-3.125735000000
H	-0.654094000000	-0.488132000000	-4.045443000000
C	0.902533000000	-1.382805000000	-2.946090000000
H	1.158795000000	-1.357017000000	-1.887107000000
C	0.505854000000	-2.806902000000	-3.361014000000
H	1.330950000000	-3.504879000000	-3.192480000000
H	-0.358061000000	-3.145348000000	-2.779405000000
H	0.249984000000	-2.834743000000	-4.427329000000
C	2.101142000000	-0.917811000000	-3.791061000000
O	1.919666000000	-0.441677000000	-4.915422000000
N	3.311698000000	-1.137148000000	-3.229729000000
H	3.365053000000	-1.454679000000	-2.259073000000
C	4.549762000000	-0.856192000000	-3.942015000000
H	5.091393000000	-0.016244000000	-3.495315000000
H	5.199442000000	-1.737391000000	-3.933010000000

C	7.291108000000	4.001105000000	-1.844195000000
H	7.109499000000	3.750886000000	-0.792874000000
C	7.396564000000	2.734030000000	-2.692560000000
H	7.566544000000	3.017884000000	-3.743315000000
C	8.525297000000	1.813917000000	-2.243727000000
H	9.494221000000	2.315273000000	-2.341656000000
H	8.384929000000	1.527774000000	-1.194706000000
H	8.539959000000	0.902520000000	-2.850384000000
O	6.187887000000	1.958761000000	-2.621345000000
H	5.425331000000	2.536569000000	-2.804625000000
C	5.129626000000	6.701190000000	4.360504000000
H	6.122900000000	7.087740000000	4.611977000000
H	4.608016000000	6.493594000000	5.304298000000
C	5.219430000000	5.462669000000	3.497291000000
C	4.076602000000	4.942609000000	2.870788000000
H	3.118790000000	5.443878000000	2.995693000000
C	4.149441000000	3.789564000000	2.088073000000
H	3.248974000000	3.405809000000	1.615946000000
C	5.370203000000	3.128544000000	1.908686000000
H	5.415818000000	2.233142000000	1.293390000000
C	6.513212000000	3.641710000000	2.526425000000
H	7.471546000000	3.142969000000	2.398425000000
C	6.437151000000	4.796010000000	3.310883000000
H	7.335688000000	5.186370000000	3.784933000000
S	5.845482000000	-5.037384000000	1.521509000000
O	3.595381000000	-1.925996000000	-0.242357000000
Fe	4.502152000000	-3.280173000000	0.521707000000
C	3.734033000000	-2.375878000000	3.746252000000
C	7.332759000000	-1.397170000000	0.674639000000
C	5.456093000000	-4.479273000000	-2.548709000000
C	1.726319000000	-5.261047000000	0.426003000000
C	4.887199000000	-1.834772000000	3.192935000000
C	5.774242000000	-0.919599000000	3.870028000000
C	6.776029000000	-0.630619000000	2.995765000000
C	6.504697000000	-1.378194000000	1.791434000000
C	7.156270000000	-2.177597000000	-0.461615000000
C	8.087515000000	-2.246076000000	-1.561125000000
C	7.570024000000	-3.126734000000	-2.461823000000
C	6.317313000000	-3.589670000000	-1.917194000000
C	4.244353000000	-4.937750000000	-2.036643000000
C	3.366811000000	-5.872640000000	-2.701681000000
C	2.314035000000	-6.087198000000	-1.862936000000
C	2.561568000000	-5.280550000000	-0.688871000000
C	1.957689000000	-4.547736000000	1.600406000000
C	1.095296000000	-4.602672000000	2.758142000000
C	1.666919000000	-3.803353000000	3.700342000000
C	2.863391000000	-3.256390000000	3.106702000000
N	5.347357000000	-2.098956000000	1.925819000000
N	6.084521000000	-3.006907000000	-0.692110000000
N	3.734135000000	-4.584405000000	-0.817587000000
N	3.020448000000	-3.715225000000	1.829195000000
H	3.485406000000	-2.081760000000	4.761441000000
H	8.222510000000	-0.775559000000	0.710924000000
H	5.755697000000	-4.851530000000	-3.524249000000
H	0.817500000000	-5.854176000000	0.375175000000
C	2.349723000000	-0.113935000000	1.031839000000
O	1.403372000000	-0.348810000000	2.032541000000
C	0.214066000000	-0.937270000000	1.687197000000
C	-0.925730000000	-0.545948000000	2.401086000000
C	-2.158771000000	-1.109593000000	2.091318000000
C	-2.263618000000	-2.106102000000	1.107275000000
C	-1.103002000000	-2.516143000000	0.436182000000
C	0.126263000000	-1.922510000000	0.699621000000
C	-3.582558000000	-2.694792000000	0.712987000000
O	-4.621784000000	-1.955443000000	0.806738000000
O	-3.601047000000	-3.877934000000	0.252782000000
H	-0.832497000000	0.211667000000	3.172452000000
H	-3.046339000000	-0.781814000000	2.623408000000
H	-1.167951000000	-3.314889000000	-0.294485000000
H	1.019425000000	-2.243695000000	0.178583000000
H	1.908262000000	0.313308000000	0.128692000000

H	3.164893000000	0.463991000000	1.460294000000
H	2.966923000000	-1.179186000000	0.524844000000
O	-6.939395000000	-2.723991000000	-0.346798000000
H	-6.656425000000	-3.389975000000	-1.003804000000
H	-6.076210000000	-2.448264000000	0.074743000000
O	-5.241140000000	-7.128630000000	-2.516512000000
H	-5.351400000000	-6.229571000000	-2.129578000000
H	-5.678045000000	-7.732130000000	-1.897720000000
O	4.841197000000	0.722265000000	-0.429013000000
H	4.639755000000	-0.229433000000	-0.522311000000
H	5.443335000000	0.970909000000	-1.155918000000
H	3.553744000000	-6.306562000000	-3.676042000000
H	1.450475000000	-6.731366000000	-1.980352000000
H	7.985027000000	-3.442731000000	-3.410492000000
H	9.016143000000	-1.692877000000	-1.617205000000
H	7.629089000000	0.019607000000	3.139879000000
H	5.631885000000	-0.553996000000	4.878331000000
H	1.317526000000	-3.579726000000	4.700148000000
H	0.163392000000	-5.150806000000	2.788491000000
H	4.574566000000	7.502223000000	3.857634000000
H	-2.208131000000	7.592481000000	1.148328000000
H	-6.621222000000	4.223882000000	1.898862000000
H	-1.740168000000	-7.480467000000	-3.314273000000
H	2.353535000000	4.935874000000	8.398546000000
H	-9.866655000000	-0.121593000000	7.818907000000
H	2.507746000000	5.170133000000	6.650276000000
H	-3.301853000000	-2.413794000000	-3.745155000000
H	6.296947000000	-5.614114000000	0.384965000000
H	6.465939000000	4.636019000000	-2.188292000000
H	8.214616000000	4.588478000000	-1.909163000000
H	4.289918000000	-0.604902000000	-4.971475000000
H	-2.231049000000	1.013552000000	-3.509966000000
H	-7.304112000000	-1.080247000000	-5.079115000000
H	-3.018913000000	-8.576942000000	0.049821000000
H	-2.219645000000	4.981344000000	-4.011423000000
H	0.661199000000	8.338316000000	-3.955624000000

²Intermediate1 / LS_I1

C	-6.959009000000	3.253332000000	0.842708000000
H	-6.923019000000	3.042984000000	-0.233417000000
H	-6.013776000000	3.732518000000	1.129023000000
N	-7.223073000000	2.052702000000	1.618198000000
H	-7.930190000000	2.085878000000	2.387065000000
C	-6.418531000000	0.983209000000	1.598828000000
N	-5.400154000000	0.866833000000	0.736713000000
H	-5.111329000000	1.570679000000	0.055919000000
H	-4.892094000000	-0.020023000000	0.745064000000
N	-6.634559000000	-0.014272000000	2.476667000000
H	-7.554439000000	-0.083265000000	2.941729000000
H	-6.076073000000	-0.853905000000	2.352554000000
C	-1.861078000000	-7.684048000000	0.629500000000
H	-2.901731000000	-7.420777000000	0.409193000000
C	-1.234517000000	-6.666302000000	1.581517000000
H	-1.775691000000	-6.665751000000	2.538698000000
H	-0.200819000000	-6.965972000000	1.777966000000
O	-1.193756000000	-5.364140000000	1.014301000000
H	-2.019720000000	-4.879690000000	1.224314000000
C	-1.052500000000	-7.808004000000	-0.664220000000
O	0.178370000000	-7.815836000000	-0.661798000000
N	-1.796006000000	-7.941235000000	-1.790915000000
H	-2.816102000000	-7.878172000000	-1.784175000000
C	5.455694000000	2.597192000000	7.303117000000
H	5.784053000000	1.553990000000	7.372747000000
C	3.933179000000	2.729889000000	7.430146000000
H	3.604756000000	2.309837000000	8.392975000000
H	3.673181000000	3.797547000000	7.461071000000
C	3.127064000000	2.068460000000	6.294378000000
H	3.492909000000	2.485590000000	5.343745000000
C	3.318640000000	0.544127000000	6.249837000000
H	2.734789000000	0.102339000000	5.432952000000
H	4.368029000000	0.266419000000	6.099124000000

H	2.982690000000	0.079364000000	7.186706000000
C	1.635628000000	2.415891000000	6.415278000000
H	1.059776000000	1.975725000000	5.592451000000
H	1.216945000000	2.034460000000	7.356272000000
H	1.477709000000	3.501272000000	6.397488000000
C	-11.271508000000	-0.265898000000	5.539698000000
H	-10.757439000000	-1.224238000000	5.425610000000
H	-12.048071000000	-0.213039000000	4.767430000000
C	-10.282197000000	0.894488000000	5.411980000000
H	-10.777760000000	1.864599000000	5.522578000000
H	-9.539816000000	0.839492000000	6.221842000000
C	-9.493153000000	0.917689000000	4.099557000000
O	-9.270254000000	-0.213814000000	3.521691000000
O	-9.085657000000	2.023321000000	3.675709000000
C	-3.441729000000	5.673735000000	-4.496056000000
H	-3.734247000000	5.451796000000	-5.530207000000
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H	-5.021338000000	7.961182000000	-4.577003000000
C	-5.505191000000	4.710827000000	-3.398009000000
H	-5.822685000000	4.246564000000	-4.341882000000
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H	-6.411792000000	4.931432000000	-2.819892000000
C	-2.441459000000	6.825720000000	-4.540415000000
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N	-1.286531000000	6.613639000000	-3.833036000000
H	-1.118809000000	5.700515000000	-3.433807000000
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C	1.131134000000	6.997743000000	-4.307817000000
H	1.019865000000	6.768364000000	-5.373788000000
H	1.894393000000	7.782851000000	-4.223901000000
C	1.569972000000	5.756818000000	-3.555421000000
C	1.473833000000	4.486236000000	-4.138614000000
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C	2.365687000000	4.702450000000	-1.509095000000
H	2.717747000000	4.793631000000	-0.485527000000
C	2.032422000000	5.847240000000	-2.231678000000
H	2.126166000000	6.824249000000	-1.761830000000
C	-2.011116000000	7.341716000000	0.274854000000
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H	-1.515827000000	8.308144000000	0.428658000000
C	-1.372753000000	6.252862000000	1.107711000000
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C	-0.412653000000	4.017804000000	1.305272000000
H	-0.132705000000	3.078115000000	0.834378000000
C	-0.205036000000	4.217994000000	2.672305000000
H	0.248185000000	3.436521000000	3.276003000000
C	-0.577852000000	5.432014000000	3.257650000000
H	-0.418680000000	5.595083000000	4.320804000000
C	-1.156343000000	6.436651000000	2.481999000000
H	-1.443198000000	7.378144000000	2.946429000000
C	-5.980561000000	-1.283789000000	-4.318136000000
H	-5.879731000000	-0.330026000000	-4.846604000000
C	-7.327525000000	-1.333411000000	-3.561490000000
H	-8.140003000000	-1.399179000000	-4.296429000000
H	-7.361264000000	-2.260632000000	-2.975927000000
C	-7.554918000000	-0.113871000000	-2.656016000000
H	-6.680716000000	0.050584000000	-2.017918000000
H	-7.660197000000	0.781482000000	-3.281925000000
C	-8.796191000000	-0.214006000000	-1.763106000000
H	-8.934168000000	0.754048000000	-1.265378000000
H	-9.696189000000	-0.405678000000	-2.364092000000

N	-8.628385000000	-1.260676000000	-0.757337000000
H	-7.862966000000	-1.939294000000	-0.873061000000
C	-9.144695000000	-1.233089000000	0.477624000000
N	-8.829118000000	-2.221813000000	1.334948000000
H	-8.064870000000	-2.843962000000	1.072567000000
H	-9.027702000000	-2.054752000000	2.316932000000
N	-10.008618000000	-0.291073000000	0.892566000000
H	-10.127927000000	0.530936000000	0.319488000000
H	-9.975230000000	-0.131874000000	1.918859000000
C	-4.793705000000	-1.410848000000	-3.370153000000
O	-4.332166000000	-0.440139000000	-2.756211000000
N	-4.307331000000	-2.662176000000	-3.197848000000
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O	-3.961552000000	2.007267000000	-1.456147000000
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O	0.029028000000	0.865903000000	-0.453207000000
N	0.186463000000	0.042147000000	-2.578284000000
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C	1.393298000000	-0.745964000000	-2.384733000000
H	1.908101000000	-0.366397000000	-1.498088000000
C	1.044222000000	-2.235701000000	-2.209201000000
H	1.942730000000	-2.847333000000	-2.094421000000
H	0.410968000000	-2.369700000000	-1.325745000000
H	0.498752000000	-2.600909000000	-3.087488000000
C	2.294136000000	-0.518021000000	-3.616572000000
O	1.829767000000	0.007058000000	-4.640750000000
N	3.560861000000	-0.940439000000	-3.477284000000
H	3.870268000000	-1.302632000000	-2.561841000000
C	4.556904000000	-0.737200000000	-4.516956000000
H	5.110868000000	0.193108000000	-4.342502000000
H	5.259411000000	-1.575113000000	-4.514831000000
C	6.245814000000	4.250412000000	-1.733085000000
H	6.060365000000	3.998240000000	-0.682979000000
C	6.433067000000	2.983382000000	-2.567814000000
H	6.626119000000	3.268073000000	-3.614461000000
C	7.584734000000	2.117819000000	-2.072902000000
H	8.529157000000	2.670992000000	-2.124051000000
H	7.411774000000	1.814824000000	-1.034122000000
H	7.674627000000	1.212203000000	-2.681224000000
O	5.256595000000	2.155491000000	-2.532734000000
H	4.493556000000	2.690428000000	-2.812915000000
C	5.397797000000	6.499486000000	4.809535000000
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H	4.672514000000	7.298496000000	4.622120000000
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H	3.149119000000	5.772089000000	3.423444000000
C	3.825896000000	4.041718000000	2.336917000000
H	2.857099000000	3.879942000000	1.870237000000
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H	4.764058000000	2.347081000000	1.369316000000
C	6.128821000000	3.417193000000	2.668308000000
H	6.966813000000	2.757829000000	2.457702000000
C	6.291765000000	4.492255000000	3.543953000000
H	7.261088000000	4.669138000000	4.006338000000
S	6.556008000000	-4.974503000000	0.841395000000
O	4.176463000000	-1.886112000000	-0.829096000000
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C	5.796098000000	-4.564742000000	-3.190086000000
C	2.500199000000	-5.323817000000	0.265858000000
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C	7.679136000000	-0.331725000000	1.870889000000
C	7.332102000000	-1.200106000000	0.769591000000
C	7.720883000000	-2.123746000000	-1.492685000000
C	8.476056000000	-2.217264000000	-2.719986000000
C	7.839800000000	-3.137266000000	-3.497335000000
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C	2.717156000000	-3.491588000000	3.344791000000
C	3.821320000000	-2.981083000000	2.564704000000
N	6.201234000000	-1.912075000000	1.062206000000
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N	4.319235000000	-4.657370000000	-1.236494000000
N	3.868474000000	-3.597024000000	1.345867000000
H	4.537656000000	-1.593535000000	4.000635000000
H	8.934808000000	-0.681088000000	-0.520237000000
H	5.974759000000	-4.979032000000	-4.178382000000
H	1.633462000000	-5.970978000000	0.360689000000
C	1.963278000000	0.763221000000	2.155050000000
O	0.912991000000	0.693550000000	2.959539000000
C	-0.167057000000	-0.123610000000	2.624128000000
C	-1.443178000000	0.353186000000	2.919166000000
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C	-2.371161000000	-1.683500000000	1.965165000000
C	-1.070345000000	-2.162611000000	1.748155000000
C	0.036331000000	-1.381906000000	2.065775000000
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O	-4.643643000000	-1.835695000000	1.265829000000
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H	-1.563846000000	1.332453000000	3.370069000000
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H	-0.910656000000	-3.149842000000	1.331693000000
H	1.040723000000	-1.757941000000	1.908579000000
H	1.896561000000	0.430703000000	1.126183000000
H	2.799292000000	1.318422000000	2.555698000000
H	3.285047000000	-2.148043000000	-0.549141000000
O	-6.555790000000	-3.049865000000	-0.250353000000
H	-6.045152000000	-3.722262000000	-0.745712000000
H	-5.856893000000	-2.598582000000	0.299055000000
O	-4.670891000000	-7.431091000000	-1.582315000000
H	-4.677419000000	-6.498990000000	-1.263598000000
H	-5.145366000000	-7.937510000000	-0.906781000000
O	3.990310000000	0.801201000000	-0.248816000000
H	4.163309000000	-0.166995000000	-0.371397000000
H	4.501379000000	1.230558000000	-0.962944000000
H	3.895357000000	-6.558908000000	-3.953347000000
H	2.039293000000	-6.981710000000	-1.989794000000
H	8.107177000000	-3.484314000000	-4.487468000000
H	9.373170000000	-1.652378000000	-2.939659000000
H	8.539666000000	0.325067000000	1.893508000000
H	6.644905000000	-0.046818000000	3.797653000000
H	2.465439000000	-3.165731000000	4.346208000000
H	1.211012000000	-5.011669000000	2.796822000000
H	6.402260000000	6.932802000000	4.746263000000
H	-3.067781000000	7.480695000000	0.539328000000
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H	-1.304648000000	-8.063928000000	-2.665786000000
H	5.964881000000	3.151698000000	8.100168000000
H	-11.769551000000	-0.250589000000	6.515859000000
H	5.805527000000	2.994604000000	6.342109000000
H	-2.245264000000	-2.790270000000	-2.768304000000

H	7.776987000000	-4.429977000000	0.635190000000
H	5.396051000000	4.840452000000	-2.096238000000
H	7.139734000000	4.883443000000	-1.785151000000
H	4.054154000000	-0.678369000000	-5.484231000000
H	-2.034448000000	1.144614000000	-2.971759000000
H	-5.957857000000	-2.081609000000	-5.070228000000
H	-1.867925000000	-8.672368000000	1.111283000000
H	-2.969894000000	4.769220000000	-4.090432000000
H	-0.514359000000	8.431206000000	-4.382345000000

⁴Intermediate1 / HS_11

C	-6.778531000000	3.090618000000	1.153850000000
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N	-6.397229000000	-0.295554000000	2.511591000000
H	-7.253505000000	-0.370787000000	3.084213000000
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C	-1.488426000000	-6.851971000000	1.693891000000
H	-2.166243000000	-6.933351000000	2.559007000000
H	-0.566133000000	-7.385987000000	1.937883000000
O	-1.116015000000	-5.507118000000	1.456792000000
H	-1.917562000000	-4.969279000000	1.274869000000
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O	0.014631000000	-7.679389000000	-0.608832000000
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H	-2.862170000000	-7.674581000000	-2.001562000000
C	3.951023000000	4.136085000000	7.733747000000
H	4.972222000000	3.767366000000	7.587522000000
C	2.914166000000	3.011202000000	7.631256000000
H	3.134719000000	2.239823000000	8.384954000000
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C	2.811897000000	2.341033000000	6.246451000000
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C	1.638649000000	1.349758000000	6.212045000000
H	1.509191000000	0.918161000000	5.212965000000
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H	-8.781794000000	0.358604000000	6.633216000000
C	-9.004257000000	0.594311000000	4.533877000000
O	-8.884237000000	-0.508172000000	3.874642000000
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C	-3.100239000000	5.724401000000	-4.348056000000
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C	-5.246535000000	4.871705000000	-3.319378000000
H	-5.588792000000	4.482048000000	-4.288078000000
H	-4.721715000000	4.065855000000	-2.793184000000
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C	-2.023953000000	6.806407000000	-4.345761000000

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N	-0.898057000000	6.502157000000	-3.624225000000
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C	0.252525000000	7.388823000000	-3.544117000000
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C	1.512082000000	6.798335000000	-4.212012000000
H	1.315609000000	6.669298000000	-5.282694000000
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C	1.944271000000	5.480335000000	-3.600728000000
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H	1.289246000000	4.280519000000	-5.265387000000
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C	2.653962000000	3.020584000000	-2.410924000000
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C	2.879215000000	4.226222000000	-1.734216000000
H	3.323234000000	4.213750000000	-0.742733000000
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H	-0.064685000000	3.081653000000	0.329843000000
C	-0.087194000000	3.898277000000	2.327599000000
H	0.315713000000	2.998078000000	2.782851000000
C	-0.390757000000	5.016136000000	3.111274000000
H	-0.225362000000	4.988540000000	4.185724000000
C	-0.908712000000	6.169052000000	2.520183000000
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Fe	4.971786000000	3.233821000000	-0.894423000000
C	3.911847000000	3.388947000000	-4.159258000000
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C	5.894911000000	2.967137000000	2.417720000000
C	2.885970000000	5.808887000000	-0.098416000000
C	4.825834000000	2.398286000000	-3.825048000000
C	5.405562000000	1.470749000000	-4.767074000000
C	6.267522000000	0.686531000000	-4.064367000000
C	6.217579000000	1.137257000000	-2.693305000000
C	6.952907000000	1.005250000000	-0.340517000000
C	7.741556000000	0.403686000000	0.707443000000
C	7.437260000000	1.069756000000	1.862331000000
C	6.462194000000	2.074343000000	1.513709000000
C	4.960984000000	3.939472000000	2.089175000000
C	4.401512000000	4.887462000000	3.020690000000
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C	3.600760000000	5.229537000000	0.942655000000
C	2.919106000000	5.399633000000	-1.424664000000
C	2.151606000000	6.020242000000	-2.481128000000
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C	3.373167000000	4.301003000000	-3.264269000000
N	5.321697000000	2.171569000000	-2.565357000000
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N	4.448038000000	4.151145000000	0.827120000000
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H	3.604089000000	3.459885000000	-5.197758000000
H	7.629088000000	-0.236214000000	-1.920823000000
H	6.217929000000	2.909233000000	3.452746000000
H	2.250631000000	6.654525000000	0.146323000000
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C	0.341953000000	2.045742000000	-1.441241000000
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C	-3.585789000000	3.239281000000	-0.116613000000
O	-4.588401000000	2.636924000000	-0.625922000000
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***Product / HS_Prod**

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H	-0.694713000000	-9.136647000000	2.727139000000

²TransitionState2 / LS_TS2

C	2.867225000000	4.320121000000	3.337044000000
H	3.232105000000	4.774691000000	2.410290000000
H	3.326579000000	3.327932000000	3.440264000000
N	1.412586000000	4.253833000000	3.362362000000
H	0.929984000000	4.465073000000	4.265369000000
C	0.698798000000	3.568353000000	2.459105000000
N	1.253883000000	3.055850000000	1.347611000000
H	2.191818000000	3.307806000000	1.028695000000
H	0.613613000000	2.668604000000	0.658116000000
N	-0.609629000000	3.363978000000	2.678988000000
H	-1.086603000000	3.894848000000	3.422696000000
H	-1.145042000000	2.959001000000	1.914648000000
C	-6.052875000000	4.693777000000	-0.692104000000
H	-5.269577000000	4.622354000000	-1.456543000000
C	-5.669084000000	3.887919000000	0.553019000000
H	-4.758614000000	4.324632000000	0.998327000000
H	-6.476421000000	3.975763000000	1.284979000000
O	-5.512743000000	2.509034000000	0.298173000000
H	-4.735808000000	2.357573000000	-0.277084000000
C	-7.410285000000	4.252996000000	-1.244397000000
O	-8.373460000000	4.048734000000	-0.510706000000
N	-7.472797000000	4.132385000000	-2.599463000000
H	-6.652794000000	4.211087000000	-3.204256000000
C	-1.057751000000	-2.399317000000	9.975150000000
H	-1.511141000000	-1.403286000000	9.924877000000
C	-0.185020000000	-2.694768000000	8.749612000000
H	0.611370000000	-1.938835000000	8.676423000000
H	0.324466000000	-3.657196000000	8.900924000000
C	-0.941539000000	-2.748574000000	7.407108000000
H	-1.745435000000	-3.495607000000	7.510598000000
C	-1.591487000000	-1.404491000000	7.042539000000
H	-2.091197000000	-1.466801000000	6.069239000000
H	-2.335639000000	-1.091263000000	7.783298000000
H	-0.833590000000	-0.612022000000	6.976939000000
C	-0.010256000000	-3.216096000000	6.278155000000
H	-0.547264000000	-3.295099000000	5.326420000000
H	0.816757000000	-2.506743000000	6.138200000000
H	0.430053000000	-4.196102000000	6.500713000000
C	-3.225965000000	5.608592000000	7.043692000000
H	-3.877242000000	5.312033000000	6.217072000000
H	-3.024390000000	6.681294000000	6.938173000000
C	-1.929624000000	4.795718000000	7.024791000000
H	-1.259729000000	5.078937000000	7.843314000000
H	-2.159059000000	3.730288000000	7.173850000000
C	-1.139995000000	4.890991000000	5.715978000000
O	-1.809952000000	5.085609000000	4.632132000000
O	0.103746000000	4.748934000000	5.762203000000
C	9.280464000000	1.173879000000	-2.143761000000
H	8.653293000000	1.799765000000	-2.791090000000
C	10.672141000000	1.840819000000	-1.987198000000
H	11.317111000000	1.128939000000	-1.450897000000
C	11.322045000000	2.156270000000	-3.341961000000
H	10.734140000000	2.908398000000	-3.884866000000
H	12.331720000000	2.560785000000	-3.200163000000
H	11.383267000000	1.267992000000	-3.975298000000
C	10.553314000000	3.106684000000	-1.125807000000
H	9.885981000000	3.839627000000	-1.599048000000
H	10.155178000000	2.877982000000	-0.130595000000
H	11.531606000000	3.585839000000	-0.998137000000
C	9.351118000000	-0.208320000000	-2.783279000000
O	9.523539000000	-0.371214000000	-3.990115000000
N	9.257479000000	-1.262702000000	-1.915523000000
H	9.032799000000	-1.089224000000	-0.943953000000
C	9.343261000000	-2.636202000000	-2.387015000000
H	9.768245000000	-3.249649000000	-1.584633000000
C	7.993515000000	-3.231727000000	-2.853692000000
H	7.579385000000	-2.558070000000	-3.611943000000
H	8.207315000000	-4.185221000000	-3.354011000000
C	7.002628000000	-3.457288000000	-1.733255000000
C	6.158226000000	-2.429082000000	-1.288666000000

H	6.190415000000	-1.457073000000	-1.773105000000
C	5.277791000000	-2.626596000000	-0.221230000000
H	4.659956000000	-1.795635000000	0.106472000000
C	5.221975000000	-3.868974000000	0.416529000000
H	4.537372000000	-4.029828000000	1.245411000000
C	6.053922000000	-4.905196000000	-0.016461000000
H	6.017523000000	-5.875471000000	0.473014000000
C	6.935399000000	-4.697415000000	-1.079474000000
H	7.577720000000	-5.510736000000	-1.412129000000
C	9.945555000000	-2.716997000000	2.306017000000
H	10.994582000000	-2.800207000000	1.997667000000
H	9.352985000000	-3.396195000000	1.684323000000
C	9.445281000000	-1.293718000000	2.198922000000
C	8.195955000000	-1.009568000000	1.628611000000
H	7.580553000000	-1.823556000000	1.253475000000
C	7.714621000000	0.302860000000	1.550578000000
H	6.744019000000	0.494544000000	1.097779000000
C	8.486594000000	1.352751000000	2.053956000000
H	8.117759000000	2.374417000000	2.005948000000
C	9.735069000000	1.085115000000	2.624052000000
H	10.340741000000	1.898169000000	3.016803000000
C	10.209704000000	-0.225027000000	2.690721000000
H	11.183904000000	-0.423120000000	3.133339000000
C	1.467794000000	6.462571000000	-3.070701000000
H	2.551635000000	6.617189000000	-3.060673000000
C	0.803327000000	7.254915000000	-1.921539000000
H	0.884906000000	8.327403000000	-2.140175000000
H	-0.268096000000	7.019205000000	-1.915034000000
C	1.428804000000	6.962887000000	-0.549109000000
H	1.513990000000	5.883993000000	-0.391253000000
H	2.451371000000	7.359973000000	-0.527421000000
C	0.661828000000	7.557915000000	0.636281000000
H	1.259244000000	7.394535000000	1.541618000000
H	0.534325000000	8.643133000000	0.517576000000
N	-0.639548000000	6.910188000000	0.782035000000
H	-0.993066000000	6.338356000000	0.004087000000
C	-1.273573000000	6.687481000000	1.940991000000
N	-2.434981000000	6.009469000000	1.921194000000
H	-2.664456000000	5.511748000000	1.060615000000
H	-2.754209000000	5.634270000000	2.810941000000
N	-0.836605000000	7.157498000000	3.122808000000
H	0.111675000000	7.499837000000	3.173694000000
H	-1.147078000000	6.568074000000	3.918573000000
C	1.216238000000	4.963081000000	-2.948342000000
O	1.957048000000	4.218511000000	-2.287850000000
N	0.104384000000	4.498978000000	-3.557053000000
H	-0.442754000000	5.139234000000	-4.115764000000
C	-0.338692000000	3.104881000000	-3.470950000000
H	-0.226431000000	2.773996000000	-2.434458000000
C	-1.792357000000	2.956423000000	-3.908080000000
H	-1.950485000000	3.423778000000	-4.889499000000
H	-2.024053000000	1.891133000000	-4.015242000000
O	-2.723848000000	3.561425000000	-3.001925000000
H	-2.904468000000	2.888219000000	-2.263397000000
C	5.085700000000	2.743711000000	-1.438565000000
H	6.151153000000	2.514597000000	-1.561037000000
C	4.930843000000	3.734485000000	-0.281512000000
H	5.306042000000	3.282151000000	0.640916000000
H	5.529993000000	4.634179000000	-0.488952000000
O	3.572797000000	4.092390000000	-0.031366000000
H	3.110939000000	4.248861000000	-0.884939000000
C	4.355775000000	1.432080000000	-1.154875000000
O	4.707285000000	0.692727000000	-0.226423000000
N	3.312264000000	1.171674000000	-1.966346000000
H	3.102289000000	1.772067000000	-2.757458000000
C	2.486582000000	-0.023985000000	-1.889278000000
H	3.143894000000	-0.902605000000	-1.842398000000
C	1.576976000000	-0.018782000000	-0.652334000000
H	1.027961000000	-0.958406000000	-0.550257000000
H	2.191443000000	0.131970000000	0.239169000000
H	0.845013000000	0.791844000000	-0.721700000000

C	1.708369000000	-0.085498000000	-3.220063000000
O	1.956895000000	0.716737000000	-4.131349000000
N	0.789832000000	-1.064347000000	-3.342862000000
H	0.407480000000	-1.563499000000	-2.529432000000
C	0.066348000000	-1.212895000000	-4.593921000000
H	-0.374825000000	-2.210079000000	-4.617866000000
H	-0.738702000000	-0.473132000000	-4.697887000000
C	2.317408000000	-6.540584000000	-0.954259000000
H	1.889339000000	-7.372234000000	-1.526108000000
C	1.708860000000	-5.212897000000	-1.404426000000
H	2.163098000000	-4.398141000000	-0.821034000000
C	1.926896000000	-4.937178000000	-2.886356000000
H	2.998096000000	-4.907000000000	-3.111698000000
H	1.464615000000	-5.723341000000	-3.494667000000
H	1.489511000000	-3.975196000000	-3.170995000000
O	0.283639000000	-5.211875000000	-1.178631000000
H	0.144540000000	-5.348207000000	-0.224218000000
C	1.264479000000	-7.635256000000	4.352461000000
H	1.158524000000	-7.383723000000	5.416203000000
H	2.312259000000	-7.911222000000	4.189538000000
C	0.852999000000	-6.475473000000	3.474606000000
C	1.740222000000	-5.418230000000	3.219895000000
H	2.740861000000	-5.448803000000	3.646015000000
C	1.357040000000	-4.330835000000	2.433975000000
H	2.058535000000	-3.520365000000	2.253393000000
C	0.071991000000	-4.275354000000	1.882564000000
H	-0.225941000000	-3.433713000000	1.263127000000
C	-0.821698000000	-5.322554000000	2.131600000000
H	-1.826417000000	-5.285587000000	1.717817000000
C	-0.430151000000	-6.411270000000	2.916137000000
H	-1.132599000000	-7.220931000000	3.102805000000
S	-6.528628000000	-3.710884000000	-2.913835000000
O	-3.452188000000	-1.686007000000	-0.874873000000
Fe	-4.868094000000	-2.389317000000	-1.669259000000
C	-7.062768000000	-2.877763000000	0.915783000000
C	-3.477240000000	-5.453923000000	-1.074931000000
C	-3.265690000000	-2.278428000000	-4.703885000000
C	-6.268247000000	0.643821000000	-2.286036000000
C	-6.155167000000	-3.900086000000	0.652749000000
C	-6.069281000000	-5.137480000000	1.386355000000
C	-5.020461000000	-5.832990000000	0.859676000000
C	-4.487121000000	-5.033628000000	-0.215479000000
C	-3.094817000000	-4.814090000000	-2.246271000000
C	-2.200552000000	-5.375061000000	-3.232346000000
C	-2.181104000000	-4.507254000000	-4.279716000000
C	-3.037700000000	-3.401056000000	-3.919074000000
C	-4.043657000000	-1.184037000000	-4.342274000000
C	-4.196557000000	0.007607000000	-5.142723000000
C	-5.012613000000	0.847422000000	-4.445450000000
C	-5.371369000000	0.152667000000	-3.230537000000
C	-6.729614000000	-0.049856000000	-1.176564000000
C	-7.792895000000	0.414670000000	-0.312927000000
C	-8.042893000000	-0.593548000000	0.562509000000
C	-7.113945000000	-1.657035000000	0.253968000000
N	-5.184348000000	-3.853346000000	-0.317033000000
N	-3.586965000000	-3.608406000000	-2.679485000000
N	-4.766312000000	-1.072313000000	-3.182915000000
N	-6.301332000000	-1.297277000000	-0.793127000000
H	-7.781954000000	-3.042631000000	1.712818000000
H	-3.012966000000	-6.412284000000	-0.862025000000
H	-2.776066000000	-2.239569000000	-5.672238000000
H	-6.679970000000	1.632673000000	-2.456569000000
C	-3.956302000000	-3.240442000000	3.852835000000
O	-2.724594000000	-2.587001000000	3.577207000000
C	-2.669013000000	-1.718109000000	2.527132000000
C	-1.453883000000	-1.015736000000	2.404658000000
C	-1.322663000000	-0.012183000000	1.446885000000
C	-2.350681000000	0.294194000000	0.558896000000
C	-3.539947000000	-0.533070000000	0.552330000000
C	-3.702755000000	-1.467594000000	1.637507000000
C	-2.257090000000	1.540060000000	-0.263047000000

O	-1.279383000000	2.340808000000	-0.035155000000
O	-3.168288000000	1.782408000000	-1.114484000000
H	-0.654772000000	-1.232048000000	3.105860000000
H	-0.415978000000	0.579491000000	1.431405000000
H	-4.442328000000	-0.063582000000	0.183194000000
H	-4.645479000000	-1.989440000000	1.714028000000
H	-4.248489000000	-3.911211000000	3.037514000000
H	-3.785305000000	-3.822060000000	4.760474000000
H	-4.759743000000	-2.513923000000	4.031121000000
O	-1.905125000000	4.907640000000	-0.697569000000
H	-2.227197000000	4.766721000000	-1.611676000000
H	-1.605270000000	3.989910000000	-0.444509000000
O	-5.082075000000	4.244739000000	-4.273125000000
H	-4.263030000000	3.971182000000	-3.792355000000
H	-4.907779000000	5.148034000000	-4.576452000000
O	-0.627352000000	-2.481502000000	-1.261059000000
H	-1.584569000000	-2.282039000000	-1.152232000000
H	-0.524814000000	-3.453027000000	-1.328381000000
H	-3.736317000000	0.162870000000	-6.110722000000
H	-5.349456000000	1.840918000000	-4.713885000000
H	-1.638598000000	-4.590488000000	-5.213027000000
H	-1.663854000000	-6.306001000000	-3.114813000000
H	-4.653924000000	-6.812490000000	1.140034000000
H	-6.731137000000	-5.424456000000	2.193852000000
H	-8.776728000000	-0.628530000000	1.357612000000
H	-8.253937000000	1.391886000000	-0.378262000000
H	0.648073000000	-8.520339000000	4.163548000000
H	9.885686000000	-3.082229000000	3.339881000000
H	3.184430000000	4.936372000000	4.180753000000
H	-8.359386000000	3.854357000000	-2.999125000000
H	-0.467306000000	-2.444166000000	10.897773000000
H	-3.767433000000	5.461624000000	7.985251000000
H	-1.871648000000	-3.130130000000	10.067069000000
H	0.303274000000	2.466557000000	-4.090307000000
H	-6.060188000000	-3.489242000000	-4.162225000000
H	2.124656000000	-6.717396000000	0.110992000000
H	3.403468000000	-6.534763000000	-1.100233000000
H	0.755061000000	-1.088408000000	-5.432823000000
H	4.734250000000	3.203357000000	-2.369882000000
H	1.091775000000	6.834268000000	-4.031933000000
H	-6.139537000000	5.754648000000	-0.416590000000
H	8.797700000000	1.117067000000	-1.160298000000
H	10.038073000000	-2.640289000000	-3.230968000000

⁴TransitionState2 / HS_TS2

C	2.867225000000	4.320121000000	3.337044000000
H	3.232105000000	4.774691000000	2.410290000000
H	3.326579000000	3.327932000000	3.440264000000
N	1.412586000000	4.253833000000	3.362362000000
H	0.929984000000	4.465073000000	4.265369000000
C	0.698798000000	3.568353000000	2.459105000000
N	1.253883000000	3.055850000000	1.347611000000
H	2.191818000000	3.307806000000	1.028695000000
H	0.613613000000	2.668604000000	0.658116000000
N	-0.609629000000	3.363978000000	2.678988000000
H	-1.086603000000	3.894848000000	3.422696000000
H	-1.145042000000	2.959001000000	1.914648000000
C	-6.052875000000	4.693777000000	-0.692104000000
H	-5.269577000000	4.622354000000	-1.456543000000
C	-5.669084000000	3.887919000000	0.553019000000
H	-4.758614000000	4.324632000000	0.998327000000
H	-6.476421000000	3.975763000000	1.284979000000
O	-5.512743000000	2.509034000000	0.298173000000
H	-4.735808000000	2.357573000000	-0.277084000000
C	-7.410285000000	4.252996000000	-1.244397000000
O	-8.373460000000	4.048734000000	-0.510706000000
N	-7.472797000000	4.132385000000	-2.599463000000
H	-6.652794000000	4.211087000000	-3.204256000000
C	-1.057751000000	-2.399317000000	9.975150000000
H	-1.511141000000	-1.403286000000	9.924877000000
C	-0.185020000000	-2.694768000000	8.749612000000

H	0.611370000000	-1.938835000000	8.676423000000
H	0.324466000000	-3.657196000000	8.900924000000
C	-0.941539000000	-2.748574000000	7.407108000000
H	-1.745435000000	-3.495607000000	7.510598000000
C	-1.591487000000	-1.404491000000	7.042539000000
H	-2.091197000000	-1.466801000000	6.069239000000
H	-2.335639000000	-1.091263000000	7.783298000000
H	-0.833590000000	-0.612022000000	6.976939000000
C	-0.010256000000	-3.216096000000	6.278155000000
H	-0.547264000000	-3.295099000000	5.326420000000
H	0.816757000000	-2.506743000000	6.138200000000
H	0.430053000000	-4.196102000000	6.500713000000
C	-3.225965000000	5.608592000000	7.043692000000
H	-3.877242000000	5.312033000000	6.217072000000
H	-3.024390000000	6.681294000000	6.938173000000
C	-1.929624000000	4.795718000000	7.024791000000
H	-1.259729000000	5.078937000000	7.843314000000
H	-2.159059000000	3.730288000000	7.173850000000
C	-1.139995000000	4.890991000000	5.715978000000
O	-1.809952000000	5.085609000000	4.632132000000
O	0.103746000000	4.748934000000	5.762203000000
C	9.280464000000	1.173879000000	-2.143761000000
H	8.653293000000	1.799765000000	-2.791090000000
C	10.672141000000	1.840819000000	-1.987198000000
H	11.317111000000	1.128939000000	-1.450897000000
C	11.322045000000	2.156270000000	-3.341961000000
H	10.734140000000	2.908398000000	-3.884866000000
H	12.331720000000	2.560785000000	-3.200163000000
H	11.383267000000	1.267992000000	-3.975298000000
C	10.553314000000	3.106684000000	-1.125807000000
H	9.885981000000	3.839627000000	-1.599048000000
H	10.155178000000	2.877982000000	-0.130595000000
H	11.531606000000	3.585839000000	-0.998137000000
C	9.351118000000	-0.208320000000	-2.783279000000
O	9.523539000000	-0.371214000000	-3.990115000000
N	9.257479000000	-1.262702000000	-1.915523000000
H	9.032799000000	-1.089224000000	-0.943953000000
C	9.343261000000	-2.636202000000	-2.387015000000
H	9.768245000000	-3.249649000000	-1.584633000000
C	7.993515000000	-3.231727000000	-2.853692000000
H	7.579385000000	-2.558070000000	-3.611943000000
H	8.207315000000	-4.185221000000	-3.354011000000
C	7.002628000000	-3.457288000000	-1.733255000000
C	6.158226000000	-2.429082000000	-1.288666000000
H	6.190415000000	-1.457073000000	-1.773105000000
C	5.277791000000	-2.626596000000	-0.221230000000
H	4.659956000000	-1.795635000000	0.106472000000
C	5.221975000000	-3.868974000000	0.416529000000
H	4.537372000000	-4.029828000000	1.245411000000
C	6.053922000000	-4.905196000000	-0.016461000000
H	6.017523000000	-5.875471000000	0.473014000000
C	6.935399000000	-4.697415000000	-1.079474000000
H	7.577720000000	-5.510736000000	-1.412129000000
C	9.945555000000	-2.716997000000	2.306017000000
H	10.994582000000	-2.800207000000	1.997667000000
H	9.352985000000	-3.396195000000	1.684323000000
C	9.445281000000	-1.293718000000	2.198922000000
C	8.195955000000	-1.009568000000	1.628611000000
H	7.580553000000	-1.823556000000	1.253475000000
C	7.714621000000	0.302860000000	1.550578000000
H	6.744019000000	0.494544000000	1.097779000000
C	8.486594000000	1.352751000000	2.053956000000
H	8.117759000000	2.374417000000	2.005948000000
C	9.735069000000	1.085115000000	2.624052000000
H	10.340741000000	1.898169000000	3.016803000000
C	10.209704000000	-0.225027000000	2.690721000000
H	11.183904000000	-0.423120000000	3.133339000000
C	1.467794000000	6.462571000000	-3.070701000000
H	2.551635000000	6.617189000000	-3.060673000000
C	0.803327000000	7.254915000000	-1.921539000000
H	0.884906000000	8.327403000000	-2.140175000000

H	-0.268096000000	7.019205000000	-1.915034000000
C	1.428804000000	6.962887000000	-0.549109000000
H	1.513990000000	5.883993000000	-0.391253000000
H	2.451371000000	7.359973000000	-0.527421000000
C	0.661828000000	7.557915000000	0.636281000000
H	1.259244000000	7.394535000000	1.541618000000
H	0.534325000000	8.643133000000	0.517576000000
N	-0.639548000000	6.910188000000	0.782035000000
H	-0.993066000000	6.338356000000	0.004087000000
C	-1.273573000000	6.687481000000	1.940991000000
N	-2.434981000000	6.009469000000	1.921194000000
H	-2.664456000000	5.511748000000	1.060615000000
H	-2.754209000000	5.634270000000	2.810941000000
N	-0.836605000000	7.157498000000	3.122808000000
H	0.111675000000	7.499837000000	3.173694000000
H	-1.147078000000	6.568074000000	3.918573000000
C	1.216238000000	4.963081000000	-2.948342000000
O	1.957048000000	4.218511000000	-2.287850000000
N	0.104384000000	4.498978000000	-3.557053000000
H	-0.442754000000	5.139234000000	-4.115764000000
C	-0.338692000000	3.104881000000	-3.470950000000
H	-0.226431000000	2.773996000000	-2.434458000000
C	-1.792357000000	2.956423000000	-3.908080000000
H	-1.950485000000	3.423778000000	-4.889499000000
H	-2.024053000000	1.891133000000	-4.015242000000
O	-2.723848000000	3.561425000000	-3.001925000000
H	-2.904468000000	2.888219000000	-2.263397000000
C	5.085700000000	2.743711000000	-1.438565000000
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C	4.930843000000	3.734485000000	-0.281512000000
H	5.306042000000	3.282151000000	0.640916000000
H	5.529993000000	4.634179000000	-0.488952000000
O	3.572797000000	4.092390000000	-0.031366000000
H	3.110939000000	4.248861000000	-0.884939000000
C	4.355775000000	1.432080000000	-1.154875000000
O	4.707285000000	0.692727000000	-0.226423000000
N	3.312264000000	1.171674000000	-1.966346000000
H	3.102289000000	1.772067000000	-2.757458000000
C	2.486582000000	-0.023985000000	-1.889278000000
H	3.143894000000	-0.902605000000	-1.842398000000
C	1.576976000000	-0.018782000000	-0.652334000000
H	1.027961000000	-0.958406000000	-0.550257000000
H	2.191443000000	0.131970000000	0.239169000000
H	0.845013000000	0.791844000000	-0.721700000000
C	1.708369000000	-0.085498000000	-3.220063000000
O	1.956895000000	0.716737000000	-4.131349000000
N	0.789832000000	-1.064347000000	-3.342862000000
H	0.407480000000	-1.563499000000	-2.529432000000
C	0.066348000000	-1.212895000000	-4.593921000000
H	-0.374825000000	-2.210079000000	-4.617866000000
H	-0.738702000000	-0.473132000000	-4.697887000000
C	2.317408000000	-6.540584000000	-0.954259000000
H	1.889339000000	-7.372234000000	-1.526108000000
C	1.708860000000	-5.212897000000	-1.404426000000
H	2.163098000000	-4.398141000000	-0.821034000000
C	1.926896000000	-4.937178000000	-2.886356000000
H	2.998096000000	-4.907000000000	-3.111698000000
H	1.464615000000	-5.723341000000	-3.494667000000
H	1.489511000000	-3.975196000000	-3.170995000000
O	0.283639000000	-5.211875000000	-1.178631000000
H	0.144540000000	-5.348207000000	-0.224218000000
C	1.264479000000	-7.635256000000	4.352461000000
H	1.158524000000	-7.383723000000	5.416203000000
H	2.312259000000	-7.911222000000	4.189538000000
C	0.852999000000	-6.475473000000	3.474606000000
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H	2.740861000000	-5.448803000000	3.646015000000
C	1.357040000000	-4.330835000000	2.433975000000
H	2.058535000000	-3.520365000000	2.253393000000
C	0.071991000000	-4.275354000000	1.882564000000
H	-0.225941000000	-3.433713000000	1.263127000000

C	-0.821698000000	-5.322554000000	2.131600000000
H	-1.826417000000	-5.285587000000	1.717817000000
C	-0.430151000000	-6.411270000000	2.916137000000
H	-1.132599000000	-7.220931000000	3.102805000000
S	-6.528628000000	-3.710884000000	-2.913835000000
O	-3.452188000000	-1.686007000000	-0.874873000000
Fe	-4.868094000000	-2.389317000000	-1.669259000000
C	-7.062768000000	-2.877763000000	0.915783000000
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C	-3.265669000000	-2.278428000000	-4.703885000000
C	-6.268247000000	0.643821000000	-2.286036000000
C	-6.155167000000	-3.900086000000	0.652749000000
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C	-5.020461000000	-5.832990000000	0.859676000000
C	-4.487121000000	-5.033628000000	-0.215479000000
C	-3.094817000000	-4.814090000000	-2.246271000000
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C	-8.042893000000	-0.593548000000	0.562509000000
C	-7.113945000000	-1.657035000000	0.253968000000
N	-5.184348000000	-3.853346000000	-0.317033000000
N	-3.586965000000	-3.608406000000	-2.679485000000
N	-4.766312000000	-1.072313000000	-3.182915000000
N	-6.301332000000	-1.297277000000	-0.793127000000
H	-7.781954000000	-3.042631000000	1.712818000000
H	-3.012966000000	-6.412284000000	-0.862025000000
H	-2.776066000000	-2.239569000000	-5.672238000000
H	-6.679970000000	1.632673000000	-2.456569000000
C	-3.956302000000	-3.240442000000	3.852835000000
O	-2.724594000000	-2.587001000000	3.577207000000
C	-2.669013000000	-1.718109000000	2.527132000000
C	-1.453883000000	-1.015736000000	2.404658000000
C	-1.322663000000	-0.012183000000	1.446885000000
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C	-2.257090000000	1.540060000000	-0.263047000000
O	-1.279383000000	2.340808000000	-0.035155000000
O	-3.168288000000	1.782408000000	-1.114484000000
H	-0.654772000000	-1.232048000000	3.105860000000
H	-0.415978000000	0.579491000000	1.431405000000
H	-4.442328000000	-0.063582000000	0.183194000000
H	-4.645479000000	-1.989440000000	1.714028000000
H	-4.248489000000	-3.911211000000	3.037514000000
H	-3.785305000000	-3.822060000000	4.760474000000
H	-4.759743000000	-2.513923000000	4.031121000000
O	-1.905125000000	4.907640000000	-0.697569000000
H	-2.227197000000	4.766721000000	-1.611676000000
H	-1.605270000000	3.989910000000	-0.444509000000
O	-5.082075000000	4.244739000000	-4.273125000000
H	-4.263030000000	3.971182000000	-3.792355000000
H	-4.907779000000	5.148034000000	-4.576452000000
O	-0.627352000000	-2.481502000000	-1.261059000000
H	-1.584569000000	-2.282039000000	-1.152232000000
H	-0.524814000000	-3.453027000000	-1.328381000000
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H	-5.349456000000	1.840918000000	-4.713885000000
H	-1.638598000000	-4.590488000000	-5.213027000000
H	-1.663854000000	-6.306001000000	-3.114813000000
H	-4.653924000000	-6.812490000000	1.140034000000
H	-6.731137000000	-5.424456000000	2.193852000000
H	-8.776728000000	-0.628530000000	1.357612000000
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H	0.648073000000	-8.520339000000	4.163548000000

H	9.885686000000	-3.082229000000	3.339881000000
H	3.184430000000	4.936372000000	4.180753000000
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H	-0.467306000000	-2.444166000000	10.897773000000
H	-3.767433000000	5.461624000000	7.985251000000
H	-1.871648000000	-3.130130000000	10.067069000000
H	0.303274000000	2.466557000000	-4.090307000000
H	-6.060188000000	-3.489242000000	-4.162225000000
H	2.124656000000	-6.717396000000	0.110992000000
H	3.403468000000	-6.534763000000	-1.100233000000
H	0.755061000000	-1.088408000000	-5.432823000000
H	4.734250000000	3.203357000000	-2.369882000000
H	1.091775000000	6.834268000000	-4.031933000000
H	-6.139537000000	5.754648000000	-0.416590000000
H	8.797700000000	1.117067000000	-1.160298000000
H	10.038073000000	-2.640289000000	-3.230968000000

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C	2.770146000000	4.339641000000	3.409052000000
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H	3.221676000000	3.345604000000	3.527085000000
N	1.314970000000	4.279516000000	3.397199000000
H	0.809771000000	4.509559000000	4.284013000000
C	0.622626000000	3.584388000000	2.485908000000
N	1.205124000000	3.048845000000	1.400263000000
H	2.150391000000	3.298165000000	1.100398000000
H	0.584328000000	2.648737000000	0.699976000000
N	-0.693658000000	3.390187000000	2.676706000000
H	-1.183966000000	3.946742000000	3.393147000000
H	-1.214637000000	2.988850000000	1.901774000000
C	-5.862506000000	4.625407000000	-0.448742000000
H	-5.107880000000	4.565292000000	-1.242491000000
C	-5.464561000000	3.750888000000	0.744303000000
H	-4.528827000000	4.141130000000	1.180817000000
H	-6.245839000000	3.825014000000	1.505262000000
O	-5.352006000000	2.381016000000	0.425550000000
H	-4.641347000000	2.243976000000	-0.231703000000
C	-7.253825000000	4.261516000000	-0.973389000000
O	-8.195121000000	4.044857000000	-0.215415000000
N	-7.370198000000	4.225586000000	-2.329309000000
H	-6.572645000000	4.319696000000	-2.961488000000
C	-1.645937000000	-3.185876000000	9.986373000000
H	-2.121433000000	-2.199314000000	10.015038000000
C	-0.627377000000	-3.300285000000	8.845906000000
H	0.152105000000	-2.533801000000	8.971940000000
H	-0.114371000000	-4.269299000000	8.926329000000
C	-1.219590000000	-3.177550000000	7.427626000000
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C	-0.155535000000	-3.492748000000	6.364970000000
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H	0.669554000000	-2.769223000000	6.414295000000
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C	-3.392977000000	5.775149000000	6.917064000000
H	-4.026502000000	5.470421000000	6.079664000000
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C	-2.111027000000	4.940339000000	6.953627000000
H	-1.459553000000	5.231493000000	7.784154000000
H	-2.363288000000	3.882892000000	7.121544000000
C	-1.282770000000	4.989441000000	5.666513000000
O	-1.915192000000	5.175053000000	4.559088000000
O	-0.044460000000	4.819739000000	5.752684000000
C	9.307835000000	1.219185000000	-1.973705000000
H	8.682102000000	1.858845000000	-2.608889000000
C	10.698636000000	1.883318000000	-1.798521000000
H	11.342879000000	1.159458000000	-1.277574000000
C	11.351537000000	2.230394000000	-3.143996000000

H	10.765136000000	2.995226000000	-3.670537000000
H	12.360992000000	2.631129000000	-2.990407000000
H	11.413657000000	1.356923000000	-3.797494000000
C	10.577037000000	3.128608000000	-0.907899000000
H	9.910432000000	3.872053000000	-1.365557000000
H	10.176480000000	2.876767000000	0.080814000000
H	11.554738000000	3.605188000000	-0.766739000000
C	9.381457000000	-0.148590000000	-2.643364000000
O	9.560709000000	-0.284657000000	-3.852550000000
N	9.282316000000	-1.222022000000	-1.800082000000
H	9.053763000000	-1.069726000000	-0.825966000000
C	9.373946000000	-2.584748000000	-2.301394000000
H	9.790202000000	-3.215726000000	-1.508135000000
C	8.030411000000	-3.170723000000	-2.796931000000
H	7.622913000000	-2.479113000000	-3.542512000000
H	8.252045000000	-4.110592000000	-3.319101000000
C	7.027645000000	-3.427864000000	-1.694112000000
C	6.179028000000	-2.412737000000	-1.228108000000
H	6.217999000000	-1.426281000000	-1.681795000000
C	5.284230000000	-2.642603000000	-0.179260000000
H	4.661893000000	-1.821849000000	0.165272000000
C	5.217974000000	-3.904469000000	0.417851000000
H	4.520189000000	-4.091286000000	1.230132000000
C	6.054882000000	-4.927487000000	-0.036258000000
H	6.010482000000	-5.912819000000	0.421435000000
C	6.950875000000	-4.687441000000	-1.080074000000
H	7.596379000000	-5.490952000000	-1.429886000000
C	9.944432000000	-2.734163000000	2.385513000000
H	10.992580000000	-2.801072000000	2.070163000000
H	9.355340000000	-3.406632000000	1.753357000000
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C	8.182272000000	-1.028002000000	1.737147000000
H	7.577242000000	-1.838304000000	1.337874000000
C	7.688845000000	0.281305000000	1.687222000000
H	6.719922000000	0.474834000000	1.231702000000
C	8.446931000000	1.326067000000	2.221392000000
H	8.068601000000	2.345083000000	2.195219000000
C	9.693955000000	1.056655000000	2.794167000000
H	10.288710000000	1.865690000000	3.211237000000
C	10.180766000000	-0.250122000000	2.832461000000
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C	1.544987000000	6.434987000000	-3.070485000000
H	2.630658000000	6.574420000000	-3.043277000000
C	0.871867000000	7.253836000000	-1.944960000000
H	0.960203000000	8.321326000000	-2.184092000000
H	-0.200805000000	7.023445000000	-1.946700000000
C	1.481102000000	6.986827000000	-0.559853000000
H	1.582784000000	5.911470000000	-0.389815000000
H	2.496054000000	7.402089000000	-0.526675000000
C	0.685923000000	7.579786000000	0.607363000000
H	1.269723000000	7.431498000000	1.524450000000
H	0.544366000000	8.662089000000	0.478659000000
N	-0.608420000000	6.914291000000	0.733532000000
H	-0.932688000000	6.315030000000	-0.035954000000
C	-1.282876000000	6.731164000000	1.876180000000
N	-2.446421000000	6.059270000000	1.838346000000
H	-2.651918000000	5.541383000000	0.983325000000
H	-2.792430000000	5.705318000000	2.727081000000
N	-0.882126000000	7.236754000000	3.057214000000
H	0.070382000000	7.563570000000	3.130226000000
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C	1.268431000000	4.941428000000	-2.929098000000
O	1.970718000000	4.202013000000	-2.222978000000
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C	-0.279839000000	3.089449000000	-3.500878000000
H	-0.166135000000	2.749821000000	-2.467823000000
C	-1.735744000000	2.953774000000	-3.936388000000
H	-1.898213000000	3.449935000000	-4.902877000000
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O	-2.664270000000	3.529987000000	-3.009047000000

H	-2.850489000000	2.832528000000	-2.297806000000
C	5.108978000000	2.737273000000	-1.301638000000
H	6.178490000000	2.512194000000	-1.390935000000
C	4.913783000000	3.724501000000	-0.147757000000
H	5.265373000000	3.273008000000	0.784347000000
H	5.511779000000	4.629106000000	-0.335974000000
O	3.546158000000	4.072001000000	0.063945000000
H	3.104214000000	4.219581000000	-0.801500000000
C	4.373767000000	1.422859000000	-1.044096000000
O	4.702625000000	0.678634000000	-0.111321000000
N	3.350294000000	1.169548000000	-1.882409000000
H	3.166117000000	1.771651000000	-2.678795000000
C	2.519081000000	-0.024350000000	-1.838780000000
H	3.171824000000	-0.906968000000	-1.799407000000
C	1.592706000000	-0.038906000000	-0.614600000000
H	1.035740000000	-0.976473000000	-0.541323000000
H	2.196717000000	0.087833000000	0.287731000000
H	0.867227000000	0.778000000000	-0.675234000000
C	1.764474000000	-0.056674000000	-3.184937000000
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N	0.824912000000	-1.010290000000	-3.336204000000
H	0.411054000000	-1.509947000000	-2.537030000000
C	0.128946000000	-1.130418000000	-4.605954000000
H	-0.339228000000	-2.114430000000	-4.648163000000
H	-0.652645000000	-0.367880000000	-4.723437000000
C	2.304204000000	-6.478222000000	-1.122220000000
H	1.896926000000	-7.312633000000	-1.705152000000
C	1.684327000000	-5.156619000000	-1.575463000000
H	2.117947000000	-4.339151000000	-0.979866000000
C	1.922615000000	-4.869466000000	-3.052027000000
H	2.996734000000	-4.826536000000	-3.261166000000
H	1.477500000000	-5.656521000000	-3.671804000000
H	1.479118000000	-3.910304000000	-3.336333000000
O	0.256358000000	-5.176401000000	-1.373965000000
H	0.105941000000	-5.337509000000	-0.425568000000
C	1.269910000000	-7.550564000000	4.241032000000
H	1.143473000000	-7.284901000000	5.299098000000
H	2.326031000000	-7.804889000000	4.097148000000
C	0.844880000000	-6.414340000000	3.339206000000
C	1.699885000000	-5.325763000000	3.105815000000
H	2.685293000000	-5.314856000000	3.567139000000
C	1.304135000000	-4.260303000000	2.296646000000
H	1.981118000000	-3.426025000000	2.131299000000
C	0.038029000000	-4.258118000000	1.700418000000
H	-0.267449000000	-3.435830000000	1.058835000000
C	-0.822742000000	-5.337178000000	1.927117000000
H	-1.811654000000	-5.344307000000	1.474555000000
C	-0.418836000000	-6.404009000000	2.735418000000
H	-1.095616000000	-7.239100000000	2.903546000000
S	-6.625954000000	-3.310606000000	-2.984227000000
O	-3.346281000000	-1.563709000000	-0.870082000000
Fe	-4.871976000000	-2.345327000000	-1.767818000000
C	-6.955654000000	-2.876792000000	0.905926000000
C	-3.502938000000	-5.441275000000	-1.314696000000
C	-3.233017000000	-2.081358000000	-4.772730000000
C	-6.257238000000	0.712937000000	-2.243818000000
C	-6.081746000000	-3.909135000000	0.568464000000
C	-6.016295000000	-5.186324000000	1.233747000000
C	-5.009780000000	-5.886441000000	0.635571000000
C	-4.478790000000	-5.041904000000	-0.407132000000
C	-3.106000000000	-4.740596000000	-2.448962000000
C	-2.225627000000	-5.270727000000	-3.463976000000
C	-2.184429000000	-4.345704000000	-4.461691000000
C	-3.016986000000	-3.244311000000	-4.036517000000
C	-4.005416000000	-1.002868000000	-4.367537000000
C	-4.188821000000	0.209610000000	-5.131912000000
C	-5.019591000000	1.007350000000	-4.405289000000
C	-5.352169000000	0.267521000000	-3.207030000000
C	-6.694939000000	-0.007123000000	-1.142849000000
C	-7.731158000000	0.437941000000	-0.236164000000
C	-7.943557000000	-0.581358000000	0.635937000000

C	-7.025514000000	-1.638873000000	0.277044000000
N	-5.135103000000	-3.835780000000	-0.421146000000
N	-3.564636000000	-3.501090000000	-2.810212000000
N	-4.717155000000	-0.938258000000	-3.197209000000
N	-6.251102000000	-1.260192000000	-0.792048000000
H	-7.649040000000	-3.058891000000	1.721936000000
H	-3.067500000000	-6.425782000000	-1.169471000000
H	-2.749057000000	-2.010163000000	-5.742230000000
H	-6.689615000000	1.697310000000	-2.389834000000
C	-3.800300000000	-3.519181000000	3.712211000000
O	-2.653972000000	-2.691832000000	3.563264000000
C	-2.612913000000	-1.836750000000	2.500261000000
C	-1.474925000000	-0.997094000000	2.467400000000
C	-1.350389000000	0.001465000000	1.492277000000
C	-2.287004000000	0.185343000000	0.494977000000
C	-3.438388000000	-0.789512000000	0.343386000000
C	-3.551808000000	-1.737761000000	1.503430000000
C	-2.207213000000	1.448002000000	-0.316989000000
O	-1.258594000000	2.271713000000	-0.053855000000
O	-3.109368000000	1.675470000000	-1.177047000000
H	-0.723613000000	-1.113378000000	3.242079000000
H	-0.509336000000	0.679855000000	1.559689000000
H	-4.366333000000	-0.194379000000	0.306177000000
H	-4.407776000000	-2.393128000000	1.481377000000
H	-3.899562000000	-4.223681000000	2.879245000000
H	-3.649787000000	-4.069341000000	4.642442000000
H	-4.715270000000	-2.917072000000	3.784264000000
O	-1.850258000000	4.861914000000	-0.715824000000
H	-2.158267000000	4.716695000000	-1.635154000000
H	-1.565818000000	3.943380000000	-0.454921000000
O	-5.060034000000	4.389490000000	-4.105964000000
H	-4.224084000000	4.042713000000	-3.711096000000
H	-4.863127000000	5.305181000000	-4.352758000000
O	-0.659920000000	-2.421843000000	-1.316375000000
H	-1.618575000000	-2.193260000000	-1.217954000000
H	-0.585369000000	-3.388000000000	-1.449197000000
H	-3.742608000000	0.402465000000	-6.099752000000
H	-5.384682000000	1.998408000000	-4.643571000000
H	-1.644035000000	-4.388736000000	-5.398964000000
H	-1.711997000000	-6.219795000000	-3.398368000000
H	-4.671072000000	-6.892831000000	0.847626000000
H	-6.664390000000	-5.496197000000	2.043921000000
H	-8.646492000000	-0.628367000000	1.457866000000
H	-8.197656000000	1.414185000000	-0.267373000000
H	0.676723000000	-8.452363000000	4.057349000000
H	9.893802000000	-3.120450000000	3.412140000000
H	3.067917000000	4.957039000000	4.258923000000
H	-8.280992000000	4.005197000000	-2.710139000000
H	-1.165814000000	-3.346124000000	10.958794000000
H	-3.962604000000	5.659051000000	7.846131000000
H	-2.441329000000	-3.935076000000	9.882451000000
H	0.357666000000	2.451779000000	-4.125685000000
H	-5.950769000000	-3.601565000000	-4.118379000000
H	2.096249000000	-6.663153000000	-0.061107000000
H	3.392439000000	-6.457169000000	-1.249405000000
H	0.840888000000	-1.019039000000	-5.427132000000
H	4.785570000000	3.198214000000	-2.242513000000
H	1.191978000000	6.798133000000	-4.043531000000
H	-5.900744000000	5.674406000000	-0.121288000000
H	8.822272000000	1.140543000000	-0.993141000000
H	10.078336000000	-2.569848000000	-3.137270000000

⁴Intermediate2 / HS_I2

C	2.779812000000	4.309173000000	3.410613000000
H	3.169745000000	4.760124000000	2.492438000000
H	3.232029000000	3.315194000000	3.527424000000
N	1.324422000000	4.249612000000	3.399597000000
H	0.823936000000	4.454187000000	4.294548000000
C	0.632723000000	3.556890000000	2.483537000000
N	1.212734000000	3.043661000000	1.386057000000
H	2.157391000000	3.295154000000	1.088151000000

H	0.589220000000	2.642077000000	0.688213000000
N	-0.679295000000	3.348592000000	2.676037000000
H	-1.173090000000	3.870082000000	3.414860000000
H	-1.197135000000	2.935440000000	1.903954000000
C	-5.936598000000	4.640576000000	-0.543291000000
H	-5.162641000000	4.615922000000	-1.319939000000
C	-5.547631000000	3.741956000000	0.635524000000
H	-4.620650000000	4.125547000000	1.093920000000
H	-6.340296000000	3.792761000000	1.386756000000
O	-5.424435000000	2.382579000000	0.278286000000
H	-4.649979000000	2.251857000000	-0.306682000000
C	-7.304980000000	4.251393000000	-1.106960000000
O	-8.265324000000	4.020942000000	-0.377134000000
N	-7.378772000000	4.199127000000	-2.465812000000
H	-6.564875000000	4.308517000000	-3.074249000000
C	-1.647676000000	-3.046307000000	9.980191000000
H	-2.095583000000	-2.046760000000	10.002880000000
C	-0.649479000000	-3.202391000000	8.826606000000
H	0.153542000000	-2.457575000000	8.932996000000
H	-0.163578000000	-4.185066000000	8.910603000000
C	-1.259242000000	-3.077494000000	7.416004000000
H	-2.084003000000	-3.805896000000	7.347708000000
C	-1.841860000000	-1.681313000000	7.145341000000
H	-2.253035000000	-1.624044000000	6.131292000000
H	-2.642182000000	-1.424388000000	7.848326000000
H	-1.062367000000	-0.912191000000	7.232787000000
C	-0.223997000000	-3.441877000000	6.340887000000
H	-0.661500000000	-3.395793000000	5.337639000000
H	0.626517000000	-2.747173000000	6.368282000000
H	0.171915000000	-4.454038000000	6.492142000000
C	-3.379412000000	5.534680000000	7.022557000000
H	-4.014877000000	5.244941000000	6.181365000000
H	-3.185146000000	6.610445000000	6.935844000000
C	-2.076189000000	4.732732000000	7.012455000000
H	-1.421380000000	5.009746000000	7.845176000000
H	-2.299160000000	3.663484000000	7.142757000000
C	-1.267675000000	4.853042000000	5.717300000000
O	-1.922650000000	5.053792000000	4.625846000000
O	-0.023042000000	4.724059000000	5.781206000000
C	9.330646000000	1.175087000000	-2.044516000000
H	8.710733000000	1.806923000000	-2.693012000000
C	10.722087000000	1.837911000000	-1.869841000000
H	11.360473000000	1.120767000000	-1.332644000000
C	11.385674000000	2.161764000000	-3.215921000000
H	10.805162000000	2.919693000000	-3.758675000000
H	12.395134000000	2.562184000000	-3.061439000000
H	11.450149000000	1.277983000000	-3.855195000000
C	10.597714000000	3.097743000000	-1.000327000000
H	9.936494000000	3.835546000000	-1.474607000000
H	10.189522000000	2.862774000000	-0.010619000000
H	11.575769000000	3.573808000000	-0.859826000000
C	9.404757000000	-0.202531000000	-2.693515000000
O	9.590425000000	-0.357013000000	-3.899569000000
N	9.297978000000	-1.263148000000	-1.835086000000
H	9.064497000000	-1.096095000000	-0.864523000000
C	9.386673000000	-2.633217000000	-2.316163000000
H	9.796451000000	-3.254420000000	-1.511898000000
C	8.042863000000	-3.220464000000	-2.809705000000
H	7.642370000000	-2.538007000000	-3.567400000000
H	8.262428000000	-4.169149000000	-3.316623000000
C	7.033691000000	-3.455952000000	-1.707857000000
C	6.189670000000	-2.428852000000	-1.259980000000
H	6.236308000000	-1.449261000000	-1.727652000000
C	5.290059000000	-2.637531000000	-0.210845000000
H	4.672578000000	-1.807492000000	0.119865000000
C	5.214233000000	-3.890025000000	0.404673000000
H	4.513327000000	-4.060163000000	1.217946000000
C	6.045894000000	-4.925001000000	-0.031717000000
H	5.993960000000	-5.903129000000	0.440483000000
C	6.946798000000	-4.706028000000	-1.075955000000
H	7.588571000000	-5.518555000000	-1.411596000000

C	9.937206000000	-2.752340000000	2.368523000000
H	10.988282000000	-2.833888000000	2.066817000000
H	9.348415000000	-3.425434000000	1.736713000000
C	9.439133000000	-1.327623000000	2.270877000000
C	8.193041000000	-1.036954000000	1.696947000000
H	7.578413000000	-1.846616000000	1.311294000000
C	7.713678000000	0.276668000000	1.628113000000
H	6.745812000000	0.473729000000	1.171848000000
C	8.484311000000	1.321139000000	2.144749000000
H	8.116853000000	2.343645000000	2.104067000000
C	9.729757000000	1.046989000000	2.718584000000
H	10.334335000000	1.855804000000	3.121726000000
C	10.202498000000	-0.264309000000	2.775766000000
H	11.174239000000	-0.467533000000	3.221456000000
C	1.524161000000	6.502961000000	-2.992887000000
H	2.607145000000	6.661117000000	-2.966656000000
C	0.842393000000	7.273978000000	-1.839514000000
H	0.930377000000	8.350500000000	-2.034723000000
H	-0.229765000000	7.041751000000	-1.855635000000
C	1.443835000000	6.951438000000	-0.463351000000
H	1.522256000000	5.869270000000	-0.326432000000
H	2.467549000000	7.343188000000	-0.416100000000
C	0.659970000000	7.523652000000	0.721671000000
H	1.239645000000	7.332936000000	1.633570000000
H	0.542031000000	8.612303000000	0.627130000000
N	-0.648405000000	6.882300000000	0.826253000000
H	-0.975097000000	6.300336000000	0.043823000000
C	-1.318529000000	6.668660000000	1.966334000000
N	-2.483232000000	5.998287000000	1.914380000000
H	-2.683928000000	5.494637000000	1.049548000000
H	-2.823886000000	5.620677000000	2.795233000000
N	-0.913603000000	7.142245000000	3.158658000000
H	0.038149000000	7.470529000000	3.235087000000
H	-1.247732000000	6.552962000000	3.944491000000
C	1.277780000000	5.000501000000	-2.897180000000
O	2.020309000000	4.248156000000	-2.247920000000
N	0.168542000000	4.542962000000	-3.515896000000
H	-0.375681000000	5.189217000000	-4.070607000000
C	-0.266040000000	3.144599000000	-3.459329000000
H	-0.160021000000	2.794770000000	-2.428509000000
C	-1.715770000000	2.993396000000	-3.909066000000
H	-1.873113000000	3.485842000000	-4.878555000000
H	-1.933470000000	1.928683000000	-4.046483000000
O	-2.658724000000	3.559351000000	-2.991505000000
H	-2.840017000000	2.856775000000	-2.275288000000
C	5.123511000000	2.761697000000	-1.327634000000
H	6.192771000000	2.538341000000	-1.423845000000
C	4.931830000000	3.732954000000	-0.159174000000
H	5.283757000000	3.267881000000	0.766165000000
H	5.532178000000	4.638466000000	-0.335810000000
O	3.565678000000	4.080716000000	0.058870000000
H	3.127315000000	4.248676000000	-0.804630000000
C	4.390803000000	1.443228000000	-1.086076000000
O	4.732266000000	0.679854000000	-0.173409000000
N	3.355183000000	1.206194000000	-1.914341000000
H	3.158014000000	1.826149000000	-2.693420000000
C	2.526831000000	0.010091000000	-1.877836000000
H	3.183399000000	-0.869928000000	-1.845045000000
C	1.603307000000	-0.014839000000	-0.651523000000
H	1.050046000000	-0.954591000000	-0.579378000000
H	2.208800000000	0.110823000000	0.249926000000
H	0.872839000000	0.797887000000	-0.706057000000
C	1.769736000000	-0.017682000000	-3.222036000000
O	2.051117000000	0.790539000000	-4.118340000000
N	0.833511000000	-0.975651000000	-3.375501000000
H	0.420324000000	-1.474883000000	-2.576673000000
C	0.131726000000	-1.089194000000	-4.642072000000
H	-0.331583000000	-2.075460000000	-4.689414000000
H	-0.653416000000	-0.328512000000	-4.750965000000
C	2.269567000000	-6.476835000000	-1.017350000000
H	1.837701000000	-7.302064000000	-1.595744000000

C	1.672991000000	-5.141995000000	-1.462974000000
H	2.132379000000	-4.333863000000	-0.874628000000
C	1.898675000000	-4.861050000000	-2.942721000000
H	2.971034000000	-4.841125000000	-3.163817000000
H	1.431505000000	-5.639627000000	-3.557197000000
H	1.472599000000	-3.893157000000	-3.223983000000
O	0.247293000000	-5.130557000000	-1.239066000000
H	0.109771000000	-5.250271000000	-0.282093000000
C	1.382889000000	-7.530300000000	4.238725000000
H	1.257462000000	-7.301443000000	5.305507000000
H	2.443586000000	-7.753650000000	4.079347000000
C	0.922739000000	-6.376633000000	3.377145000000
C	1.772263000000	-5.289753000000	3.118594000000
H	2.779889000000	-5.292571000000	3.529201000000
C	1.342522000000	-4.207148000000	2.350062000000
H	2.014722000000	-3.372969000000	2.166339000000
C	0.047244000000	-4.186506000000	1.821065000000
H	-0.287137000000	-3.347695000000	1.217110000000
C	-0.809367000000	-5.263034000000	2.074930000000
H	-1.822092000000	-5.251883000000	1.679600000000
C	-0.371105000000	-6.347006000000	2.840833000000
H	-1.045030000000	-7.179651000000	3.031406000000
S	-6.478725000000	-3.601674000000	-3.025090000000
O	-3.391956000000	-1.529575000000	-0.874476000000
Fe	-4.829461000000	-2.345216000000	-1.758630000000
C	-7.049696000000	-2.970964000000	0.776933000000
C	-3.370961000000	-5.385088000000	-1.244325000000
C	-3.237174000000	-2.115000000000	-4.791138000000
C	-6.238824000000	0.695940000000	-2.249957000000
C	-6.116323000000	-3.964061000000	0.489125000000
C	-6.006883000000	-5.221227000000	1.183832000000
C	-4.926252000000	-5.867263000000	0.658690000000
C	-4.398328000000	-5.019173000000	-0.381045000000
C	-3.013108000000	-4.711730000000	-2.407750000000
C	-2.128948000000	-5.240102000000	-3.420894000000
C	-2.139372000000	-4.350462000000	-4.449750000000
C	-2.999395000000	-3.261621000000	-4.048032000000
C	-4.015064000000	-1.030514000000	-4.384465000000
C	-4.176188000000	0.190174000000	-5.138044000000
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C	-7.110151000000	-1.720477000000	0.171429000000
N	-5.128574000000	-3.856326000000	-0.460423000000
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N	-4.725415000000	-0.968773000000	-3.220550000000
N	-6.290652000000	-1.309292000000	-0.847853000000
H	-7.774502000000	-3.181890000000	1.557846000000
H	-2.877970000000	-6.333736000000	-1.053942000000
H	-2.755846000000	-2.042244000000	-5.761772000000
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C	-3.939985000000	-3.343795000000	3.785278000000
O	-2.749905000000	-2.598259000000	3.589720000000
C	-2.682411000000	-1.773700000000	2.496467000000
C	-1.486765000000	-0.999705000000	2.438092000000
C	-1.343421000000	-0.015823000000	1.457053000000
C	-2.294254000000	0.208008000000	0.474303000000
C	-3.484115000000	-0.735746000000	0.332955000000
C	-3.638650000000	-1.641805000000	1.532182000000
C	-2.205175000000	1.465420000000	-0.319600000000
O	-1.255226000000	2.293747000000	-0.055772000000
O	-3.102611000000	1.708813000000	-1.190400000000
H	-0.733373000000	-1.146274000000	3.204653000000
H	-0.476971000000	0.632736000000	1.503951000000
H	-4.382425000000	-0.111211000000	0.257650000000
H	-4.544237000000	-2.229271000000	1.561689000000
H	-4.108160000000	-4.058440000000	2.970574000000
H	-3.804251000000	-3.884549000000	4.723953000000
H	-4.813774000000	-2.683125000000	3.866147000000

O	-1.882182000000	4.868587000000	-0.668378000000
H	-2.182901000000	4.738650000000	-1.591784000000
H	-1.589938000000	3.945028000000	-0.423439000000
O	-5.017518000000	4.371823000000	-4.171381000000
H	-4.191701000000	4.050603000000	-3.732469000000
H	-4.825963000000	5.283182000000	-4.437613000000
O	-0.658843000000	-2.379060000000	-1.359979000000
H	-1.609510000000	-2.152641000000	-1.224344000000
H	-0.573326000000	-3.352292000000	-1.400731000000
H	-3.724183000000	0.385509000000	-6.102535000000
H	-5.332064000000	2.000623000000	-4.630359000000
H	-1.612044000000	-4.406655000000	-5.393618000000
H	-1.580812000000	-6.167528000000	-3.332493000000
H	-4.535638000000	-6.843703000000	0.915837000000
H	-6.674167000000	-5.553711000000	1.968913000000
H	-8.787560000000	-0.749420000000	1.306308000000
H	-8.242882000000	1.355185000000	-0.324600000000
H	0.810126000000	-8.440252000000	4.031097000000
H	9.869714000000	-3.126821000000	3.398600000000
H	3.078487000000	4.925926000000	4.260732000000
H	-8.274519000000	3.963933000000	-2.872540000000
H	-1.158413000000	-3.207988000000	10.947897000000
H	-3.934545000000	5.369561000000	7.953092000000
H	-2.464701000000	-3.774473000000	9.896391000000
H	0.385421000000	2.523077000000	-4.085670000000
H	-5.954433000000	-3.433347000000	-4.259556000000
H	2.070320000000	-6.658003000000	0.045865000000
H	3.356340000000	-6.478952000000	-1.158291000000
H	0.838919000000	-0.968498000000	-5.466028000000
H	4.795940000000	3.235732000000	-2.260459000000
H	1.158618000000	6.888717000000	-3.952660000000
H	-6.009356000000	5.679533000000	-0.191246000000
H	8.838393000000	1.111951000000	-1.066153000000
H	10.095117000000	-2.633199000000	-3.148750000000

Part 3.3 Mutant CYP199A4 system

Part 3.3.1 QM cluster energies, charges, and spin densities

Table S8: Absolute (free) energies (in au) of UB3LYP/BS1 optimized geometries of mutant CYP199A4 cluster model as obtained in Gaussian-09. Also shown are the degree of spin contamination in the structures (S^2 values).

	E [BS1, au]	ZPE	G [au]	E [BS2, au]	S^2
$^2\text{RC}_{\text{MUT}}$	-5401.26	1.90	-5399.55	-5402.67	1.7900
$^4\text{RC}_{\text{MUT}}$	-5401.26	1.90	-5399.55	-5402.67	3.7928
$^2\text{TS1}_{\text{MUT}}$	-5401.21	1.90	-5399.50	-5402.63	1.7150
$^4\text{TS1}_{\text{MUT}}$	-5401.21	1.90	-5399.50	-5402.63	3.8182
$^2\text{IM1}_{\text{MUT}}$	-5401.22	1.90	-5399.51	-5402.64	1.7648
$^4\text{IM1}_{\text{MUT}}$	-5401.22	1.90	-5399.51	-5402.64	3.8000
$^2\text{PR1}_{\text{MUT}}$	-5401.34	1.91	-5399.62	-5402.76	0.9003
$^4\text{PR1}_{\text{MUT}}$	-5401.34	1.91	-5399.63	-5402.75	3.7909
$^2\text{TS2}_{\text{MUT}}$	-5401.19	1.90	-5399.47	-5402.62	1.7962
$^4\text{TS2}_{\text{MUT}}$	-5401.19	1.90	-5399.47	-5402.62	3.8161
$^2\text{IM2}_{\text{MUT}}$	-5401.21	1.90	-5399.50	-5402.63	1.2911
$^4\text{IM2}_{\text{MUT}}$	-5401.20	1.90	-5399.49	-5402.63	3.8428

Table S9: Relative (free) energies (in au) of UB3LYP/BS1 optimized geometries of mutant CYP199A4 cluster model as obtained in Gaussian-09.

	ΔE	$\Delta E + \text{ZPE}$	ΔG	ΔE [BS2]	ΔE [BS2] + ZPE	ΔG [BS2]
$^2\text{RC}_{\text{MUT}}$	0.00	0.00	0.00	0.00	0.00	0.00
$^4\text{RC}_{\text{MUT}}$	0.16	0.16	-0.43	0.20	0.20	-0.39
$^2\text{TS1}_{\text{MUT}}$	30.86	26.53	29.55	28.47	24.14	27.16
$^4\text{TS1}_{\text{MUT}}$	31.37	26.86	29.41	29.19	24.68	27.22
$^2\text{IM1}_{\text{MUT}}$	22.78	20.91	23.23	19.49	17.63	19.95
$^4\text{IM1}_{\text{MUT}}$	23.34	21.36	23.13	20.02	18.03	19.80
$^2\text{PR1}_{\text{MUT}}$	-51.23	-48.91	-47.58	-55.38	-53.06	-51.73
$^4\text{PR1}_{\text{MUT}}$	-51.18	-49.38	-51.52	-46.91	-45.11	-47.24
$^2\text{TS2}_{\text{MUT}}$	40.31	39.34	49.73	35.13	34.16	44.54
$^4\text{TS2}_{\text{MUT}}$	39.76	38.80	49.73	35.61	34.64	45.57
$^2\text{IM2}_{\text{MUT}}$	29.83	29.15	30.67	24.83	24.15	25.67
$^4\text{IM2}_{\text{MUT}}$	33.56	32.69	35.47	28.71	27.84	30.62

Table S10: Group charges and spin densities (in au) of UB3LYP/BS1 optimized geometries of mutant CYP199A4 cluster model as obtained in Gaussian-09.

(a) Charges

	Fe	O	Por	Axial	SubH	Prot	Total
² RC _{MUT}	0.50	-0.52	-0.60	-0.01	-0.63	1.25	0.00
⁴ RC _{MUT}	0.50	-0.51	-0.59	-0.01	-0.63	1.25	0.00
² TS1 _{MUT}	0.37	-0.62	-0.69	-0.05	-0.33	1.32	0.00
⁴ TS1 _{MUT}	0.37	-0.62	-0.68	-0.05	-0.34	1.32	0.00
² IM1 _{MUT}	0.32	-0.71	-0.68	-0.04	-0.21	1.32	0.00
⁴ IM1 _{MUT}	0.32	-0.71	-0.66	-0.05	-0.22	1.32	0.00
² PR1 _{MUT}	0.35	-0.64	-0.98	-0.03	-0.02	1.32	0.00
⁴ PR1 _{MUT}	0.52	-0.64	-1.00	-0.19	-0.02	1.33	0.00
² TS2 _{MUT}	0.43	-0.49	-0.87	0.00	-0.35	1.28	0.00
⁴ TS2 _{MUT}	0.41	-0.48	-0.85	0.00	-0.34	1.26	0.00
² IM2 _{MUT}	0.27	-0.56	-0.77	-0.07	-0.14	1.27	0.00
⁴ IM2 _{MUT}	0.34	-0.55	-0.66	-0.02	-0.36	1.25	0.00

(b) Spin densities

	Fe	O	Por	Axial	SubH	Prot	Total
² RC _{MUT}	1.37	0.73	-0.57	-0.54	0.00	0.01	1.00
⁴ RC _{MUT}	1.24	0.78	0.48	0.49	0.00	0.01	3.00
² TS1 _{MUT}	1.03	0.52	-0.64	-0.39	0.48	0.00	1.00
⁴ TS1 _{MUT}	0.90	0.60	0.57	0.40	0.53	0.00	3.00
² IM1 _{MUT}	1.00	0.11	-0.68	-0.38	0.95	0.00	1.00
⁴ IM1 _{MUT}	0.88	0.18	0.61	0.36	0.97	0.00	3.00
² PR1 _{MUT}	1.21	0.00	-0.13	-0.07	0.00	0.00	1.00
⁴ PR1 _{MUT}	2.47	0.00	0.06	0.46	0.00	0.00	3.00
² TS2 _{MUT}	1.85	0.27	-0.40	-0.18	-0.53	-0.01	1.00
⁴ TS2 _{MUT}	1.30	0.72	0.13	0.32	0.52	0.00	3.00
² IM2 _{MUT}	1.04	0.07	-0.53	-0.12	0.54	0.00	1.00
⁴ IM2 _{MUT}	0.86	0.25	0.58	0.37	0.94	0.00	3.00

Part 3.3.2: Cartesian coordinates of optimized geometries

²Reactant_mut / LS_React_mut

C	37.518371000000	36.716146000000	26.887638000000
H	37.803570000000	36.897702000000	27.928705000000
C	36.613974000000	37.820929000000	26.327352000000
H	37.155360000000	38.779212000000	26.330981000000
H	36.396086000000	37.601233000000	25.271948000000
C	35.278678000000	38.004678000000	27.077234000000
H	34.802451000000	37.013631000000	27.151913000000
C	35.480038000000	38.543962000000	28.502309000000
H	34.518091000000	38.642087000000	29.021473000000
H	36.126361000000	37.900814000000	29.108449000000
H	35.937692000000	39.542706000000	28.471344000000
C	34.332546000000	38.919360000000	26.284019000000
H	33.369614000000	39.038175000000	26.795736000000
H	34.767746000000	39.920525000000	26.163275000000
H	34.134074000000	38.520514000000	25.281392000000
C	29.010644000000	36.051379000000	35.310993000000
H	28.155257000000	35.377261000000	35.190532000000
H	29.676376000000	35.909182000000	34.453109000000
C	29.730993000000	35.804365000000	36.617483000000
C	31.120711000000	35.958486000000	36.717049000000
H	31.691565000000	36.226305000000	35.829947000000
C	31.791382000000	35.752549000000	37.926954000000
H	32.871342000000	35.877971000000	37.976704000000
C	31.066976000000	35.377046000000	39.061853000000
H	31.582484000000	35.198368000000	40.002073000000
C	29.681634000000	35.217054000000	38.979325000000
H	29.113477000000	34.917706000000	39.856805000000
C	29.022225000000	35.429726000000	37.767872000000
H	27.943619000000	35.296833000000	37.710781000000
C	40.941357000000	37.629480000000	40.375664000000
H	41.417638000000	36.641286000000	40.383890000000
C	39.943959000000	37.728826000000	39.224735000000
H	39.517567000000	38.748286000000	39.226096000000
C	40.594832000000	37.478312000000	37.860990000000
H	41.013072000000	36.466500000000	37.814746000000
H	39.848903000000	37.563500000000	37.063519000000
H	41.395536000000	38.202670000000	37.664010000000
O	38.907892000000	36.785781000000	39.487040000000
H	38.285656000000	36.811101000000	38.726108000000
C	39.580433000000	33.467779000000	39.360566000000
H	39.633708000000	32.833140000000	40.257430000000
C	38.268229000000	33.199871000000	38.597842000000
H	38.286200000000	33.844705000000	37.710497000000
C	38.154378000000	31.740495000000	38.138018000000
H	38.994538000000	31.438342000000	37.503819000000
H	38.126130000000	31.058028000000	38.999093000000
H	37.232259000000	31.583887000000	37.565145000000
C	37.068622000000	33.602152000000	39.467908000000
H	37.146161000000	34.643691000000	39.795453000000
H	36.129478000000	33.497909000000	38.913579000000
H	37.004115000000	32.965862000000	40.361958000000
C	40.829362000000	33.303687000000	38.511798000000
O	40.928679000000	33.731709000000	37.365074000000
N	41.890034000000	32.660133000000	39.117234000000
H	41.805649000000	32.431851000000	40.097595000000
C	43.220082000000	32.701613000000	38.529866000000
H	43.391827000000	33.675059000000	38.061848000000
C	43.522716000000	31.657007000000	37.445931000000
O	44.532651000000	31.760477000000	36.754889000000
N	42.639532000000	30.632894000000	37.340649000000
H	41.773032000000	30.658659000000	37.865724000000
C	42.694613000000	29.695428000000	36.240431000000
H	43.272331000000	30.142536000000	35.426760000000
C	41.266410000000	29.339522000000	35.827702000000
O	40.360232000000	29.287854000000	36.662111000000
N	41.080084000000	29.065733000000	34.516499000000
H	41.833890000000	29.114682000000	33.839766000000

C	39.800170000000	28.622051000000	33.999603000000
H	39.411006000000	27.839096000000	34.660294000000
C	38.740553000000	29.774527000000	33.941263000000
H	38.943375000000	30.414252000000	34.804430000000
H	38.891583000000	30.369619000000	33.035053000000
C	37.311154000000	29.278146000000	34.016038000000
C	36.462401000000	29.315669000000	32.898819000000
H	36.834273000000	29.718845000000	31.960654000000
C	35.148629000000	28.843474000000	32.994733000000
H	34.499344000000	28.884185000000	32.123707000000
C	34.668711000000	28.333728000000	34.201671000000
H	33.646150000000	27.972553000000	34.274936000000
C	35.507788000000	28.296787000000	35.319634000000
H	35.138271000000	27.909131000000	36.265537000000
C	36.818026000000	28.764615000000	35.227618000000
H	37.470431000000	28.746487000000	36.098053000000
C	40.066703000000	28.041009000000	32.606791000000
O	41.142957000000	28.200931000000	32.028961000000
N	39.041919000000	27.336767000000	32.052316000000
H	38.116894000000	27.465229000000	32.447660000000
C	39.128567000000	26.962365000000	30.656462000000
H	40.040106000000	26.377400000000	30.501347000000
C	39.094525000000	28.189267000000	29.725721000000
O	38.413188000000	29.174021000000	29.987527000000
N	39.821862000000	28.056892000000	28.582456000000
H	40.464326000000	27.279424000000	28.511203000000
C	39.908402000000	29.108837000000	27.577561000000
H	39.048568000000	29.762186000000	27.742111000000
C	41.226370000000	29.899251000000	27.619927000000
H	42.062530000000	29.197015000000	27.497029000000
H	41.247423000000	30.555400000000	26.738313000000
C	41.473571000000	30.742408000000	28.882114000000
H	41.507565000000	30.103309000000	29.772210000000
H	42.475025000000	31.185052000000	28.775836000000
C	40.442876000000	31.867364000000	29.079521000000
H	40.079944000000	32.228209000000	28.105786000000
H	39.580226000000	31.489854000000	29.635398000000
N	41.054686000000	32.994208000000	29.803968000000
H	42.065226000000	33.007875000000	29.828619000000
C	40.444769000000	34.201429000000	29.946733000000
N	39.113335000000	34.272705000000	29.951052000000
H	38.595432000000	33.482267000000	30.352434000000
H	38.693173000000	35.215821000000	30.118027000000
N	41.171204000000	35.316753000000	30.051438000000
H	42.174447000000	35.275779000000	29.949165000000
H	40.731588000000	36.191959000000	30.454638000000
C	44.447905000000	34.838338000000	34.632560000000
H	44.865926000000	34.832630000000	33.616133000000
C	42.946470000000	35.154959000000	34.617193000000
H	42.540579000000	35.059727000000	35.632984000000
H	42.802175000000	36.204297000000	34.322641000000
C	42.101008000000	34.274129000000	33.675258000000
H	42.500226000000	34.398732000000	32.654027000000
C	42.175448000000	32.783241000000	34.036978000000
H	43.204911000000	32.408756000000	34.023116000000
H	41.771146000000	32.621564000000	35.043096000000
H	41.586790000000	32.182267000000	33.330680000000
C	40.640212000000	34.749849000000	33.675247000000
H	40.023328000000	34.123913000000	33.015345000000
H	40.219986000000	34.689288000000	34.686557000000
H	40.552244000000	35.782532000000	33.318415000000
S	34.347172000000	43.814603000000	34.003990000000
C	32.789987000000	38.690929000000	40.614798000000
H	32.607992000000	39.679157000000	40.173859000000
H	32.403536000000	37.942334000000	39.916731000000
C	34.279955000000	38.456317000000	40.899417000000
H	34.417929000000	37.463376000000	41.338203000000
H	34.655983000000	39.177800000000	41.634464000000
N	35.128294000000	38.508349000000	39.714813000000
H	35.256574000000	37.634629000000	39.158041000000
C	35.667522000000	39.625167000000	39.221767000000

N	36.566627000000	39.560702000000	38.243609000000
H	36.785086000000	40.419959000000	37.745268000000
H	36.869086000000	38.637442000000	37.875928000000
N	35.366117000000	40.848372000000	39.747465000000
H	35.666244000000	41.637395000000	39.173009000000
H	34.450043000000	40.956152000000	40.158368000000
O	36.289524000000	42.343021000000	37.389015000000
Fe	35.519467000000	42.776613000000	36.007290000000
N	36.939004000000	42.017094000000	34.797464000000
N	36.415718000000	44.588021000000	35.909014000000
N	33.957754000000	43.631806000000	36.972132000000
N	34.473625000000	41.073415000000	35.838690000000
C	37.053341000000	40.713310000000	34.371837000000
C	38.302408000000	40.509256000000	33.648587000000
C	38.919393000000	41.726000000000	33.649900000000
C	38.076821000000	42.645809000000	34.368229000000
C	37.624569000000	44.880003000000	35.317723000000
C	37.991621000000	46.248787000000	35.582423000000
C	37.009999000000	46.776347000000	36.362553000000
C	36.033613000000	45.736283000000	36.569479000000
C	33.903398000000	44.902585000000	37.488066000000
C	32.668785000000	45.099016000000	38.203545000000
C	31.969525000000	43.933503000000	38.108246000000
C	32.784706000000	43.022479000000	37.346577000000
C	33.236155000000	40.800876000000	36.366744000000
C	32.875192000000	39.427074000000	36.119644000000
C	33.914734000000	38.867050000000	35.442203000000
C	34.899489000000	39.905332000000	35.267325000000
C	36.106709000000	39.726926000000	34.595728000000
H	36.313846000000	38.731276000000	34.219482000000
C	38.395381000000	43.980337000000	34.599420000000
H	39.335934000000	44.341869000000	34.195294000000
C	34.879946000000	45.878036000000	37.321139000000
H	34.707611000000	46.840467000000	37.793071000000
C	32.441179000000	41.708040000000	37.055370000000
H	31.476789000000	41.354681000000	37.408127000000
C	38.793881000000	39.224834000000	33.048286000000
H	38.678952000000	38.409980000000	33.775105000000
H	39.866193000000	39.304348000000	32.849875000000
C	38.104116000000	38.821783000000	31.727155000000
H	38.198433000000	39.645024000000	31.005920000000
H	37.034517000000	38.639331000000	31.865379000000
C	38.751252000000	37.570696000000	31.103365000000
O	40.010111000000	37.499344000000	31.152918000000
O	37.971394000000	36.714708000000	30.581888000000
C	35.541100000000	34.458272000000	33.323559000000
C	36.647111000000	35.290872000000	33.522817000000
C	36.844074000000	35.866957000000	34.776535000000
C	35.944651000000	35.641751000000	35.828500000000
C	34.855290000000	34.786497000000	35.613494000000
C	34.654037000000	34.189396000000	34.368207000000
C	36.127235000000	36.378149000000	37.139458000000
O	37.196710000000	37.063268000000	37.258924000000
O	35.206979000000	36.307908000000	37.998302000000
O	35.325173000000	33.833850000000	32.100105000000
C	35.114812000000	34.729304000000	30.990156000000
H	37.327152000000	35.501204000000	32.702816000000
H	37.702947000000	36.502388000000	34.963758000000
H	34.163927000000	34.600526000000	36.428199000000
H	33.815649000000	33.522695000000	34.189975000000
H	35.015942000000	34.094449000000	30.106813000000
H	35.949231000000	35.426156000000	30.859609000000
H	34.185042000000	35.291008000000	31.141188000000
O	37.742726000000	32.427808000000	31.671600000000
H	36.822001000000	32.755588000000	31.776647000000
H	38.179350000000	32.709609000000	32.491379000000
H	32.212605000000	38.626378000000	41.544428000000
H	39.568541000000	34.516503000000	39.691078000000
H	43.961782000000	32.576791000000	39.325243000000
H	43.205885000000	28.764862000000	36.532074000000
H	38.270780000000	26.324667000000	30.419224000000

H	39.793569000000	28.653209000000	26.586327000000
H	28.622437000000	37.077613000000	35.254731000000
H	38.439498000000	36.630629000000	26.298215000000
H	37.012569000000	35.742264000000	26.850623000000
H	40.431535000000	37.770401000000	41.334902000000
H	41.726048000000	38.388998000000	40.281345000000
H	34.029811000000	37.848179000000	35.097468000000
H	31.955809000000	38.957349000000	36.444527000000
H	30.991558000000	43.698309000000	38.508501000000
H	32.382360000000	46.019211000000	38.696366000000
H	39.877941000000	41.981473000000	33.215049000000
H	38.892700000000	46.724725000000	35.217614000000
H	36.936151000000	47.777125000000	36.768303000000
H	35.423022000000	43.912091000000	33.190796000000
H	44.996897000000	35.595677000000	35.205647000000
H	44.657998000000	33.867228000000	35.093218000000

⁴Reactant_mut / HS_React_mut

C	37.526189000000	36.723752000000	26.891111000000
H	37.809069000000	36.903532000000	27.933120000000
C	36.624892000000	37.830682000000	26.330057000000
H	37.167801000000	38.788091000000	26.336166000000
H	36.409156000000	37.612662000000	25.273862000000
C	35.288138000000	38.015634000000	27.077042000000
H	34.809956000000	37.025332000000	27.149040000000
C	35.487079000000	38.552305000000	28.503433000000
H	34.524076000000	38.651516000000	29.020412000000
H	36.130630000000	37.906897000000	29.110111000000
H	35.946803000000	39.550179000000	28.475142000000
C	34.345534000000	38.933254000000	26.283019000000
H	33.381618000000	39.053010000000	26.792654000000
H	34.782816000000	39.933822000000	26.164865000000
H	34.148711000000	38.536323000000	25.279308000000
C	29.011312000000	36.063088000000	35.330870000000
H	28.154972000000	35.390297000000	35.209705000000
H	29.674658000000	35.924031000000	34.470637000000
C	29.734894000000	35.809575000000	36.634335000000
C	31.125354000000	35.959224000000	36.730128000000
H	31.694053000000	36.228560000000	35.842120000000
C	31.799169000000	35.746917000000	37.937186000000
H	32.879605000000	35.869340000000	37.984103000000
C	31.077159000000	35.369499000000	39.072975000000
H	31.595058000000	35.185727000000	40.010900000000
C	29.691059000000	35.214093000000	38.994216000000
H	29.124733000000	34.913458000000	39.872442000000
C	29.028525000000	35.433075000000	37.785604000000
H	27.949332000000	35.303784000000	37.731421000000
C	40.938819000000	37.618876000000	40.387190000000
H	41.415585000000	36.630921000000	40.396117000000
C	39.944589000000	37.718406000000	39.233530000000
H	39.517616000000	38.737621000000	39.234335000000
C	40.599433000000	37.469239000000	37.871428000000
H	41.018190000000	36.457631000000	37.825538000000
H	39.855716000000	37.554700000000	37.071929000000
H	41.400404000000	38.194065000000	37.677245000000
O	38.908360000000	36.774585000000	39.492205000000
H	38.287773000000	36.800884000000	38.729897000000
C	39.579060000000	33.456545000000	39.363371000000
H	39.631932000000	32.821182000000	40.259752000000
C	38.266793000000	33.189910000000	38.600289000000
H	38.285316000000	33.835301000000	37.713360000000
C	38.152036000000	31.730879000000	38.139583000000
H	38.992095000000	31.428489000000	37.505357000000
H	38.123116000000	31.047931000000	39.000258000000
H	37.229935000000	31.575241000000	37.566418000000
C	37.067340000000	33.592471000000	39.470441000000
H	37.145538000000	34.633787000000	39.798505000000
H	36.128196000000	33.489120000000	38.915956000000
H	37.002364000000	32.955718000000	40.364135000000
C	40.827989000000	33.292536000000	38.514605000000
O	40.927908000000	33.722139000000	37.368537000000

N	41.887976000000	32.647060000000	39.119246000000
H	41.803235000000	32.417435000000	40.099265000000
C	43.218207000000	32.688495000000	38.532270000000
H	43.390354000000	33.662307000000	38.065159000000
C	43.520775000000	31.644794000000	37.447455000000
O	44.531406000000	31.748109000000	36.757397000000
N	42.636523000000	30.621842000000	37.340051000000
H	41.769664000000	30.647814000000	37.864520000000
C	42.691625000000	29.685468000000	36.238911000000
H	43.271068000000	30.132483000000	35.426407000000
C	41.263431000000	29.331920000000	35.824135000000
O	40.356387000000	29.279881000000	36.657590000000
N	41.078088000000	29.060417000000	34.512324000000
H	41.832529000000	29.109989000000	33.836349000000
C	39.798204000000	28.618904000000	33.993469000000
H	39.407762000000	27.835119000000	34.652416000000
C	38.739643000000	29.772417000000	33.936332000000
H	38.942688000000	30.410676000000	34.800532000000
H	38.891604000000	30.368682000000	33.031044000000
C	37.309781000000	29.277166000000	34.009791000000
C	36.461472000000	29.317198000000	32.892316000000
H	36.833994000000	29.721659000000	31.954967000000
C	35.147250000000	28.846010000000	32.986998000000
H	34.498327000000	28.888683000000	32.115796000000
C	34.666434000000	28.334780000000	34.192950000000
H	33.643527000000	27.974393000000	34.265272000000
C	35.505062000000	28.295350000000	35.311164000000
H	35.134847000000	27.906545000000	36.256323000000
C	36.815746000000	28.762166000000	35.220377000000
H	37.467797000000	28.742097000000	36.091033000000
C	40.065438000000	28.040089000000	32.599863000000
O	41.142273000000	28.200217000000	32.023182000000
N	39.040572000000	27.337572000000	32.043312000000
H	38.115277000000	27.466285000000	32.437957000000
C	39.128191000000	26.965382000000	30.646921000000
H	40.039383000000	26.379906000000	30.491703000000
C	39.096022000000	28.193768000000	29.718088000000
O	38.415439000000	29.178773000000	29.980939000000
N	39.824329000000	28.062595000000	28.575304000000
H	40.466278000000	27.284755000000	28.503476000000
C	39.912624000000	29.115991000000	27.572088000000
H	39.052830000000	29.769442000000	27.736437000000
C	41.230830000000	29.905865000000	27.617259000000
H	42.066895000000	29.203535000000	27.494269000000
H	41.253113000000	30.563336000000	26.736662000000
C	41.476855000000	30.747040000000	28.880995000000
H	41.510029000000	30.106567000000	29.770143000000
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N	41.056224000000	32.996384000000	29.807963000000
H	42.066718000000	33.009972000000	29.834680000000
C	40.446007000000	34.203327000000	29.952076000000
N	39.114551000000	34.274498000000	29.953577000000
H	38.595836000000	33.483215000000	30.352156000000
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N	41.172140000000	35.318421000000	30.060872000000
H	42.175589000000	35.277719000000	29.960544000000
H	40.731685000000	36.192777000000	30.465053000000
C	44.448731000000	34.830813000000	34.640386000000
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C	42.947417000000	35.147994000000	34.624955000000
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H	42.803584000000	36.197873000000	34.332108000000
C	42.101957000000	34.268993000000	33.681303000000
H	42.501470000000	34.395211000000	32.660376000000
C	42.175902000000	32.777474000000	34.040504000000
H	43.205255000000	32.402705000000	34.026611000000
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C	40.641249000000	34.745000000000	33.681830000000
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H	40.221151000000	34.683394000000	34.693126000000
H	40.553254000000	35.778059000000	33.326114000000
S	34.337100000000	43.787490000000	33.995173000000
C	32.800461000000	38.682718000000	40.619913000000
H	32.616100000000	39.669266000000	40.176187000000
H	32.414008000000	37.931364000000	39.924835000000
C	34.291277000000	38.451517000000	40.902701000000
H	34.431857000000	37.460050000000	41.343991000000
H	34.667284000000	39.175719000000	41.635050000000
N	35.137567000000	38.501948000000	39.716511000000
H	35.264790000000	37.627502000000	39.160535000000
C	35.673758000000	39.618456000000	39.219724000000
N	36.571551000000	39.553436000000	38.240348000000
H	36.785752000000	40.411611000000	37.738476000000
H	36.874562000000	38.629779000000	37.874017000000
N	35.370828000000	40.842455000000	39.742992000000
H	35.668297000000	41.630496000000	39.166138000000
H	34.454854000000	40.949475000000	40.154365000000
O	36.282667000000	42.335924000000	37.375296000000
Fe	35.512208000000	42.794426000000	36.000733000000
N	36.933590000000	42.026325000000	34.792537000000
N	36.404545000000	44.600441000000	35.890532000000
N	33.953773000000	43.647097000000	36.965507000000
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C	37.047575000000	40.719941000000	34.373920000000
C	38.297192000000	40.512170000000	33.652072000000
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C	38.070654000000	42.652153000000	34.360222000000
C	37.609188000000	44.893047000000	35.288488000000
C	37.966475000000	46.268245000000	35.531516000000
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C	36.015540000000	45.756721000000	36.532873000000
C	33.892803000000	44.923316000000	37.467230000000
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C	32.782490000000	43.036504000000	37.345749000000
C	33.236507000000	40.808015000000	36.382553000000
C	32.879383000000	39.430883000000	36.147014000000
C	33.917117000000	38.870934000000	35.466715000000
C	34.896631000000	39.912554000000	35.279655000000
C	36.101661000000	39.734229000000	34.603156000000
H	36.309030000000	38.737307000000	34.230305000000
C	38.384651000000	43.990176000000	34.580290000000
H	39.322849000000	44.352624000000	34.171586000000
C	34.863971000000	45.901664000000	37.287086000000
H	34.687213000000	46.869306000000	37.746512000000
C	32.441656000000	41.718776000000	37.066947000000
H	31.479022000000	41.366450000000	37.425488000000
C	38.788489000000	39.225491000000	33.056513000000
H	38.670839000000	38.412407000000	33.784819000000
H	39.861325000000	39.303234000000	32.860215000000
C	38.101018000000	38.820805000000	31.734663000000
H	38.195194000000	39.643853000000	31.013173000000
H	37.031435000000	38.637243000000	31.871636000000
C	38.750149000000	37.570415000000	31.111514000000
O	40.008857000000	37.498931000000	31.164460000000
O	37.971720000000	36.715297000000	30.586474000000
C	35.540017000000	34.458299000000	33.322821000000
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C	35.947134000000	35.637379000000	35.829219000000
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C	34.653479000000	34.188957000000	34.367758000000
C	36.132049000000	36.371273000000	37.141187000000
O	37.202723000000	37.054575000000	37.260927000000
O	35.212457000000	36.301301000000	38.000767000000
O	35.322747000000	33.835651000000	32.098707000000
C	35.113491000000	34.732501000000	30.989775000000
H	37.326834000000	35.499883000000	32.702174000000

H	37.705694000000	36.497347000000	34.964326000000
H	34.165608000000	34.597311000000	36.428762000000
H	33.814232000000	33.523504000000	34.189167000000
H	35.013267000000	34.098719000000	30.105807000000
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H	34.184726000000	35.295596000000	31.141678000000
O	37.739994000000	32.429069000000	31.670529000000
H	36.819188000000	32.756689000000	31.775107000000
H	38.175365000000	32.709200000000	32.491526000000
H	32.224811000000	38.620112000000	41.550742000000
H	39.567685000000	34.505044000000	39.694618000000
H	43.959708000000	32.562736000000	39.327680000000
H	43.201190000000	28.753868000000	36.530259000000
H	38.270101000000	26.328767000000	30.407865000000
H	39.798920000000	28.661843000000	26.580046000000
H	28.623934000000	37.089921000000	35.280111000000
H	38.448638000000	36.637550000000	26.303861000000
H	37.018945000000	35.750720000000	26.851611000000
H	40.426242000000	37.758907000000	41.345089000000
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H	34.034417000000	37.850309000000	35.127960000000
H	31.963541000000	38.959662000000	36.479716000000
H	30.987253000000	43.716540000000	38.501489000000
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H	39.873190000000	41.982086000000	33.212073000000
H	38.862674000000	46.745267000000	35.156276000000
H	36.903227000000	47.806845000000	36.696957000000
H	35.405869000000	43.860818000000	33.170253000000
H	44.997784000000	35.586998000000	35.214936000000
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²TransitionState1_mut / LS_TS1_mut

C	0.751463000000	-1.831371000000	7.168449000000
H	1.060854000000	-2.344553000000	6.251416000000
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H	-0.666252000000	-1.989694000000	8.787858000000
C	-1.758160000000	-2.450590000000	6.988093000000
H	-1.943548000000	-1.401982000000	6.714872000000
C	-1.621754000000	-3.263315000000	5.690277000000
H	-2.550008000000	-3.215170000000	5.101381000000
H	-0.799035000000	-2.896960000000	5.068789000000
H	-1.427961000000	-4.322189000000	5.911322000000
C	-2.956384000000	-2.947851000000	7.810918000000
H	-3.889257000000	-2.898752000000	7.233587000000
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H	-3.093758000000	-2.346622000000	8.717830000000
C	-2.688302000000	-2.188680000000	-4.573276000000
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H	-2.022352000000	-1.511480000000	-4.028658000000
C	-1.913672000000	-3.285509000000	-5.269377000000
C	-2.485886000000	-4.001569000000	-6.332111000000
H	-3.485906000000	-3.740145000000	-6.672693000000
C	-1.791790000000	-5.036317000000	-6.960787000000
H	-2.253706000000	-5.573482000000	-7.785657000000
C	-0.503570000000	-5.374956000000	-6.538681000000
H	0.041834000000	-6.175515000000	-7.031675000000
C	0.080242000000	-4.667728000000	-5.485989000000
H	1.086708000000	-4.913208000000	-5.155850000000
C	-0.618191000000	-3.632378000000	-4.856731000000
H	-0.150281000000	-3.092797000000	-4.035778000000
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H	-1.827530000000	7.156301000000	1.910409000000
C	-0.702377000000	6.582393000000	0.158385000000
H	-0.031826000000	7.065376000000	-0.571519000000
C	0.048688000000	5.444364000000	0.851146000000
H	-0.597799000000	4.967694000000	1.595084000000
H	0.365241000000	4.689706000000	0.121171000000
H	0.947020000000	5.819780000000	1.356277000000
O	-1.851474000000	6.075680000000	-0.538187000000
H	-1.527413000000	5.416673000000	-1.190973000000

C	-4.920654000000	5.435539000000	2.861140000000
H	-5.888773000000	5.115365000000	3.272074000000
C	-4.858236000000	5.121127000000	1.349247000000
H	-3.876225000000	5.446442000000	0.985833000000
C	-4.985917000000	3.614670000000	1.079262000000
H	-4.170130000000	3.054629000000	1.549718000000
H	-5.935021000000	3.210542000000	1.456439000000
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C	-5.939979000000	5.912586000000	0.601212000000
H	-5.839943000000	6.991400000000	0.775991000000
H	-5.868245000000	5.736930000000	-0.479642000000
H	-6.948792000000	5.615074000000	0.918085000000
C	-3.761038000000	4.802965000000	3.619065000000
O	-2.593051000000	4.996234000000	3.303550000000
N	-4.106535000000	3.977067000000	4.664985000000
H	-5.073337000000	3.945775000000	4.956860000000
C	-3.105918000000	3.295432000000	5.466094000000
H	-2.133242000000	3.694486000000	5.166797000000
C	-3.046193000000	1.769686000000	5.308219000000
O	-2.261775000000	1.109976000000	5.985070000000
N	-3.887739000000	1.229609000000	4.395490000000
H	-4.543768000000	1.805455000000	3.883253000000
C	-3.922253000000	-0.189071000000	4.128447000000
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C	-4.907784000000	-0.443439000000	2.991045000000
O	-5.833536000000	0.335227000000	2.752083000000
N	-4.702442000000	-1.584420000000	2.290874000000
H	-3.921355000000	-2.198147000000	2.490849000000
C	-5.619310000000	-2.029777000000	1.260592000000
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C	-5.571449000000	-1.137878000000	-0.029989000000
H	-5.297810000000	-0.133783000000	0.302798000000
H	-4.781338000000	-1.498915000000	-0.695616000000
C	-6.901811000000	-1.074600000000	-0.752929000000
C	-7.110901000000	-1.727682000000	-1.976918000000
H	-6.298294000000	-2.295185000000	-2.422953000000
C	-8.352604000000	-1.652907000000	-2.617954000000
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C	-9.397882000000	-0.928618000000	-2.044502000000
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C	-9.198401000000	-0.276248000000	-0.823617000000
H	-10.007058000000	0.293116000000	-0.372493000000
C	-7.961964000000	-0.348293000000	-0.183595000000
H	-7.800503000000	0.163824000000	0.762388000000
C	-5.256829000000	-3.480218000000	0.922928000000
O	-4.192595000000	-3.991993000000	1.286474000000
N	-6.184819000000	-4.155462000000	0.196522000000
H	-6.915570000000	-3.602048000000	-0.237745000000
C	-5.839914000000	-5.407138000000	-0.442595000000
H	-5.412804000000	-6.080426000000	0.306541000000
C	-4.836646000000	-5.203900000000	-1.601737000000
O	-4.617017000000	-4.086068000000	-2.063106000000
N	-4.249441000000	-6.342284000000	-2.049128000000
H	-4.434613000000	-7.199477000000	-1.543282000000
C	-3.135846000000	-6.346741000000	-3.000979000000
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C	-1.797408000000	-6.771663000000	-2.362981000000
H	-1.799956000000	-7.859493000000	-2.205926000000
H	-1.010605000000	-6.570175000000	-3.101001000000
C	-1.470021000000	-6.092551000000	-1.024044000000
H	-2.245923000000	-6.345630000000	-0.289332000000
H	-0.531518000000	-6.505002000000	-0.634178000000
C	-1.349023000000	-4.560105000000	-1.083568000000
H	-0.474341000000	-4.255413000000	-1.660655000000
H	-2.219615000000	-4.116770000000	-1.571672000000
N	-1.288501000000	-3.962239000000	0.254499000000
H	-2.184228000000	-3.912391000000	0.732003000000
C	-0.187643000000	-3.994715000000	1.051193000000
N	1.036870000000	-4.031746000000	0.520792000000
H	1.184020000000	-3.602025000000	-0.393524000000
H	1.843758000000	-4.095405000000	1.185331000000

N	-0.327817000000	-3.985123000000	2.378377000000
H	-1.236725000000	-4.137565000000	2.790095000000
H	0.488732000000	-3.698941000000	2.991220000000
C	1.302694000000	1.830385000000	4.398963000000
H	1.936456000000	1.066750000000	4.867755000000
C	1.353835000000	1.718089000000	2.869715000000
H	0.714166000000	2.494280000000	2.422455000000
H	2.376724000000	1.934469000000	2.533610000000
C	0.942462000000	0.343323000000	2.305442000000
H	1.550655000000	-0.426666000000	2.801163000000
C	-0.530376000000	0.018453000000	2.595968000000
H	-0.734052000000	0.005894000000	3.671822000000
H	-1.193340000000	0.763908000000	2.133408000000
H	-0.794765000000	-0.967457000000	2.192478000000
C	1.225596000000	0.271866000000	0.797352000000
H	0.991279000000	-0.728040000000	0.407865000000
H	0.617041000000	1.002602000000	0.247018000000
H	2.277858000000	0.474542000000	0.567424000000
S	8.553712000000	0.019645000000	0.687737000000
C	-4.970007000000	3.879989000000	-6.376824000000
H	-4.307216000000	4.408270000000	-7.069192000000
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C	-5.393364000000	4.796493000000	-5.229157000000
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N	-4.225285000000	5.185009000000	-4.446411000000
H	-3.384648000000	4.534601000000	-4.438974000000
C	-4.193296000000	6.190321000000	-3.581373000000
N	-3.031654000000	6.570536000000	-3.039066000000
H	-3.018780000000	6.919850000000	-2.081687000000
H	-2.214804000000	5.930750000000	-3.186730000000
N	-5.327023000000	6.902841000000	-3.308849000000
H	-5.266500000000	7.625777000000	-2.606010000000
H	-6.220509000000	6.438934000000	-3.383402000000
O	4.703048000000	0.719536000000	-0.841305000000
Fe	6.379477000000	0.485742000000	-0.344700000000
N	5.714817000000	0.190251000000	1.560320000000
N	6.567699000000	2.456949000000	0.040280000000
N	7.182163000000	0.740164000000	-2.177534000000
N	6.352999000000	-1.488427000000	-0.676949000000
C	5.261583000000	-0.985914000000	2.110107000000
C	4.830462000000	-0.777167000000	3.497072000000
C	5.046025000000	0.550492000000	3.732917000000
C	5.570271000000	1.142431000000	2.532599000000
C	6.282987000000	3.108131000000	1.204237000000
C	6.481327000000	4.531055000000	1.050249000000
C	6.883231000000	4.728831000000	-0.235034000000
C	6.940357000000	3.424144000000	-0.853414000000
C	7.497912000000	1.941531000000	-2.760728000000
C	8.049680000000	1.731619000000	-4.076321000000
C	8.085289000000	0.383474000000	-4.275457000000
C	7.540546000000	-0.222592000000	-3.086710000000
C	6.791886000000	-2.182880000000	-1.784048000000
C	6.504191000000	-3.588763000000	-1.635984000000
C	5.863346000000	-3.732594000000	-0.443059000000
C	5.787561000000	-2.419511000000	0.153660000000
C	5.251599000000	-2.192066000000	1.418681000000
H	4.786484000000	-3.055274000000	1.878855000000
C	5.845438000000	2.494389000000	2.376479000000
H	5.670006000000	3.136133000000	3.234967000000
C	7.360106000000	3.188766000000	-2.157416000000
H	7.643238000000	4.054839000000	-2.748918000000
C	7.370936000000	-1.594312000000	-2.899554000000
H	7.687551000000	-2.250720000000	-3.705119000000
C	4.299555000000	-1.715814000000	4.566858000000
H	3.323825000000	-1.335528000000	4.894059000000
H	4.967426000000	-1.605593000000	5.432045000000
C	4.120422000000	-3.220366000000	4.297751000000
H	3.945823000000	-3.691620000000	5.273012000000
H	5.025164000000	-3.671769000000	3.880735000000
C	2.898465000000	-3.554880000000	3.423115000000

O	1.774852000000	-3.160724000000	3.855577000000
O	3.101360000000	-4.191700000000	2.349040000000
C	1.834645000000	0.633957000000	-3.322910000000
C	2.050268000000	1.858326000000	-2.684670000000
C	1.061425000000	2.840012000000	-2.773005000000
C	-0.124856000000	2.616304000000	-3.481799000000
C	-0.313205000000	1.379882000000	-4.115312000000
C	0.656736000000	0.385798000000	-4.036740000000
C	-1.188154000000	3.685305000000	-3.573974000000
O	-1.007363000000	4.750503000000	-2.901359000000
O	-2.178137000000	3.449150000000	-4.324081000000
O	2.741481000000	-0.413807000000	-3.266650000000
C	4.097812000000	-0.122864000000	-3.145895000000
H	2.949819000000	2.020981000000	-2.099012000000
H	1.200776000000	3.798441000000	-2.284403000000
H	-1.228140000000	1.219899000000	-4.675460000000
H	0.531171000000	-0.569737000000	-4.536964000000
H	4.663529000000	-1.039287000000	-3.301194000000
H	4.438139000000	0.268307000000	-1.877132000000
H	4.410410000000	0.722095000000	-3.764622000000
O	1.068629000000	-2.349445000000	-1.929015000000
H	1.832956000000	-1.888258000000	-2.328176000000
H	0.537369000000	-1.622954000000	-1.565284000000
H	-5.850970000000	3.537523000000	-6.929044000000
H	-4.847992000000	6.520880000000	3.008284000000
H	-3.239582000000	3.508820000000	6.532214000000
H	-4.257038000000	-0.747273000000	5.015717000000
H	-6.757919000000	-5.866219000000	-0.823909000000
H	-3.377592000000	-7.016333000000	-3.834414000000
H	-3.398259000000	-2.608758000000	-3.849072000000
H	1.607969000000	-1.832258000000	7.854228000000
H	0.533394000000	-0.787183000000	6.911160000000
H	-1.782515000000	8.403315000000	0.633238000000
H	-0.354804000000	8.116100000000	1.648971000000
H	5.475885000000	-4.630566000000	0.020586000000
H	6.755081000000	-4.349500000000	-2.364506000000
H	8.441895000000	-0.161655000000	-5.140267000000
H	8.376523000000	2.520201000000	-4.742278000000
H	4.857366000000	1.091828000000	4.652348000000
H	6.324779000000	5.265227000000	1.830225000000
H	7.129914000000	5.659454000000	-0.730164000000
H	9.073619000000	-0.742487000000	-0.301306000000
H	1.665231000000	2.811695000000	4.729653000000
H	0.290107000000	1.704439000000	4.797697000000

***TransitionState1 _mut/ HS_TS1_mut**

C	0.802675000000	-1.983943000000	7.118876000000
H	1.102967000000	-2.488250000000	6.193939000000
C	-0.417880000000	-2.640514000000	7.777467000000
H	-0.191346000000	-3.692000000000	8.013855000000
H	-0.610849000000	-2.147726000000	8.741214000000
C	-1.712001000000	-2.583209000000	6.940447000000
H	-1.891014000000	-1.530645000000	6.678352000000
C	-1.585915000000	-3.384961000000	5.634838000000
H	-2.514349000000	-3.320942000000	5.047797000000
H	-0.759947000000	-3.022458000000	5.015403000000
H	-1.403717000000	-4.447933000000	5.845749000000
C	-2.911103000000	-3.079179000000	7.762790000000
H	-3.845214000000	-3.018885000000	7.188568000000
H	-2.777337000000	-4.127096000000	8.064556000000
H	-3.041769000000	-2.484521000000	8.675001000000
C	-2.773357000000	-2.054921000000	-4.630451000000
H	-3.365017000000	-1.455326000000	-5.331837000000
H	-2.098152000000	-1.378890000000	-4.095787000000
C	-2.010529000000	-3.147222000000	-5.346493000000
C	-2.591975000000	-3.842422000000	-6.417926000000
H	-3.590816000000	-3.567704000000	-6.751385000000
C	-1.908408000000	-4.873462000000	-7.064183000000
H	-2.377315000000	-5.394329000000	-7.895553000000
C	-0.621805000000	-5.229018000000	-6.651399000000
H	-0.084559000000	-6.026433000000	-7.158273000000

C	-0.028857000000	-4.542613000000	-5.589935000000
H	0.976543000000	-4.801227000000	-5.266675000000
C	-0.716762000000	-3.511209000000	-4.943041000000
H	-0.242022000000	-2.988446000000	-4.115208000000
C	-1.077078000000	7.582163000000	1.300312000000
H	-1.711291000000	7.105946000000	2.055689000000
C	-0.595646000000	6.542601000000	0.294096000000
H	0.080248000000	7.027129000000	-0.429790000000
C	0.140922000000	5.384403000000	0.968874000000
H	-0.510817000000	4.905745000000	1.706986000000
H	0.446076000000	4.636071000000	0.227621000000
H	1.045026000000	5.740154000000	1.477938000000
O	-1.752577000000	6.062156000000	-0.407719000000
H	-1.438393000000	5.414281000000	-1.076334000000
C	-4.829238000000	5.420963000000	2.976209000000
H	-5.803685000000	5.111047000000	3.380035000000
C	-4.767255000000	5.125541000000	1.460323000000
H	-3.779735000000	5.441395000000	1.103570000000
C	-4.915932000000	3.624877000000	1.169631000000
H	-4.107891000000	3.047081000000	1.631960000000
H	-5.870647000000	3.228722000000	1.541119000000
H	-4.872573000000	3.434416000000	0.090870000000
C	-5.835295000000	5.942691000000	0.720249000000
H	-5.719222000000	7.017578000000	0.908991000000
H	-5.763936000000	5.779532000000	-0.362577000000
H	-6.849197000000	5.656687000000	1.031381000000
C	-3.682188000000	4.759881000000	3.728753000000
O	-2.509996000000	4.944903000000	3.423968000000
N	-4.044331000000	3.917894000000	4.756046000000
H	-5.013174000000	3.893442000000	5.041704000000
C	-3.057359000000	3.207452000000	5.548933000000
H	-2.077839000000	3.599258000000	5.262733000000
C	-3.016969000000	1.684346000000	5.362102000000
O	-2.241190000000	1.002230000000	6.026618000000
N	-3.865423000000	1.171857000000	4.439951000000
H	-4.513779000000	1.765185000000	3.938044000000
C	-3.919169000000	-0.241601000000	4.148969000000
H	-2.923703000000	-0.619152000000	3.895042000000
C	-4.910552000000	-0.463997000000	3.009943000000
O	-5.830154000000	0.327532000000	2.790210000000
N	-4.717285000000	-1.592210000000	2.286293000000
H	-3.939837000000	-2.215462000000	2.470456000000
C	-5.641791000000	-2.010025000000	1.251348000000
H	-6.659164000000	-1.971073000000	1.657608000000
C	-5.594838000000	-1.091856000000	-0.020916000000
H	-5.310894000000	-0.096999000000	0.330447000000
H	-4.812178000000	-1.445387000000	-0.699220000000
C	-6.929519000000	-1.003346000000	-0.733215000000
C	-7.152116000000	-1.629986000000	-1.968621000000
H	-6.347243000000	-2.194848000000	-2.431757000000
C	-8.397650000000	-1.532482000000	-2.599112000000
H	-8.553046000000	-2.017272000000	-3.559669000000
C	-9.433182000000	-0.811913000000	-2.003729000000
H	-10.399433000000	-0.735403000000	-2.495358000000
C	-9.220192000000	-0.185962000000	-0.771353000000
H	-10.021187000000	0.380390000000	-0.303094000000
C	-7.979953000000	-0.280625000000	-0.141738000000
H	-7.807828000000	0.210635000000	0.813381000000
C	-5.290067000000	-3.455259000000	0.881776000000
O	-4.226287000000	-3.980149000000	1.227351000000
N	-6.227489000000	-4.110194000000	0.148814000000
H	-6.957459000000	-3.543518000000	-0.269402000000
C	-5.895139000000	-5.350904000000	-0.517711000000
H	-5.464056000000	-6.040279000000	0.214293000000
C	-4.902193000000	-5.130152000000	-1.682459000000
O	-4.679890000000	-4.004471000000	-2.122919000000
N	-4.326599000000	-6.262703000000	-2.158725000000
H	-4.512327000000	-7.129026000000	-1.668915000000
C	-3.223163000000	-6.254301000000	-3.122240000000
H	-3.161522000000	-5.236550000000	-3.507830000000
C	-1.881265000000	-6.702132000000	-2.507926000000

H	-1.889372000000	-7.793209000000	-2.375458000000
H	-1.100752000000	-6.488826000000	-3.249213000000
C	-1.535569000000	-6.055412000000	-1.157407000000
H	-2.305381000000	-6.320069000000	-0.420352000000
H	-0.595664000000	-6.482065000000	-0.786725000000
C	-1.405617000000	-4.522839000000	-1.184400000000
H	-0.535302000000	-4.210518000000	-1.763943000000
H	-2.278603000000	-4.063911000000	-1.653403000000
N	-1.327349000000	-3.954353000000	0.165476000000
H	-2.217756000000	-3.906611000000	0.652895000000
C	-0.218307000000	-4.008986000000	0.949564000000
N	1.000273000000	-4.045996000000	0.406452000000
H	1.141637000000	-3.605049000000	-0.503594000000
H	1.813620000000	-4.126718000000	1.061615000000
N	-0.345470000000	-4.021151000000	2.278320000000
H	-1.251732000000	-4.172658000000	2.696094000000
H	0.478917000000	-3.754577000000	2.888869000000
C	1.308369000000	1.710926000000	4.424135000000
H	1.930716000000	0.932668000000	4.884091000000
C	1.359451000000	1.617398000000	2.893517000000
H	0.727261000000	2.405270000000	2.456201000000
H	2.384369000000	1.828605000000	2.560359000000
C	0.935922000000	0.253816000000	2.311606000000
H	1.540378000000	-0.527580000000	2.793883000000
C	-0.538410000000	-0.062772000000	2.603611000000
H	-0.737112000000	-0.090015000000	3.680193000000
H	-1.196963000000	0.695484000000	2.155667000000
H	-0.813105000000	-1.039922000000	2.186256000000
C	1.212464000000	0.201087000000	0.801336000000
H	0.965264000000	-0.790572000000	0.399026000000
H	0.610319000000	0.946518000000	0.263524000000
H	2.266175000000	0.394151000000	0.569864000000
S	8.690780000000	0.382086000000	0.391813000000
C	-4.899203000000	4.096772000000	-6.322454000000
H	-4.219633000000	4.630735000000	-6.993854000000
H	-4.384107000000	3.200166000000	-5.964663000000
C	-5.309773000000	4.987096000000	-5.149857000000
H	-6.058936000000	4.463183000000	-4.534226000000
H	-5.774899000000	5.910963000000	-5.517586000000
N	-4.138417000000	5.326953000000	-4.349594000000
H	-3.309030000000	4.662057000000	-4.360366000000
C	-4.091820000000	6.303198000000	-3.452443000000
N	-2.926156000000	6.643159000000	-2.892780000000
H	-2.910982000000	6.964343000000	-1.925746000000
H	-2.120196000000	5.993045000000	-3.056393000000
N	-5.213483000000	7.028106000000	-3.162398000000
H	-5.143522000000	7.724851000000	-2.434445000000
H	-6.114911000000	6.583509000000	-3.256587000000
O	4.663108000000	0.599007000000	-0.848389000000
Fe	6.333893000000	0.428579000000	-0.312128000000
N	5.685519000000	0.067665000000	1.572952000000
N	6.494713000000	2.383988000000	0.117120000000
N	7.142461000000	0.760051000000	-2.148250000000
N	6.372071000000	-1.540969000000	-0.702878000000
C	5.286220000000	-1.141740000000	2.098947000000
C	4.838374000000	-0.979739000000	3.485590000000
C	4.981395000000	0.354576000000	3.743336000000
C	5.492648000000	0.986778000000	2.558660000000
C	6.187795000000	3.005772000000	1.304969000000
C	6.362528000000	4.433665000000	1.182373000000
C	6.753008000000	4.672289000000	-0.098403000000
C	6.834692000000	3.389955000000	-0.757838000000
C	7.404815000000	1.981316000000	-2.711014000000
C	7.967112000000	1.817810000000	-4.030103000000
C	8.068305000000	0.477050000000	-4.248886000000
C	7.545547000000	-0.174255000000	-3.073008000000
C	6.835972000000	-2.183846000000	-1.819528000000
C	6.591493000000	-3.602087000000	-1.720447000000
C	5.957172000000	-3.802565000000	-0.530322000000
C	5.846110000000	-2.508781000000	0.100222000000
C	5.326072000000	-2.332295000000	1.385182000000

H	4.897250000000	-3.220619000000	1.830826000000
C	5.733692000000	2.356656000000	2.442151000000
H	5.521239000000	2.970288000000	3.312722000000
C	7.221613000000	3.207912000000	-2.077592000000
H	7.461378000000	4.099778000000	-2.649353000000
C	7.419330000000	-1.549487000000	-2.914163000000
H	7.767768000000	-2.179097000000	-3.727996000000
C	4.375705000000	-1.964925000000	4.544460000000
H	3.449256000000	-1.569354000000	4.977718000000
H	5.121376000000	-1.931339000000	5.351479000000
C	4.119166000000	-3.443699000000	4.209311000000
H	3.919998000000	-3.946574000000	5.163941000000
H	5.002356000000	-3.921169000000	3.775339000000
C	2.889477000000	-3.680780000000	3.314969000000
O	1.780240000000	-3.262453000000	3.762585000000
O	3.075700000000	-4.270380000000	2.212386000000
C	1.841330000000	0.639236000000	-3.360794000000
C	2.073547000000	1.836602000000	-2.678463000000
C	1.102158000000	2.837665000000	-2.736361000000
C	-0.084256000000	2.659855000000	-3.457900000000
C	-0.290263000000	1.449842000000	-4.135406000000
C	0.662594000000	0.437383000000	-4.088041000000
C	-1.129072000000	3.748928000000	-3.515789000000
O	-0.933551000000	4.787102000000	-2.805733000000
O	-2.120220000000	3.555922000000	-4.276758000000
O	2.728300000000	-0.425938000000	-3.336295000000
C	4.092187000000	-0.163856000000	-3.203045000000
H	2.971931000000	1.962039000000	-2.082106000000
H	1.254785000000	3.775392000000	-2.212752000000
H	-1.205075000000	1.325045000000	-4.704668000000
H	0.522579000000	-0.498118000000	-4.621243000000
H	4.636963000000	-1.090131000000	-3.373637000000
H	4.431749000000	0.201108000000	-1.910345000000
H	4.424691000000	0.683181000000	-3.808814000000
O	1.028214000000	-2.332699000000	-2.012851000000
H	1.795582000000	-1.881966000000	-2.418859000000
H	0.522197000000	-1.600860000000	-1.624568000000
H	-5.783767000000	3.791727000000	-6.890632000000
H	-4.739491000000	6.502909000000	3.137848000000
H	-3.194163000000	3.401964000000	6.618302000000
H	-4.259214000000	-0.809948000000	5.027741000000
H	-6.819073000000	-5.798298000000	-0.898631000000
H	-3.478566000000	-6.904140000000	-3.967199000000
H	-3.468067000000	-2.479996000000	-3.894427000000
H	1.662246000000	-2.000549000000	7.800697000000
H	0.592415000000	-0.934878000000	6.875282000000
H	-1.648565000000	8.371907000000	0.797988000000
H	-0.224800000000	8.047910000000	1.807984000000
H	5.599379000000	-4.725853000000	-0.093503000000
H	6.865834000000	-4.331256000000	-2.472383000000
H	8.454462000000	-0.036773000000	-5.120122000000
H	8.259862000000	2.631191000000	-4.681859000000
H	4.757677000000	0.871376000000	4.668951000000
H	6.192187000000	5.145844000000	1.979696000000
H	6.975098000000	5.621400000000	-0.569469000000
H	8.551532000000	1.018596000000	1.576740000000
H	1.683146000000	2.683241000000	4.767788000000
H	0.293874000000	1.593333000000	4.820432000000

²Intermediate1_mut / LS_I1_mut

C	42.731870000000	37.795537000000	29.470670000000
H	41.661058000000	37.673055000000	29.274804000000
C	43.540319000000	36.536375000000	29.132112000000
H	43.412827000000	36.289231000000	28.066671000000
H	44.609727000000	36.752681000000	29.267584000000
C	43.188445000000	35.295289000000	29.977242000000
H	43.271116000000	35.580097000000	31.036686000000
C	41.749957000000	34.817329000000	29.719857000000
H	41.516648000000	33.930670000000	30.327624000000
H	41.016391000000	35.595569000000	29.951249000000
H	41.618373000000	34.534243000000	28.666036000000

C	44.189244000000	34.160083000000	29.712025000000
H	43.972058000000	33.278331000000	30.329636000000
H	44.155312000000	33.841394000000	28.661190000000
H	45.216569000000	34.475014000000	29.931334000000
C	33.467374000000	31.715058000000	34.952541000000
H	33.202538000000	31.036909000000	35.771306000000
H	33.871252000000	32.633800000000	35.391257000000
C	32.275023000000	32.002941000000	34.068149000000
C	31.229863000000	31.076313000000	33.940401000000
H	31.266179000000	30.150911000000	34.511693000000
C	30.143400000000	31.325075000000	33.098948000000
H	29.342529000000	30.593729000000	33.021292000000
C	30.079541000000	32.513521000000	32.368306000000
H	29.230638000000	32.713491000000	31.719664000000
C	31.111156000000	33.447869000000	32.489132000000
H	31.069076000000	34.382150000000	31.934579000000
C	32.198215000000	33.195112000000	33.330440000000
H	32.993606000000	33.932917000000	33.409476000000
C	40.457351000000	37.847525000000	41.334309000000
H	41.219708000000	37.374045000000	40.706190000000
C	39.096256000000	37.766622000000	40.651658000000
H	38.351439000000	38.297853000000	41.267008000000
C	39.119707000000	38.378261000000	39.251253000000
H	39.865471000000	37.867206000000	38.633804000000
H	38.139595000000	38.283947000000	38.768857000000
H	39.370149000000	39.445119000000	39.294023000000
O	38.736652000000	36.377445000000	40.589017000000
H	37.863166000000	36.315666000000	40.143331000000
C	42.632305000000	34.349422000000	39.361108000000
H	43.261017000000	33.467857000000	39.170496000000
C	41.157547000000	33.918650000000	39.529938000000
H	40.571029000000	34.822026000000	39.733650000000
C	40.604649000000	33.273117000000	38.251008000000
H	40.627019000000	33.975170000000	37.410105000000
H	41.175706000000	32.380496000000	37.962053000000
H	39.560503000000	32.969997000000	38.391825000000
C	41.020641000000	32.974810000000	40.732823000000
H	41.401328000000	33.440315000000	41.651102000000
H	39.968518000000	32.710921000000	40.898090000000
H	41.576178000000	32.040023000000	40.577124000000
C	42.800236000000	35.394879000000	38.265884000000
O	42.175317000000	36.449544000000	38.269030000000
N	43.680419000000	35.067587000000	37.259846000000
H	44.238610000000	34.231645000000	37.361480000000
C	43.931171000000	35.946947000000	36.131866000000
H	43.490484000000	36.917056000000	36.373414000000
C	43.340473000000	35.499298000000	34.785837000000
O	43.532225000000	36.167707000000	33.773560000000
N	42.611780000000	34.358702000000	34.805214000000
H	42.531299000000	33.805568000000	35.648614000000
C	41.999528000000	33.821111000000	33.613181000000
H	41.297578000000	34.540850000000	33.178938000000
C	41.305979000000	32.510605000000	33.973890000000
O	41.652790000000	31.843933000000	34.951874000000
N	40.308777000000	32.130753000000	33.138978000000
H	40.024195000000	32.703650000000	32.352555000000
C	39.635988000000	30.855167000000	33.284283000000
H	40.395338000000	30.069472000000	33.374260000000
C	38.720255000000	30.789287000000	34.558071000000
H	39.178143000000	31.451744000000	35.296306000000
H	37.729400000000	31.185547000000	34.316633000000
C	38.617267000000	29.394862000000	35.142996000000
C	37.436972000000	28.641494000000	35.055084000000
H	36.570284000000	29.067914000000	34.556839000000
C	37.372909000000	27.355100000000	35.602219000000
H	36.449022000000	26.786480000000	35.531806000000
C	38.484871000000	26.806682000000	36.241456000000
H	38.433907000000	25.808206000000	36.667611000000
C	39.665246000000	27.551009000000	36.334308000000
H	40.534264000000	27.132264000000	36.835390000000
C	39.731387000000	28.833022000000	35.790355000000

H	40.645079000000	29.418179000000	35.867104000000
C	38.806962000000	30.623745000000	32.016175000000
O	38.600854000000	31.522973000000	31.194715000000
N	38.317363000000	29.364801000000	31.865682000000
H	38.358529000000	28.761300000000	32.680122000000
C	37.258710000000	29.105497000000	30.914560000000
H	37.544817000000	29.527210000000	29.946483000000
C	35.913880000000	29.719676000000	31.371227000000
O	35.784315000000	30.201973000000	32.494059000000
N	34.925268000000	29.679084000000	30.442457000000
H	35.156769000000	29.331453000000	29.520106000000
C	33.654732000000	30.391945000000	30.599247000000
H	33.605428000000	30.700460000000	31.643724000000
C	33.517346000000	31.601562000000	29.651036000000
H	33.291171000000	31.242758000000	28.637080000000
H	32.638178000000	32.170847000000	29.978220000000
C	34.754800000000	32.509409000000	29.574266000000
H	35.608032000000	31.921829000000	29.209644000000
H	34.580988000000	33.290364000000	28.824055000000
C	35.164338000000	33.175716000000	30.900542000000
H	34.460110000000	33.956893000000	31.189645000000
H	35.176666000000	32.450938000000	31.717208000000
N	36.518864000000	33.732509000000	30.835067000000
H	37.263633000000	33.044904000000	30.912249000000
C	36.844282000000	34.886123000000	30.197382000000
N	35.958512000000	35.881424000000	30.086455000000
H	35.236429000000	35.963644000000	30.802761000000
H	36.279937000000	36.757562000000	29.611749000000
N	38.061868000000	35.025995000000	29.668445000000
H	38.688132000000	34.233950000000	29.653620000000
H	38.444324000000	35.994302000000	29.472607000000
C	40.753411000000	38.418415000000	35.350428000000
H	40.730527000000	39.484967000000	35.091818000000
C	39.362112000000	37.793205000000	35.185542000000
H	39.376108000000	36.758150000000	35.561148000000
H	38.652628000000	38.337181000000	35.823826000000
C	38.833773000000	37.795586000000	33.737298000000
H	39.001470000000	38.799667000000	33.322760000000
C	39.575713000000	36.791253000000	32.842434000000
H	40.664093000000	36.897470000000	32.916399000000
H	39.315210000000	35.762015000000	33.135693000000
H	39.301337000000	36.925230000000	31.790651000000
C	37.319296000000	37.536622000000	33.698965000000
H	36.967597000000	37.465539000000	32.661736000000
H	37.084167000000	36.591018000000	34.215230000000
H	36.762142000000	38.345361000000	34.184320000000
S	35.382872000000	44.419005000000	32.885557000000
C	33.915540000000	31.370324000000	41.613311000000
H	33.238324000000	31.988333000000	42.210995000000
H	33.790854000000	31.651936000000	40.563195000000
C	35.364001000000	31.572091000000	42.057271000000
H	36.018582000000	30.878621000000	41.504592000000
H	35.469944000000	31.342375000000	43.125505000000
N	35.768746000000	32.953467000000	41.822659000000
H	35.275710000000	33.503699000000	41.059466000000
C	36.839962000000	33.528617000000	42.354037000000
N	37.038617000000	34.841722000000	42.203124000000
H	37.990922000000	35.200423000000	42.140464000000
H	36.440126000000	35.329260000000	41.494626000000
N	37.696816000000	32.804341000000	43.134722000000
H	38.532485000000	33.268292000000	43.461467000000
H	37.789058000000	31.814346000000	42.959897000000
O	35.381969000000	40.473502000000	34.429770000000
Fe	35.386098000000	42.102586000000	33.631834000000
N	37.124526000000	41.705385000000	32.677322000000
N	36.429877000000	42.836481000000	35.204988000000
N	33.643380000000	42.642056000000	34.519613000000
N	34.333436000000	41.464151000000	32.053787000000
C	37.279971000000	41.093605000000	31.453038000000
C	38.699603000000	40.960002000000	31.116927000000
C	39.361673000000	41.489293000000	32.189808000000

C	38.384924000000	41.932193000000	33.145194000000
C	37.792137000000	42.895188000000	35.349901000000
C	38.138659000000	43.417421000000	36.652579000000
C	36.966680000000	43.656515000000	37.299210000000
C	35.905072000000	43.292634000000	36.386557000000
C	33.504343000000	43.147122000000	35.787393000000
C	32.112557000000	43.395847000000	36.077000000000
C	31.410526000000	43.048017000000	34.962559000000
C	32.373504000000	42.569902000000	34.001185000000
C	32.977445000000	41.511664000000	31.850143000000
C	32.635566000000	40.892184000000	30.592631000000
C	33.806165000000	40.463379000000	30.041425000000
C	34.856809000000	40.847357000000	30.954057000000
C	36.212137000000	40.659721000000	30.675694000000
H	36.420868000000	40.092810000000	29.777044000000
C	38.702236000000	42.488501000000	34.385362000000
H	39.757280000000	42.590107000000	34.622999000000
C	34.550072000000	43.416680000000	36.665196000000
H	34.281661000000	43.800327000000	37.645407000000
C	32.062043000000	42.056845000000	32.746255000000
H	31.015182000000	42.051212000000	32.455882000000
C	39.429465000000	40.452398000000	29.885657000000
H	40.182508000000	39.729018000000	30.220799000000
H	39.995073000000	41.306996000000	29.488478000000
C	38.678598000000	39.806559000000	28.707659000000
H	39.409128000000	39.705474000000	27.895459000000
H	37.874438000000	40.447987000000	28.336129000000
C	38.147129000000	38.392056000000	28.999783000000
O	39.016839000000	37.522355000000	29.309733000000
O	36.901580000000	38.201481000000	28.906144000000
C	33.446551000000	37.034790000000	35.788765000000
C	34.372008000000	37.790281000000	36.511820000000
C	34.891421000000	37.250800000000	37.690401000000
C	34.504795000000	35.983743000000	38.141960000000
C	33.575056000000	35.249760000000	37.391692000000
C	33.042380000000	35.767435000000	36.214949000000
C	35.077272000000	35.401769000000	39.414678000000
O	35.956732000000	36.084134000000	40.029975000000
O	34.629663000000	34.277382000000	39.781114000000
O	32.898801000000	37.480472000000	34.585443000000
C	32.676933000000	38.818994000000	34.417665000000
H	34.706819000000	38.757323000000	36.145864000000
H	35.613945000000	37.812662000000	38.272324000000
H	33.274612000000	34.272928000000	37.754591000000
H	32.315786000000	35.213719000000	35.628289000000
H	32.242790000000	39.050158000000	33.453271000000
H	34.534491000000	40.046801000000	34.194533000000
H	32.432438000000	39.396492000000	35.304147000000
O	34.425948000000	35.952838000000	32.626634000000
H	33.806514000000	36.545430000000	33.093156000000
H	35.254269000000	36.044905000000	33.125511000000
H	33.628104000000	30.320872000000	41.732878000000
H	42.985041000000	34.802820000000	40.296424000000
H	45.006232000000	36.095975000000	35.984369000000
H	42.759249000000	33.619473000000	32.843793000000
H	37.154051000000	28.022336000000	30.792614000000
H	32.827844000000	29.692773000000	30.429496000000
H	34.273447000000	31.240572000000	34.377902000000
H	43.082949000000	38.648890000000	28.877199000000
H	42.850955000000	38.057129000000	30.529831000000
H	40.433702000000	37.344669000000	42.308558000000
H	40.743489000000	38.892793000000	41.496576000000
H	33.972558000000	39.948589000000	29.104039000000
H	31.630533000000	40.804223000000	30.199290000000
H	30.342086000000	43.099132000000	34.794996000000
H	31.738704000000	43.795465000000	37.011176000000
H	40.433962000000	41.573832000000	32.321711000000
H	39.149828000000	43.566261000000	37.009428000000
H	36.814732000000	44.047088000000	38.297456000000
H	36.710827000000	44.656238000000	32.979752000000
H	41.103555000000	38.327089000000	36.384655000000

H	41.499585000000	37.941231000000	34.704682000000
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⁴Intermediate1_mut / HS_I1_mut

C	42.733441000000	37.794455000000	29.477364000000
H	41.662274000000	37.673946000000	29.282219000000
C	43.540319000000	36.536500000000	29.130692000000
H	43.411050000000	36.295255000000	28.064111000000
H	44.610116000000	36.751109000000	29.265806000000
C	43.188560000000	35.291213000000	29.969640000000
H	43.272779000000	35.570370000000	31.030447000000
C	41.749408000000	34.815698000000	29.711511000000
H	41.516077000000	33.926269000000	30.315218000000
H	41.016734000000	35.593372000000	29.947610000000
H	41.616430000000	34.537961000000	28.656430000000
C	44.188122000000	34.156615000000	29.697221000000
H	43.970907000000	33.271803000000	30.310419000000
H	44.152762000000	33.843532000000	28.644743000000
H	45.215948000000	34.469539000000	29.917044000000
C	33.463405000000	31.692845000000	34.944218000000
H	33.198154000000	31.011453000000	35.760137000000
H	33.862631000000	32.611778000000	35.386822000000
C	32.273106000000	31.979156000000	34.056592000000
C	31.229302000000	31.051409000000	33.926073000000
H	31.265102000000	30.126066000000	34.497487000000
C	30.144857000000	31.298986000000	33.081667000000
H	29.344962000000	30.566797000000	33.001876000000
C	30.081704000000	32.487356000000	32.350846000000
H	29.234293000000	32.686451000000	31.699982000000
C	31.112000000000	33.422819000000	32.474416000000
H	31.070270000000	34.357152000000	31.919923000000
C	32.197075000000	33.171189000000	33.318597000000
H	32.991381000000	33.909841000000	33.400188000000
C	40.458539000000	37.874207000000	41.300014000000
H	41.218562000000	37.395959000000	40.672682000000
C	39.095405000000	37.790255000000	40.621892000000
H	38.352755000000	38.325845000000	41.236114000000
C	39.115022000000	38.393210000000	39.217716000000
H	39.858692000000	37.878023000000	38.601171000000
H	38.133401000000	38.296376000000	38.738919000000
H	39.366050000000	39.460202000000	39.253131000000
O	38.734562000000	36.400941000000	40.568817000000
H	37.860983000000	36.336816000000	40.123616000000
C	42.622270000000	34.349437000000	39.354311000000
H	43.247013000000	33.464313000000	39.167114000000
C	41.145298000000	33.926338000000	39.522835000000
H	40.562900000000	34.833195000000	39.722953000000
C	40.590765000000	33.279153000000	38.245417000000
H	40.617339000000	33.978248000000	37.402167000000
H	41.157968000000	32.382893000000	37.960122000000
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C	41.002342000000	32.987219000000	40.728700000000
H	41.384443000000	33.453909000000	41.645803000000
H	39.948734000000	32.729277000000	40.893770000000
H	41.553311000000	32.049100000000	40.576774000000
C	42.796656000000	35.390677000000	38.256056000000
O	42.175439000000	36.447529000000	38.254017000000
N	43.678391000000	35.056962000000	37.253454000000
H	44.233488000000	34.219517000000	37.359481000000
C	43.935186000000	35.931663000000	36.123224000000
H	43.498712000000	36.904625000000	36.360823000000
C	43.344883000000	35.482611000000	34.777479000000
O	43.538736000000	36.148883000000	33.764154000000
N	42.615154000000	34.342740000000	34.797854000000
H	42.531816000000	33.791585000000	35.642273000000
C	42.002694000000	33.804602000000	33.606136000000
H	41.302909000000	34.525437000000	33.170269000000
C	41.305678000000	32.496315000000	33.968278000000
O	41.648907000000	31.831368000000	34.948714000000
N	40.309458000000	32.116670000000	33.132122000000
H	40.027547000000	32.688511000000	32.343959000000
C	39.633980000000	30.842614000000	33.278473000000

H	40.391709000000	30.055700000000	33.371396000000
C	38.715396000000	30.780572000000	34.550419000000
H	39.172244000000	31.444215000000	35.288234000000
H	37.725464000000	31.177221000000	34.305876000000
C	38.609642000000	29.387503000000	35.138149000000
C	37.428716000000	28.635260000000	35.049103000000
H	36.563701000000	29.061520000000	34.547835000000
C	37.361887000000	27.350161000000	35.598950000000
H	36.437519000000	26.782437000000	35.527616000000
C	38.471702000000	26.801931000000	36.242052000000
H	38.418601000000	25.804487000000	36.670357000000
C	39.652696000000	27.545138000000	36.336023000000
H	40.520028000000	27.126551000000	36.840154000000
C	39.721601000000	28.825854000000	35.789380000000
H	40.635743000000	29.410177000000	35.867042000000
C	38.807123000000	30.610381000000	32.009056000000
O	38.604059000000	31.508475000000	31.185695000000
N	38.316065000000	29.351779000000	31.859709000000
H	38.354590000000	28.749782000000	32.675400000000
C	37.258439000000	29.092586000000	30.907410000000
H	37.546416000000	29.512732000000	29.939203000000
C	35.913761000000	29.708853000000	31.361696000000
O	35.783032000000	30.191031000000	32.484447000000
N	34.926722000000	29.670193000000	30.431197000000
H	35.159193000000	29.322184000000	29.509234000000
C	33.657014000000	30.385022000000	30.585998000000
H	33.607610000000	30.695586000000	31.629864000000
C	33.521854000000	31.593071000000	29.635576000000
H	33.295732000000	31.232852000000	28.622108000000
H	32.643232000000	32.164014000000	29.961323000000
C	34.760468000000	32.499248000000	29.557825000000
H	35.612592000000	31.910669000000	29.192167000000
H	34.586867000000	33.280653000000	28.808000000000
C	35.172344000000	33.164803000000	30.883724000000
H	34.467820000000	33.944630000000	31.175632000000
H	35.187808000000	32.439256000000	31.699688000000
N	36.525767000000	33.723562000000	30.814622000000
H	37.271992000000	33.037266000000	30.888803000000
C	36.847877000000	34.882193000000	30.184869000000
N	35.960404000000	35.877201000000	30.083392000000
H	35.240611000000	35.952801000000	30.802941000000
H	36.280738000000	36.758832000000	29.618451000000
N	38.063816000000	35.027375000000	29.653453000000
H	38.691747000000	34.236778000000	29.633282000000
H	38.444979000000	35.997589000000	29.464820000000
C	40.766921000000	38.405917000000	35.333435000000
H	40.743694000000	39.471209000000	35.069726000000
C	39.374900000000	37.780477000000	35.175803000000
H	39.389794000000	36.747198000000	35.556225000000
H	38.667668000000	38.327692000000	35.813773000000
C	38.841994000000	37.776430000000	33.729321000000
H	39.008563000000	38.778631000000	33.309722000000
C	39.580828000000	36.767905000000	32.836591000000
H	40.669435000000	36.874242000000	32.906728000000
H	39.320803000000	35.740019000000	33.134991000000
H	39.303146000000	36.897862000000	31.785229000000
C	37.327373000000	37.517667000000	33.696797000000
H	36.972134000000	37.445227000000	32.660820000000
H	37.093820000000	36.572887000000	34.215182000000
H	36.772694000000	38.327437000000	34.183177000000
S	35.402863000000	44.415281000000	32.883858000000
C	33.911484000000	31.408302000000	41.644158000000
H	33.234214000000	32.032424000000	42.235392000000
H	33.787076000000	31.679340000000	40.591230000000
C	35.359881000000	31.614457000000	42.086395000000
H	36.014501000000	30.915234000000	41.541046000000
H	35.465501000000	31.395687000000	43.156969000000
N	35.764709000000	32.993262000000	41.837544000000
H	35.272176000000	33.535572000000	41.068104000000
C	36.835777000000	33.574066000000	42.362862000000
N	37.034454000000	34.885499000000	42.197547000000

H	37.986931000000	35.243072000000	42.130284000000
H	36.436316000000	35.364954000000	41.483268000000
N	37.692542000000	32.858455000000	43.151642000000
H	38.528166000000	33.326127000000	43.473189000000
H	37.785170000000	31.866710000000	42.987220000000
O	35.401750000000	40.457269000000	34.416054000000
Fe	35.387348000000	42.113028000000	33.677349000000
N	37.134394000000	41.715366000000	32.714491000000
N	36.432201000000	42.840557000000	35.245152000000
N	33.654937000000	42.656836000000	34.556884000000
N	34.336824000000	41.480612000000	32.088251000000
C	37.287399000000	41.099998000000	31.492656000000
C	38.706951000000	40.963269000000	31.155576000000
C	39.370191000000	41.496023000000	32.226590000000
C	38.392676000000	41.941897000000	33.180092000000
C	37.797041000000	42.907596000000	35.384110000000
C	38.145230000000	43.434486000000	36.684285000000
C	36.974871000000	43.668586000000	37.335361000000
C	35.911856000000	43.298330000000	36.427250000000
C	33.512675000000	43.161768000000	35.824934000000
C	32.121777000000	43.421618000000	36.108043000000
C	31.422369000000	43.080866000000	34.990214000000
C	32.384788000000	42.594875000000	34.032380000000
C	32.984103000000	41.531738000000	31.881640000000
C	32.641582000000	40.912226000000	30.624470000000
C	33.812564000000	40.478682000000	30.076492000000
C	34.861914000000	40.860324000000	30.991594000000
C	36.217806000000	40.668644000000	30.715539000000
H	36.425416000000	40.099733000000	29.817674000000
C	38.707550000000	42.502309000000	34.420885000000
H	39.762101000000	42.607682000000	34.659197000000
C	34.556572000000	43.423469000000	36.706587000000
H	34.287979000000	43.807657000000	37.686508000000
C	32.071042000000	42.081677000000	32.779308000000
H	31.023817000000	42.080342000000	32.490068000000
C	39.435943000000	40.449769000000	29.926292000000
H	40.178003000000	39.715049000000	30.261511000000
H	40.014886000000	41.298355000000	29.535687000000
C	38.682069000000	39.818491000000	28.742036000000
H	39.411816000000	39.722360000000	27.928640000000
H	37.880017000000	40.466432000000	28.377230000000
C	38.146893000000	38.402610000000	29.021133000000
O	39.016133000000	37.526725000000	29.314460000000
O	36.900074000000	38.216980000000	28.934546000000
C	33.428918000000	37.012021000000	35.766766000000
C	34.354787000000	37.776117000000	36.480320000000
C	34.878782000000	37.248842000000	37.662516000000
C	34.496286000000	35.985278000000	38.127166000000
C	33.565994000000	35.242285000000	37.386470000000
C	33.028946000000	35.747802000000	36.206506000000
C	35.073001000000	35.416625000000	39.403907000000
O	35.953898000000	36.105368000000	40.009974000000
O	34.627003000000	34.295655000000	39.782926000000
O	32.875997000000	37.443831000000	34.561323000000
C	32.651819000000	38.781957000000	34.379364000000
H	34.686119000000	38.740968000000	36.105397000000
H	35.601675000000	37.817820000000	38.237050000000
H	33.268484000000	34.268397000000	37.759570000000
H	32.301528000000	35.187615000000	35.627024000000
H	32.206342000000	38.999074000000	33.416725000000
H	34.567837000000	40.019982000000	34.156421000000
H	32.408765000000	39.367980000000	35.260819000000
O	34.429500000000	35.930246000000	32.621719000000
H	33.801996000000	36.516075000000	33.086317000000
H	35.253604000000	36.026649000000	33.126666000000
H	33.623896000000	30.360144000000	41.774263000000
H	42.976214000000	34.804016000000	40.288614000000
H	45.011237000000	36.075040000000	35.977345000000
H	42.762605000000	33.599763000000	32.837776000000
H	37.152659000000	28.009390000000	30.786695000000
H	32.829153000000	29.686783000000	30.417149000000

H	34.272918000000	31.222865000000	34.370744000000
H	43.084382000000	38.650844000000	28.888215000000
H	42.854198000000	38.049972000000	30.537818000000
H	40.437268000000	37.377651000000	42.277546000000
H	40.746109000000	38.920237000000	41.454715000000
H	33.979532000000	39.962209000000	29.140140000000
H	31.637236000000	40.827514000000	30.228711000000
H	30.355179000000	43.141040000000	34.817848000000
H	31.747025000000	43.823798000000	37.040732000000
H	40.442549000000	41.580636000000	32.357822000000
H	39.157029000000	43.589573000000	37.036638000000
H	36.824815000000	44.061124000000	38.333103000000
H	36.729697000000	44.653168000000	32.990077000000
H	41.120029000000	38.319247000000	36.367029000000
H	41.510976000000	37.925341000000	34.687777000000

²Product_mut / LS_Prod_mut

C	41.557328000000	38.195938000000	29.984464000000
H	40.554101000000	37.813939000000	29.765645000000
C	42.668219000000	37.327229000000	29.379398000000
H	42.511238000000	37.233620000000	28.293642000000
H	43.629823000000	37.844685000000	29.503496000000
C	42.803906000000	35.917743000000	29.989647000000
H	42.957691000000	36.034917000000	31.072321000000
C	41.538735000000	35.070526000000	29.776200000000
H	41.667612000000	34.060789000000	30.191184000000
H	40.663736000000	35.524862000000	30.253006000000
H	41.320261000000	34.959048000000	28.704595000000
C	44.034486000000	35.199533000000	29.415188000000
H	44.168875000000	34.208794000000	29.868014000000
H	43.939270000000	35.057942000000	28.329815000000
H	44.949760000000	35.775062000000	29.597181000000
C	33.341240000000	30.733204000000	34.221180000000
H	33.054501000000	30.194067000000	35.132038000000
H	33.577929000000	31.764054000000	34.503337000000
C	32.241542000000	30.688024000000	33.183251000000
C	31.613761000000	29.474212000000	32.861324000000
H	31.909820000000	28.566123000000	33.383243000000
C	30.614305000000	29.416335000000	31.889058000000
H	30.137461000000	28.466254000000	31.660245000000
C	30.219022000000	30.577868000000	31.219541000000
H	29.435620000000	30.536668000000	30.467230000000
C	30.831027000000	31.792482000000	31.534650000000
H	30.524636000000	32.704828000000	31.029023000000
C	31.833236000000	31.847922000000	32.508587000000
H	32.298947000000	32.802253000000	32.745903000000
C	40.620514000000	37.805749000000	41.388893000000
H	41.318394000000	37.310748000000	40.704870000000
C	39.247679000000	37.927426000000	40.735694000000
H	38.576373000000	38.487471000000	41.408672000000
C	39.313035000000	38.649010000000	39.390895000000
H	39.984976000000	38.114196000000	38.711796000000
H	38.317716000000	38.705567000000	38.935794000000
H	39.686627000000	39.672767000000	39.517803000000
O	38.736503000000	36.594848000000	40.574972000000
H	37.894550000000	36.659080000000	40.071542000000
C	42.674041000000	34.322583000000	39.323428000000
H	43.272269000000	33.422105000000	39.123984000000
C	41.185883000000	33.936077000000	39.491871000000
H	40.626723000000	34.855443000000	39.703535000000
C	40.612103000000	33.317006000000	38.208833000000
H	40.635861000000	34.029331000000	37.376646000000
H	41.167230000000	32.418752000000	37.905879000000
H	39.565129000000	33.027594000000	38.355699000000
C	41.022439000000	32.986012000000	40.686152000000
H	41.405182000000	33.435105000000	41.610998000000
H	39.964983000000	32.742271000000	40.842954000000
H	41.559916000000	32.041800000000	40.524096000000
C	42.875957000000	35.371282000000	38.238343000000
O	42.314338000000	36.461235000000	38.273656000000
N	43.707244000000	35.008385000000	37.203185000000

H	44.217334000000	34.139523000000	37.279688000000
C	43.983432000000	35.884123000000	36.078000000000
H	43.578930000000	36.867779000000	36.328906000000
C	43.375692000000	35.460002000000	34.730596000000
O	43.634159000000	36.087162000000	33.708544000000
N	42.556802000000	34.380378000000	34.766728000000
H	42.459876000000	33.840225000000	35.616820000000
C	41.951274000000	33.828637000000	33.579536000000
H	41.143789000000	34.471765000000	33.206904000000
C	41.426842000000	32.431981000000	33.910445000000
O	41.825706000000	31.811097000000	34.898041000000
N	40.512282000000	31.925392000000	33.047498000000
H	40.186628000000	32.447329000000	32.241983000000
C	40.019992000000	30.568403000000	33.185970000000
H	40.878837000000	29.903390000000	33.331563000000
C	39.061012000000	30.388412000000	34.416764000000
H	39.373142000000	31.128572000000	35.157274000000
H	38.034478000000	30.623387000000	34.118815000000
C	39.141821000000	29.005583000000	35.032479000000
C	38.100378000000	28.074921000000	34.899099000000
H	37.209558000000	28.349305000000	34.340337000000
C	38.205639000000	26.804753000000	35.476904000000
H	37.387353000000	26.096904000000	35.371065000000
C	39.349262000000	26.449826000000	36.192301000000
H	39.428465000000	25.464303000000	36.643520000000
C	40.392415000000	27.371160000000	36.329012000000
H	41.284720000000	27.103421000000	36.889040000000
C	40.290411000000	28.637121000000	35.754116000000
H	41.096909000000	29.358595000000	35.863362000000
C	39.299526000000	30.196143000000	31.886695000000
O	38.979958000000	31.040696000000	31.044141000000
N	39.038441000000	28.870853000000	31.733924000000
H	39.136937000000	28.290589000000	32.560252000000
C	38.096997000000	28.425366000000	30.729534000000
H	38.380778000000	28.854106000000	29.763927000000
C	36.647844000000	28.830837000000	31.083382000000
O	36.351873000000	29.210742000000	32.214237000000
N	35.760158000000	28.726834000000	30.062195000000
H	36.113571000000	28.479925000000	29.146441000000
C	34.385636000000	29.222837000000	30.154028000000
H	34.215074000000	29.446507000000	31.206844000000
C	34.122376000000	30.461232000000	29.273437000000
H	34.020190000000	30.146561000000	28.225421000000
H	33.146376000000	30.866107000000	29.568615000000
C	35.204169000000	31.551272000000	29.338692000000
H	36.154978000000	31.138727000000	28.975267000000
H	34.936985000000	32.360033000000	28.647274000000
C	35.454653000000	32.156840000000	30.731548000000
H	34.595556000000	32.745535000000	31.059020000000
H	35.607963000000	31.376084000000	31.479539000000
N	36.658352000000	32.991874000000	30.735074000000
H	37.537326000000	32.483826000000	30.693055000000
C	36.685208000000	34.311051000000	30.426015000000
N	35.604347000000	35.071352000000	30.599574000000
H	34.929280000000	34.805434000000	31.323311000000
H	35.709276000000	36.101984000000	30.459449000000
N	37.815364000000	34.856001000000	29.957813000000
H	38.525083000000	34.259844000000	29.557838000000
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C	40.251528000000	37.598973000000	35.579391000000
H	39.692673000000	38.531123000000	35.733545000000
C	39.291814000000	36.414291000000	35.417322000000
H	39.877158000000	35.502646000000	35.218743000000
H	38.777326000000	36.241771000000	36.372970000000
C	38.226952000000	36.580532000000	34.317134000000
H	37.630146000000	37.470410000000	34.558497000000
C	38.830784000000	36.798231000000	32.923989000000
H	39.509995000000	37.656368000000	32.900469000000
H	39.402056000000	35.916934000000	32.597279000000
H	38.050450000000	36.980117000000	32.179108000000
C	37.273962000000	35.375865000000	34.308113000000

H	36.475308000000	35.521675000000	33.571824000000
H	37.809861000000	34.452216000000	34.044434000000
H	36.810184000000	35.228855000000	35.290929000000
S	37.183761000000	45.083497000000	33.652098000000
C	32.517326000000	33.562663000000	42.278598000000
H	32.091026000000	34.518261000000	42.599216000000
H	32.515152000000	33.542907000000	41.184435000000
C	33.938248000000	33.397556000000	42.817576000000
H	34.314826000000	32.393817000000	42.561733000000
H	33.942875000000	33.480323000000	43.912170000000
N	34.804919000000	34.426869000000	42.256115000000
H	34.558389000000	34.845364000000	41.308287000000
C	35.983601000000	34.781576000000	42.749915000000
N	36.609916000000	35.859192000000	42.269339000000
H	37.627370000000	35.882506000000	42.226477000000
H	36.206780000000	36.307845000000	41.409550000000
N	36.522723000000	34.105738000000	43.808419000000
H	37.437528000000	34.390266000000	44.127657000000
H	36.300224000000	33.128001000000	43.923545000000
O	35.475352000000	38.706619000000	32.904515000000
Fe	35.867331000000	43.305728000000	33.937057000000
N	36.856997000000	42.105885000000	32.673426000000
N	36.881211000000	42.527160000000	35.478841000000
N	34.615909000000	44.165874000000	35.250620000000
N	34.617427000000	43.778613000000	32.441886000000
C	36.656523000000	41.933411000000	31.319885000000
C	37.656233000000	41.041147000000	30.752602000000
C	38.479913000000	40.713528000000	31.786301000000
C	37.981575000000	41.370343000000	32.967204000000
C	38.021663000000	41.761660000000	35.393635000000
C	38.565813000000	41.516329000000	36.705753000000
C	37.739164000000	42.131628000000	37.595440000000
C	36.700466000000	42.766338000000	36.826190000000
C	34.711455000000	44.188952000000	36.626032000000
C	33.688386000000	45.028894000000	37.190545000000
C	32.976985000000	45.536023000000	36.145623000000
C	33.558136000000	44.995240000000	34.944597000000
C	33.573338000000	44.676604000000	32.506186000000
C	33.016456000000	44.896269000000	31.195888000000
C	33.728646000000	44.122259000000	30.331511000000
C	34.725892000000	43.437833000000	31.113485000000
C	35.666010000000	42.563043000000	30.587517000000
H	35.627193000000	42.377964000000	29.519478000000
C	38.548465000000	41.236265000000	34.223098000000
H	39.447938000000	40.634576000000	34.305133000000
C	35.679301000000	43.528570000000	37.368147000000
H	35.647319000000	43.635402000000	38.448095000000
C	33.085121000000	45.253306000000	33.666827000000
H	32.245239000000	45.935088000000	33.572660000000
C	37.719849000000	40.573492000000	29.326754000000
H	38.688064000000	40.095885000000	29.145128000000
H	37.658497000000	41.436220000000	28.649268000000
C	36.606665000000	39.568307000000	28.948328000000
H	36.642166000000	39.412147000000	27.862490000000
H	35.620601000000	39.965206000000	29.204030000000
C	36.777429000000	38.192097000000	29.605458000000
O	37.806241000000	37.533339000000	29.311381000000
O	35.839461000000	37.792918000000	30.378333000000
C	34.049693000000	37.223986000000	35.158148000000
C	35.000980000000	37.986932000000	35.848287000000
C	35.293753000000	37.671333000000	37.176742000000
C	34.658644000000	36.612519000000	37.835211000000
C	33.691909000000	35.876146000000	37.135435000000
C	33.387321000000	36.173394000000	35.811906000000
C	34.998941000000	36.250880000000	39.259426000000
O	35.979162000000	36.850083000000	39.810272000000
O	34.277023000000	35.370288000000	39.812365000000
O	33.717449000000	37.410185000000	33.832419000000
C	34.131280000000	38.643390000000	33.175422000000
H	35.538221000000	38.783848000000	35.348427000000
H	36.037714000000	38.249435000000	37.714702000000

H	33.184287000000	35.068499000000	37.651963000000
H	32.635745000000	35.606685000000	35.269630000000
H	33.514738000000	38.660109000000	32.271161000000
H	35.650022000000	38.373778000000	31.986799000000
H	33.857073000000	39.464619000000	33.845161000000
O	33.856734000000	34.751622000000	32.872790000000
H	33.690902000000	35.705464000000	33.049390000000
H	34.426349000000	34.494969000000	33.615662000000
H	31.878089000000	32.753635000000	42.646353000000
H	43.042321000000	34.755726000000	40.262037000000
H	45.062066000000	35.997614000000	35.924957000000
H	42.695165000000	33.760458000000	32.773812000000
H	38.165838000000	27.335603000000	30.647733000000
H	33.692142000000	28.420037000000	29.878611000000
H	34.262618000000	30.268106000000	33.846088000000
H	41.609290000000	39.216554000000	29.586060000000
H	41.666029000000	38.260717000000	31.074850000000
H	40.559179000000	37.224337000000	42.316789000000
H	41.018637000000	38.797214000000	41.633254000000
H	33.602993000000	44.011899000000	29.261815000000
H	32.181555000000	45.552453000000	30.984424000000
H	32.127694000000	46.207212000000	36.169646000000
H	33.547582000000	45.199591000000	38.250385000000
H	39.344640000000	40.062106000000	31.761490000000
H	39.456068000000	40.933319000000	36.903340000000
H	37.810651000000	42.160966000000	38.675239000000
H	37.337366000000	45.410012000000	34.956287000000
H	40.905604000000	37.451583000000	36.444815000000
H	40.889581000000	37.731655000000	34.697891000000

***Product_mut / HS_Prod_mut**

C	41.544114000000	38.188268000000	30.011300000000
H	40.540438000000	37.807712000000	29.791856000000
C	42.653146000000	37.324442000000	29.395983000000
H	42.492642000000	37.238993000000	28.310094000000
H	43.615012000000	37.841123000000	29.520966000000
C	42.790961000000	35.910456000000	29.995272000000
H	42.947847000000	36.020164000000	31.078302000000
C	41.525494000000	35.064309000000	29.779070000000
H	41.655733000000	34.051528000000	30.186160000000
H	40.651411000000	35.514743000000	30.261306000000
H	41.304278000000	34.960728000000	28.707256000000
C	44.020125000000	35.196948000000	29.411976000000
H	44.155875000000	34.202629000000	29.856515000000
H	43.922078000000	35.063970000000	28.325783000000
H	44.935750000000	35.771229000000	29.596072000000
C	33.338672000000	30.729928000000	34.219343000000
H	33.055627000000	30.191868000000	35.131986000000
H	33.571734000000	31.762355000000	34.498740000000
C	32.237335000000	30.677863000000	33.183462000000
C	31.616693000000	29.459984000000	32.862892000000
H	31.919736000000	28.553861000000	33.384217000000
C	30.615424000000	29.395615000000	31.892952000000
H	30.144220000000	28.442461000000	31.665277000000
C	30.211119000000	30.554568000000	31.224279000000
H	29.426330000000	30.508281000000	30.473723000000
C	30.816062000000	31.773054000000	31.537904000000
H	30.502782000000	32.683395000000	31.032897000000
C	31.820127000000	31.834957000000	32.509590000000
H	32.280118000000	32.792397000000	32.745460000000
C	40.632558000000	37.806184000000	41.372352000000
H	41.325553000000	37.326718000000	40.672505000000
C	39.249653000000	37.922610000000	40.739852000000
H	38.581485000000	38.465029000000	41.430152000000
C	39.287619000000	38.665951000000	39.405774000000
H	39.955111000000	38.149470000000	38.708275000000
H	38.284802000000	38.717827000000	38.966718000000
H	39.651477000000	39.691742000000	39.544022000000
O	38.750747000000	36.587177000000	40.565395000000
H	37.907378000000	36.648748000000	40.064077000000
C	42.703489000000	34.322085000000	39.330265000000

H	43.306654000000	33.425069000000	39.130176000000
C	41.218188000000	33.926859000000	39.504433000000
H	40.654063000000	34.844100000000	39.712250000000
C	40.645399000000	33.297141000000	38.226295000000
H	40.665570000000	34.003756000000	37.389216000000
H	41.203787000000	32.399204000000	37.928504000000
H	39.599789000000	33.004362000000	38.376201000000
C	41.063668000000	32.982328000000	40.704312000000
H	41.445496000000	33.439031000000	41.625808000000
H	40.008204000000	32.732286000000	40.864780000000
H	41.607074000000	32.040855000000	40.546263000000
C	42.894420000000	35.370528000000	38.243084000000
O	42.326644000000	36.457314000000	38.280243000000
N	43.721654000000	35.011413000000	37.203483000000
H	44.239072000000	34.146810000000	37.279027000000
C	43.988852000000	35.890305000000	36.078452000000
H	43.583692000000	36.872514000000	36.333808000000
C	43.374254000000	35.468383000000	34.733556000000
O	43.617239000000	36.105240000000	33.713662000000
N	42.568481000000	34.378998000000	34.768227000000
H	42.480980000000	33.832530000000	35.615337000000
C	41.959450000000	33.830533000000	33.581173000000
H	41.154851000000	34.477781000000	33.209922000000
C	41.430591000000	32.435636000000	33.911673000000
O	41.830620000000	31.812030000000	34.897103000000
N	40.512004000000	31.933211000000	33.050582000000
H	40.186136000000	32.457088000000	32.246370000000
C	40.020085000000	30.575681000000	33.185453000000
H	40.879356000000	29.910497000000	33.327717000000
C	39.063193000000	30.391277000000	34.417105000000
H	39.376679000000	31.128736000000	35.159749000000
H	38.036149000000	30.627403000000	34.121780000000
C	39.145183000000	29.006087000000	35.027327000000
C	38.104160000000	28.075395000000	34.891092000000
H	37.212616000000	28.351561000000	34.334371000000
C	38.210775000000	26.802854000000	35.463401000000
H	37.392844000000	26.094933000000	35.355331000000
C	39.355336000000	26.445591000000	36.176140000000
H	39.435601000000	25.458195000000	36.623045000000
C	40.398062000000	27.366971000000	36.315717000000
H	41.291118000000	27.097398000000	36.873660000000
C	40.294724000000	28.635282000000	35.746250000000
H	41.100995000000	29.356689000000	35.857577000000
C	39.298073000000	30.207441000000	31.885831000000
O	38.975357000000	31.055095000000	31.047564000000
N	39.039783000000	28.882327000000	31.727847000000
H	39.141449000000	28.298399000000	32.551192000000
C	38.099573000000	28.438192000000	30.721839000000
H	38.380916000000	28.873589000000	29.758481000000
C	36.648794000000	28.835590000000	31.078198000000
O	36.352595000000	29.214507000000	32.209308000000
N	35.760076000000	28.725722000000	30.058466000000
H	36.113495000000	28.479491000000	29.142519000000
C	34.382670000000	29.213428000000	30.151844000000
H	34.211391000000	29.434761000000	31.205030000000
C	34.110932000000	30.451154000000	29.272809000000
H	34.009198000000	30.136894000000	28.224633000000
H	33.133012000000	30.850163000000	29.569580000000
C	35.186783000000	31.547094000000	29.337702000000
H	36.139645000000	31.139249000000	28.974355000000
H	34.915666000000	32.354269000000	28.645968000000
C	35.434213000000	32.154197000000	30.730492000000
H	34.574440000000	32.743288000000	31.055615000000
H	35.586065000000	31.374209000000	31.479554000000
N	36.637978000000	32.988996000000	30.736143000000
H	37.517385000000	32.481202000000	30.698612000000
C	36.667164000000	34.307801000000	30.426739000000
N	35.587042000000	35.069947000000	30.596470000000
H	34.908113000000	34.805743000000	31.317223000000
H	35.692327000000	36.100850000000	30.454465000000
N	37.799721000000	34.850810000000	29.961892000000

H	38.509921000000	34.253632000000	29.564354000000
H	37.840685000000	35.880292000000	29.761742000000
C	40.222079000000	37.545153000000	35.610959000000
H	39.659669000000	38.473637000000	35.775082000000
C	39.266499000000	36.358453000000	35.439305000000
H	39.854979000000	35.449468000000	35.238030000000
H	38.749352000000	36.179700000000	36.392335000000
C	38.205029000000	36.527912000000	34.336185000000
H	37.611223000000	37.420352000000	34.575539000000
C	38.813281000000	36.741394000000	32.944247000000
H	39.508638000000	37.586694000000	32.924652000000
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H	38.036805000000	36.940343000000	32.199611000000
C	37.246856000000	35.327415000000	34.325139000000
H	36.454430000000	35.473592000000	33.582103000000
H	37.780658000000	34.400567000000	34.068865000000
H	36.775291000000	35.186465000000	35.305061000000
S	37.285450000000	45.358490000000	33.539461000000
C	32.554568000000	33.497485000000	42.256401000000
H	32.123134000000	34.447357000000	42.587002000000
H	32.548730000000	33.487395000000	41.162112000000
C	33.978333000000	33.336780000000	42.789080000000
H	34.360595000000	32.337931000000	42.522809000000
H	33.986123000000	33.409630000000	43.884351000000
N	34.836482000000	34.376808000000	42.234203000000
H	34.583616000000	34.803509000000	41.292099000000
C	36.014747000000	34.734271000000	42.727085000000
N	36.632713000000	35.820100000000	42.254196000000
H	37.649901000000	35.850580000000	42.208289000000
H	36.224223000000	36.273937000000	41.400054000000
N	36.561892000000	34.052174000000	43.777276000000
H	37.476146000000	34.339143000000	44.095894000000
H	36.344972000000	33.072372000000	43.885237000000
O	35.469908000000	38.708631000000	32.904604000000
Fe	35.882594000000	43.418867000000	33.924992000000
N	36.833119000000	42.110019000000	32.714109000000
N	36.862031000000	42.635968000000	35.493084000000
N	34.568494000000	44.263083000000	35.216896000000
N	34.625183000000	43.847630000000	32.420773000000
C	36.669574000000	41.959372000000	31.354878000000
C	37.643691000000	41.022693000000	30.814989000000
C	38.406810000000	40.637779000000	31.875594000000
C	37.904947000000	41.314150000000	33.042199000000
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C	38.480571000000	41.586836000000	36.769225000000
C	37.698063000000	42.305052000000	37.623936000000
C	36.691918000000	42.951533000000	36.826533000000
C	34.692432000000	44.353811000000	36.584771000000
C	33.651133000000	45.184167000000	37.130586000000
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C	33.478360000000	45.039780000000	34.892955000000
C	33.542156000000	44.701759000000	32.462665000000
C	33.018513000000	44.906938000000	31.140299000000
C	33.787475000000	44.167034000000	30.291547000000
C	34.780843000000	43.509148000000	31.095472000000
C	35.729876000000	42.629437000000	30.592972000000
H	35.721049000000	42.451680000000	29.523323000000
C	38.447421000000	41.177919000000	34.308003000000
H	39.307878000000	40.527117000000	34.421014000000
C	35.685246000000	43.751498000000	37.341843000000
H	35.668374000000	43.910683000000	38.415337000000
C	33.002865000000	45.260178000000	33.610203000000
H	32.139704000000	45.908423000000	33.496736000000
C	37.737038000000	40.568501000000	29.386947000000
H	38.703026000000	40.080046000000	29.223549000000
H	37.702614000000	41.438153000000	28.717210000000
C	36.620257000000	39.579665000000	28.976422000000
H	36.672723000000	39.436766000000	27.889526000000
H	35.634056000000	39.983381000000	29.221290000000
C	36.770520000000	38.194645000000	29.620328000000
O	37.799355000000	37.532627000000	29.333827000000

O	35.819853000000	37.794489000000	30.376825000000
C	34.049064000000	37.220112000000	35.157638000000
C	35.003362000000	37.979658000000	35.847489000000
C	35.300190000000	37.658901000000	37.173800000000
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C	33.696730000000	35.865330000000	37.131148000000
C	33.387547000000	36.168113000000	35.809942000000
C	35.012213000000	36.229434000000	39.251767000000
O	35.992029000000	36.828696000000	39.803179000000
O	34.294843000000	35.343241000000	39.801412000000
O	33.712874000000	37.411349000000	33.833769000000
C	34.126415000000	38.645933000000	33.179456000000
H	35.539638000000	38.777696000000	35.348208000000
H	36.046452000000	38.234132000000	37.711675000000
H	33.190185000000	35.056157000000	37.646321000000
H	32.633206000000	35.604448000000	35.268353000000
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H	35.640790000000	38.373373000000	31.987068000000
H	33.855501000000	39.465859000000	33.852143000000
O	33.835998000000	34.752287000000	32.867202000000
H	33.677085000000	35.706960000000	33.045323000000
H	34.404815000000	34.490479000000	33.608889000000
H	31.921888000000	32.681043000000	42.619046000000
H	43.072062000000	34.759233000000	40.266854000000
H	45.066352000000	36.006534000000	35.919528000000
H	42.701668000000	33.758833000000	32.774027000000
H	38.173098000000	27.349222000000	30.633698000000
H	33.694130000000	28.406511000000	29.876057000000
H	34.261238000000	30.267597000000	33.843806000000
H	41.594920000000	39.212095000000	29.621181000000
H	41.656203000000	38.244396000000	31.101830000000
H	40.589356000000	37.212019000000	42.293161000000
H	41.024229000000	38.798192000000	41.624870000000
H	33.696411000000	44.060229000000	29.218078000000
H	32.166694000000	45.533015000000	30.906767000000
H	32.027091000000	46.254544000000	36.089466000000
H	33.528041000000	45.403361000000	38.183614000000
H	39.239503000000	39.945828000000	31.875287000000
H	39.333361000000	40.961196000000	36.999120000000
H	37.776501000000	42.389040000000	38.700383000000
H	38.113162000000	45.132182000000	34.584854000000
H	40.878511000000	37.393290000000	36.473710000000
H	40.858448000000	37.689232000000	34.730064000000

²TransitionState2_mut / LS_TS2_mut

C	-5.652832000000	6.038667000000	-3.175725000000
H	-4.663987000000	5.578083000000	-3.253126000000
C	-5.582214000000	7.534983000000	-2.851857000000
H	-5.086878000000	8.070225000000	-3.675897000000
H	-6.605445000000	7.935929000000	-2.804068000000
C	-4.856973000000	7.877011000000	-1.534444000000
H	-5.279427000000	7.234221000000	-0.745400000000
C	-3.345217000000	7.608810000000	-1.609788000000
H	-2.858695000000	7.880639000000	-0.663888000000
H	-3.099605000000	6.562154000000	-1.820626000000
H	-2.887243000000	8.224309000000	-2.396599000000
C	-5.119041000000	9.338891000000	-1.138637000000
H	-4.629694000000	9.590361000000	-0.189623000000
H	-4.730442000000	10.025984000000	-1.902233000000
H	-6.192093000000	9.539190000000	-1.027880000000
C	6.327661000000	-1.447598000000	2.879956000000
H	6.136043000000	-1.802264000000	3.900092000000
H	5.509431000000	-1.818212000000	2.248551000000
C	7.677403000000	-1.915773000000	2.388470000000
C	8.597986000000	-1.022096000000	1.822356000000
H	8.330184000000	0.029180000000	1.745776000000
C	9.846341000000	-1.456021000000	1.365664000000
H	10.548310000000	-0.738341000000	0.946964000000
C	10.200646000000	-2.803535000000	1.463491000000
H	11.175914000000	-3.142528000000	1.123733000000
C	9.293432000000	-3.709100000000	2.025212000000

H	9.563185000000	-4.757970000000	2.124902000000
C	8.049199000000	-3.267092000000	2.481125000000
H	7.355025000000	-3.978354000000	2.922718000000
C	2.595399000000	-4.189984000000	-4.749993000000
H	1.735276000000	-4.743778000000	-4.357063000000
C	2.803881000000	-2.911317000000	-3.943469000000
H	3.630954000000	-2.338586000000	-4.402379000000
C	1.550122000000	-2.031734000000	-3.928791000000
H	0.700856000000	-2.595680000000	-3.526271000000
H	1.713250000000	-1.143891000000	-3.306839000000
H	1.294244000000	-1.696736000000	-4.942231000000
O	3.178512000000	-3.302016000000	-2.623523000000
H	3.244432000000	-2.487329000000	-2.076650000000
C	0.306169000000	-6.316141000000	-1.550037000000
H	0.009546000000	-7.171060000000	-0.924601000000
C	0.838735000000	-5.171277000000	-0.664429000000
H	1.217200000000	-4.391876000000	-1.334211000000
C	-0.260030000000	-4.572345000000	0.224903000000
H	-1.065901000000	-4.137826000000	-0.376104000000
H	-0.703445000000	-5.329706000000	0.885703000000
H	0.151501000000	-3.775662000000	0.855404000000
C	2.019207000000	-5.666322000000	0.182013000000
H	2.792549000000	-6.123646000000	-0.447935000000
H	2.475335000000	-4.828202000000	0.720062000000
H	1.698577000000	-6.417732000000	0.917542000000
C	-0.846393000000	-5.902048000000	-2.456634000000
O	-0.895017000000	-4.819939000000	-3.032735000000
N	-1.848214000000	-6.839188000000	-2.593781000000
H	-1.718584000000	-7.747211000000	-2.170459000000
C	-2.994392000000	-6.622552000000	-3.456799000000
H	-2.746391000000	-5.803004000000	-4.135451000000
C	-4.303302000000	-6.236200000000	-2.750570000000
O	-5.309770000000	-5.972723000000	-3.403054000000
N	-4.257469000000	-6.218226000000	-1.395983000000
H	-3.376375000000	-6.348838000000	-0.912461000000
C	-5.339669000000	-5.698428000000	-0.591533000000
H	-5.891738000000	-4.945991000000	-1.162693000000
C	-4.739220000000	-5.137862000000	0.698928000000
O	-3.705792000000	-5.614567000000	1.173850000000
N	-5.417472000000	-4.121148000000	1.275798000000
H	-6.272985000000	-3.745245000000	0.880842000000
C	-5.015758000000	-3.558590000000	2.550895000000
H	-4.802796000000	-4.382031000000	3.242601000000
C	-3.723982000000	-2.680916000000	2.432816000000
H	-3.096290000000	-3.175532000000	1.686528000000
H	-3.981002000000	-1.687907000000	2.048946000000
C	-2.947673000000	-2.579609000000	3.730416000000
C	-2.971788000000	-1.418521000000	4.518959000000
H	-3.561501000000	-0.564336000000	4.196393000000
C	-2.247992000000	-1.358778000000	5.715381000000
H	-2.270353000000	-0.449833000000	6.311014000000
C	-1.491908000000	-2.453457000000	6.136804000000
H	-0.926591000000	-2.403758000000	7.063707000000
C	-1.462341000000	-3.614205000000	5.356865000000
H	-0.871186000000	-4.468981000000	5.675155000000
C	-2.184598000000	-3.676418000000	4.165897000000
H	-2.156505000000	-4.575041000000	3.553584000000
C	-6.209004000000	-2.745517000000	3.066090000000
O	-7.179955000000	-2.489355000000	2.352528000000
N	-6.126670000000	-2.330346000000	4.359047000000
H	-5.218283000000	-2.365165000000	4.807333000000
C	-7.082478000000	-1.360983000000	4.851055000000
H	-8.092898000000	-1.768787000000	4.748055000000
C	-6.957888000000	-0.004828000000	4.129723000000
O	-5.869915000000	0.443310000000	3.783678000000
N	-8.135022000000	0.659575000000	3.974118000000
H	-8.992624000000	0.158197000000	4.163234000000
C	-8.238432000000	1.943032000000	3.291507000000
H	-7.223860000000	2.344244000000	3.237841000000
C	-8.877500000000	1.838752000000	1.897939000000
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H	-9.045942000000	2.861075000000	1.531570000000
C	-8.080933000000	1.049382000000	0.845845000000
H	-7.935583000000	0.011655000000	1.168189000000
H	-8.703325000000	1.012591000000	-0.060195000000
C	-6.724576000000	1.690564000000	0.501860000000
H	-6.773962000000	2.780687000000	0.639187000000
H	-5.946799000000	1.307194000000	1.168352000000
N	-6.367002000000	1.410679000000	-0.898830000000
H	-7.108225000000	1.045869000000	-1.482019000000
C	-5.376476000000	2.078391000000	-1.554544000000
N	-4.335927000000	2.553152000000	-0.870047000000
H	-4.039111000000	2.049962000000	-0.030372000000
H	-3.630608000000	3.120303000000	-1.397679000000
N	-5.454814000000	2.267379000000	-2.871365000000
H	-6.329929000000	2.114820000000	-3.350845000000
H	-4.614278000000	2.625327000000	-3.422134000000
C	-4.790417000000	-2.892551000000	-5.531322000000
H	-5.729008000000	-2.322278000000	-5.550402000000
C	-3.641850000000	-2.042500000000	-4.971775000000
H	-2.720495000000	-2.642489000000	-4.940326000000
H	-3.443422000000	-1.212549000000	-5.664496000000
C	-3.889976000000	-1.451894000000	-3.568738000000
H	-4.840438000000	-0.894637000000	-3.604194000000
C	-4.016447000000	-2.542992000000	-2.495338000000
H	-4.835596000000	-3.234428000000	-2.719237000000
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C	-2.779987000000	-0.455226000000	-3.203982000000
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H	-1.797411000000	-0.944993000000	-3.221117000000
H	-2.757515000000	0.391862000000	-3.898583000000
S	4.314308000000	5.359346000000	-0.797688000000
C	6.088912000000	-5.877832000000	0.154881000000
H	7.030049000000	-5.641686000000	0.664239000000
H	5.277912000000	-5.788968000000	0.885207000000
C	5.850695000000	-4.949188000000	-1.037496000000
H	4.918664000000	-5.205425000000	-1.552326000000
H	6.659811000000	-5.038218000000	-1.768743000000
N	5.729885000000	-3.542802000000	-0.656032000000
H	4.838457000000	-3.216271000000	-0.217775000000
C	6.578985000000	-2.578888000000	-0.990743000000
N	6.144464000000	-1.326643000000	-1.103836000000
H	6.772563000000	-0.536921000000	-1.018063000000
H	5.116386000000	-1.142156000000	-1.101428000000
N	7.885433000000	-2.882389000000	-1.277984000000
H	8.480026000000	-2.091499000000	-1.487316000000
H	8.326216000000	-3.543499000000	-0.648532000000
O	2.926859000000	1.863993000000	0.881197000000
Fe	3.528442000000	3.346654000000	0.230322000000
N	2.681005000000	2.966804000000	-1.590010000000
N	5.277354000000	2.606355000000	-0.421027000000
N	4.376963000000	3.800882000000	1.983312000000
N	1.869342000000	4.371177000000	0.748746000000
C	1.381414000000	3.200388000000	-1.971845000000
C	1.136737000000	2.653930000000	-3.306075000000
C	2.336874000000	2.154333000000	-3.716021000000
C	3.286889000000	2.352381000000	-2.649742000000
C	5.547174000000	2.140809000000	-1.685793000000
C	6.939992000000	1.781914000000	-1.789064000000
C	7.499999000000	2.012164000000	-0.564173000000
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C	5.642049000000	3.478706000000	2.401948000000
C	5.850235000000	3.933708000000	3.757098000000
C	4.707091000000	4.563452000000	4.138594000000
C	3.796388000000	4.489798000000	3.019736000000
C	1.661001000000	5.049915000000	1.918971000000
C	0.361374000000	5.677337000000	1.903130000000
C	-0.224035000000	5.338616000000	0.718855000000
C	0.724042000000	4.514117000000	0.008268000000
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H	2.238747000000	5.642324000000	3.873314000000
C	-0.177524000000	2.530208000000	-4.027124000000
H	-0.785727000000	1.795752000000	-3.482827000000
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C	-1.030155000000	3.826536000000	-4.232045000000
H	-1.181357000000	3.996437000000	-5.301364000000
H	-0.519366000000	4.699293000000	-3.816760000000
C	-2.396801000000	3.642622000000	-3.557993000000
O	-3.299223000000	3.083574000000	-4.241531000000
O	-2.496246000000	3.990894000000	-2.338540000000
C	-0.030091000000	0.682162000000	2.243523000000
C	0.459698000000	1.217271000000	1.071202000000
C	1.631635000000	0.654867000000	0.448538000000
C	2.127480000000	-0.598365000000	0.971924000000
C	1.615611000000	-1.098122000000	2.163753000000
C	0.551734000000	-0.469652000000	2.816554000000
C	3.146591000000	-1.389627000000	0.203716000000
O	3.421400000000	-0.996150000000	-0.979470000000
O	3.653542000000	-2.405095000000	0.763140000000
O	-1.144716000000	1.184325000000	2.899982000000
C	-1.284659000000	2.610702000000	2.932233000000
H	0.009867000000	2.092886000000	0.622609000000
H	1.761415000000	0.804756000000	-0.616492000000
H	2.039082000000	-2.015317000000	2.558947000000
H	0.140875000000	-0.859832000000	3.741922000000
H	-2.053036000000	2.817262000000	3.680929000000
H	-1.606731000000	3.011112000000	1.965605000000
H	-0.339852000000	3.081743000000	3.218598000000
O	-3.263074000000	0.631632000000	1.053817000000
H	-2.661004000000	0.758607000000	1.816543000000
H	-2.726856000000	0.146509000000	0.406689000000
H	6.130751000000	-6.920241000000	-0.181454000000
H	1.118406000000	-6.667867000000	-2.202013000000
H	-3.193170000000	-7.512098000000	-4.064293000000
H	-6.056223000000	-6.489717000000	-0.321852000000
H	-6.888155000000	-1.203282000000	5.916838000000
H	-8.832345000000	2.625880000000	3.911810000000
H	6.264239000000	-0.354656000000	2.888539000000
H	-6.174321000000	5.867928000000	-4.125390000000
H	-6.201224000000	5.496894000000	-2.393987000000
H	3.483839000000	-4.829294000000	-4.692086000000
H	2.402759000000	-3.958794000000	-5.804097000000
H	-1.198333000000	5.611387000000	0.334091000000
H	-0.036086000000	6.290019000000	2.702848000000
H	4.486695000000	5.051594000000	5.079555000000
H	6.766203000000	3.797946000000	4.318248000000
H	2.561116000000	1.664473000000	-4.655781000000
H	7.414377000000	1.421450000000	-2.693821000000
H	8.531325000000	1.886482000000	-0.257822000000
H	3.146828000000	6.037582000000	-0.842141000000
H	-4.576280000000	-3.202154000000	-6.561505000000
H	-4.965074000000	-3.801961000000	-4.946125000000

⁴TransitionState2_mut / HS_TS2_mut

C	-5.652832000000	6.038667000000	-3.175725000000
H	-4.663987000000	5.578083000000	-3.253126000000
C	-5.582214000000	7.534983000000	-2.851857000000
H	-5.086878000000	8.070225000000	-3.675897000000
H	-6.605445000000	7.935929000000	-2.804068000000
C	-4.856973000000	7.877011000000	-1.534444000000
H	-5.279427000000	7.234221000000	-0.745400000000
C	-3.345217000000	7.608810000000	-1.609788000000
H	-2.858695000000	7.880639000000	-0.663888000000
H	-3.099605000000	6.562154000000	-1.820626000000
H	-2.887243000000	8.224309000000	-2.396599000000
C	-5.119041000000	9.338891000000	-1.138637000000

H	-4.629694000000	9.590361000000	-0.189623000000
H	-4.730442000000	10.025984000000	-1.902233000000
H	-6.192093000000	9.539190000000	-1.027880000000
C	6.327661000000	-1.447598000000	2.879956000000
H	6.136043000000	-1.802264000000	3.900092000000
H	5.509431000000	-1.818212000000	2.248551000000
C	7.677403000000	-1.915773000000	2.388470000000
C	8.597986000000	-1.022096000000	1.822356000000
H	8.330184000000	0.029180000000	1.745776000000
C	9.846341000000	-1.456021000000	1.365664000000
H	10.548310000000	-0.738341000000	0.946964000000
C	10.200646000000	-2.803535000000	1.463491000000
H	11.175914000000	-3.142528000000	1.123733000000
C	9.293432000000	-3.709100000000	2.025212000000
H	9.563185000000	-4.757970000000	2.124902000000
C	8.049199000000	-3.267092000000	2.481125000000
H	7.355025000000	-3.978354000000	2.922718000000
C	2.595399000000	-4.189984000000	-4.749993000000
H	1.735276000000	-4.743778000000	-4.357063000000
C	2.803881000000	-2.911317000000	-3.943469000000
H	3.630954000000	-2.338586000000	-4.402379000000
C	1.550122000000	-2.031734000000	-3.928791000000
H	0.700856000000	-2.595680000000	-3.526271000000
H	1.713250000000	-1.143891000000	-3.306839000000
H	1.294244000000	-1.696736000000	-4.942231000000
O	3.178512000000	-3.302016000000	-2.623523000000
H	3.244432000000	-2.487329000000	-2.076650000000
C	0.306169000000	-6.316141000000	-1.550037000000
H	0.009546000000	-7.171060000000	-0.924601000000
C	0.838735000000	-5.171277000000	-0.664429000000
H	1.217200000000	-4.391876000000	-1.334211000000
C	-0.260030000000	-4.572345000000	0.224903000000
H	-1.065901000000	-4.137826000000	-0.376104000000
H	-0.703445000000	-5.329706000000	0.885703000000
H	0.151501000000	-3.775662000000	0.855404000000
C	2.019207000000	-5.666322000000	0.182013000000
H	2.792549000000	-6.123646000000	-0.447935000000
H	2.475335000000	-4.828202000000	0.720062000000
H	1.698577000000	-6.417732000000	0.917542000000
C	-0.846393000000	-5.902048000000	-2.456634000000
O	-0.895017000000	-4.819939000000	-3.032735000000
N	-1.848214000000	-6.839188000000	-2.593781000000
H	-1.718584000000	-7.747211000000	-2.170459000000
C	-2.994392000000	-6.622552000000	-3.456799000000
H	-2.746391000000	-5.803004000000	-4.135451000000
C	-4.303302000000	-6.236200000000	-2.750570000000
O	-5.309770000000	-5.972723000000	-3.403054000000
N	-4.257469000000	-6.218226000000	-1.395983000000
H	-3.376375000000	-6.348838000000	-0.912461000000
C	-5.339669000000	-5.698428000000	-0.591533000000
H	-5.891738000000	-4.945991000000	-1.162693000000
C	-4.739220000000	-5.137862000000	0.698928000000
O	-3.705792000000	-5.614567000000	1.173850000000
N	-5.417472000000	-4.121148000000	1.275798000000
H	-6.272985000000	-3.745245000000	0.880842000000
C	-5.015758000000	-3.558590000000	2.550895000000
H	-4.802796000000	-4.382031000000	3.242601000000
C	-3.723982000000	-2.680916000000	2.432816000000
H	-3.096290000000	-3.175532000000	1.686528000000
H	-3.981002000000	-1.687907000000	2.048946000000
C	-2.947673000000	-2.579609000000	3.730416000000
C	-2.971788000000	-1.418521000000	4.518959000000
H	-3.561501000000	-0.564336000000	4.196393000000
C	-2.247992000000	-1.358778000000	5.715381000000
H	-2.270353000000	-0.449833000000	6.311014000000
C	-1.491908000000	-2.453457000000	6.136804000000
H	-0.926591000000	-2.403758000000	7.063707000000
C	-1.462341000000	-3.614205000000	5.356865000000
H	-0.871186000000	-4.468981000000	5.675155000000
C	-2.184598000000	-3.676418000000	4.165897000000
H	-2.156505000000	-4.575041000000	3.553584000000

C	-6.209004000000	-2.745517000000	3.066090000000
O	-7.179955000000	-2.489355000000	2.352528000000
N	-6.126670000000	-2.330346000000	4.359047000000
H	-5.218283000000	-2.365165000000	4.807333000000
C	-7.082478000000	-1.360983000000	4.851055000000
H	-8.092898000000	-1.768787000000	4.748055000000
C	-6.957888000000	-0.004828000000	4.129723000000
O	-5.869915000000	0.443310000000	3.783678000000
N	-8.135022000000	0.659575000000	3.974118000000
H	-8.992624000000	0.158197000000	4.163234000000
C	-8.238432000000	1.943032000000	3.291507000000
H	-7.223860000000	2.344244000000	3.237841000000
C	-8.877500000000	1.838752000000	1.897939000000
H	-9.873541000000	1.385338000000	1.999990000000
H	-9.045942000000	2.861075000000	1.531570000000
C	-8.080933000000	1.049382000000	0.845845000000
H	-7.935583000000	0.011655000000	1.168189000000
H	-8.703325000000	1.012591000000	-0.060195000000
C	-6.724576000000	1.690564000000	0.501860000000
H	-6.773962000000	2.780687000000	0.639187000000
H	-5.946799000000	1.307194000000	1.168352000000
N	-6.367002000000	1.410679000000	-0.898830000000
H	-7.108225000000	1.045869000000	-1.482019000000
C	-5.376476000000	2.078391000000	-1.554544000000
N	-4.335927000000	2.553152000000	-0.870047000000
H	-4.039111000000	2.049962000000	-0.030372000000
H	-3.630608000000	3.120303000000	-1.397679000000
N	-5.454814000000	2.267379000000	-2.871365000000
H	-6.329929000000	2.114820000000	-3.350845000000
H	-4.614278000000	2.625327000000	-3.422134000000
C	-4.790417000000	-2.892551000000	-5.531322000000
H	-5.729008000000	-2.322278000000	-5.550402000000
C	-3.641850000000	-2.042500000000	-4.971775000000
H	-2.720495000000	-2.642489000000	-4.940326000000
H	-3.443422000000	-1.212549000000	-5.664496000000
C	-3.889976000000	-1.451894000000	-3.568738000000
H	-4.840438000000	-0.894637000000	-3.604194000000
C	-4.016447000000	-2.542992000000	-2.495338000000
H	-4.835596000000	-3.234428000000	-2.719237000000
H	-3.090198000000	-3.129367000000	-2.433457000000
H	-4.206781000000	-2.102509000000	-1.507196000000
C	-2.779987000000	-0.455226000000	-3.203982000000
H	-2.931226000000	-0.045124000000	-2.195896000000
H	-1.797411000000	-0.944993000000	-3.221117000000
H	-2.757515000000	0.391862000000	-3.898583000000
S	4.314308000000	5.359346000000	-0.797688000000
C	6.088912000000	-5.877832000000	0.154881000000
H	7.030049000000	-5.641686000000	0.664239000000
H	5.277912000000	-5.788968000000	0.885207000000
C	5.850695000000	-4.949188000000	-1.037496000000
H	4.918664000000	-5.205425000000	-1.552326000000
H	6.659811000000	-5.038218000000	-1.768743000000
N	5.729885000000	-3.542802000000	-0.656032000000
H	4.838457000000	-3.216271000000	-0.217775000000
C	6.578985000000	-2.578888000000	-0.990743000000
N	6.144464000000	-1.326643000000	-1.103836000000
H	6.772563000000	-0.536921000000	-1.018063000000
H	5.116386000000	-1.142156000000	-1.101428000000
N	7.885433000000	-2.882389000000	-1.277984000000
H	8.480026000000	-2.091499000000	-1.487316000000
H	8.326216000000	-3.543499000000	-0.648532000000
O	2.926859000000	1.863993000000	0.881197000000
Fe	3.528442000000	3.346654000000	0.230322000000
N	2.681005000000	2.966804000000	-1.590010000000
N	5.277354000000	2.606355000000	-0.421027000000
N	4.376963000000	3.800882000000	1.983312000000
N	1.869342000000	4.371177000000	0.748746000000
C	1.381414000000	3.200388000000	-1.971845000000
C	1.136737000000	2.653930000000	-3.306075000000
C	2.336874000000	2.154333000000	-3.716021000000
C	3.286889000000	2.352381000000	-2.649742000000

C	5.547174000000	2.140809000000	-1.685793000000
C	6.939992000000	1.781914000000	-1.789064000000
C	7.499999000000	2.012164000000	-0.564173000000
C	6.451246000000	2.525454000000	0.282514000000
C	5.642049000000	3.478706000000	2.401948000000
C	5.850235000000	3.933708000000	3.757098000000
C	4.707091000000	4.563452000000	4.138594000000
C	3.796388000000	4.489798000000	3.019736000000
C	1.661001000000	5.049915000000	1.918971000000
C	0.361374000000	5.677337000000	1.903130000000
C	-0.224035000000	5.338616000000	0.718855000000
C	0.724042000000	4.514117000000	0.008268000000
C	0.462200000000	3.929086000000	-1.228205000000
H	-0.540122000000	4.069347000000	-1.629201000000
C	4.624813000000	1.989882000000	-2.711596000000
H	4.980069000000	1.554746000000	-3.640429000000
C	6.619133000000	2.888492000000	1.613918000000
H	7.600993000000	2.744465000000	2.054689000000
C	2.547570000000	5.090428000000	2.990577000000
H	2.238747000000	5.642324000000	3.873314000000
C	-0.177524000000	2.530208000000	-4.027124000000
H	-0.785727000000	1.795752000000	-3.482827000000
H	0.022603000000	2.070521000000	-5.000420000000
C	-1.030155000000	3.826536000000	-4.232045000000
H	-1.181357000000	3.996437000000	-5.301364000000
H	-0.519366000000	4.699293000000	-3.816760000000
C	-2.396801000000	3.642622000000	-3.557993000000
O	-3.299223000000	3.083574000000	-4.241531000000
O	-2.496246000000	3.990894000000	-2.338540000000
C	-0.030091000000	0.682162000000	2.243523000000
C	0.459698000000	1.217271000000	1.071202000000
C	1.631635000000	0.654867000000	0.448538000000
C	2.127480000000	-0.598365000000	0.971924000000
C	1.615611000000	-1.098122000000	2.163753000000
C	0.551734000000	-0.469652000000	2.816554000000
C	3.146591000000	-1.389627000000	0.203716000000
O	3.421400000000	-0.996150000000	-0.979470000000
O	3.653542000000	-2.405095000000	0.763140000000
O	-1.144716000000	1.184325000000	2.899982000000
C	-1.284659000000	2.610702000000	2.932233000000
H	0.009867000000	2.092886000000	0.622609000000
H	1.761415000000	0.804756000000	-0.616492000000
H	2.039082000000	-2.015317000000	2.558947000000
H	0.140875000000	-0.859832000000	3.741922000000
H	-2.053036000000	2.817262000000	3.680929000000
H	-1.606731000000	3.011112000000	1.965605000000
H	-0.339852000000	3.081743000000	3.218598000000
O	-3.263074000000	0.631632000000	1.053817000000
H	-2.661004000000	0.758607000000	1.816543000000
H	-2.726856000000	0.146509000000	0.406689000000
H	6.130751000000	-6.920241000000	-0.181454000000
H	1.118406000000	-6.667867000000	-2.202013000000
H	-3.193170000000	-7.512098000000	-4.064293000000
H	-6.056223000000	-6.489717000000	-0.321852000000
H	-6.888155000000	-1.203282000000	5.916838000000
H	-8.832345000000	2.625880000000	3.911810000000
H	6.264239000000	-0.354656000000	2.888539000000
H	-6.174321000000	5.867928000000	-4.125390000000
H	-6.201224000000	5.496894000000	-2.393987000000
H	3.483839000000	-4.829294000000	-4.692086000000
H	2.402759000000	-3.958794000000	-5.804097000000
H	-1.198333000000	5.611387000000	0.334091000000
H	-0.036086000000	6.290019000000	2.702848000000
H	4.486695000000	5.051594000000	5.079555000000
H	6.766203000000	3.797946000000	4.318248000000
H	2.561116000000	1.664473000000	-4.655781000000
H	7.414377000000	1.421450000000	-2.693821000000
H	8.531325000000	1.886482000000	-0.257822000000
H	3.146828000000	6.037582000000	-0.842141000000
H	-4.576280000000	-3.202154000000	-6.561505000000
H	-4.965074000000	-3.801961000000	-4.946125000000

²Intermediate2_mut / LS_I2_mut

C	41.063916000000	37.792469000000	26.480593000000
H	40.841861000000	38.095302000000	27.508404000000
C	40.352769000000	38.665151000000	25.439393000000
H	40.653623000000	39.715053000000	25.574162000000
H	40.702261000000	38.377414000000	24.436920000000
C	38.812810000000	38.583245000000	25.460449000000
H	38.537839000000	37.518394000000	25.386035000000
C	38.210765000000	39.138025000000	26.760675000000
H	37.114841000000	39.081757000000	26.734749000000
H	38.547868000000	38.597546000000	27.650712000000
H	38.479537000000	40.195619000000	26.888743000000
C	38.220231000000	39.305529000000	24.240343000000
H	37.126687000000	39.222134000000	24.219616000000
H	38.468746000000	40.375000000000	24.261129000000
H	38.607549000000	38.892894000000	23.300248000000
C	32.191739000000	36.750111000000	40.020805000000
H	31.941641000000	35.788773000000	40.482409000000
H	33.210885000000	36.670083000000	39.619443000000
C	32.068542000000	37.880820000000	41.014981000000
C	31.896905000000	39.205278000000	40.581668000000
H	31.842918000000	39.409124000000	39.514674000000
C	31.791282000000	40.256654000000	41.495149000000
H	31.638424000000	41.271460000000	41.134410000000
C	31.858977000000	40.007973000000	42.869398000000
H	31.760282000000	40.823086000000	43.581729000000
C	32.031915000000	38.695300000000	43.317312000000
H	32.065641000000	38.482929000000	44.383358000000
C	32.131325000000	37.646671000000	42.397119000000
H	32.243948000000	36.626251000000	42.756752000000
C	41.028197000000	37.845248000000	39.823322000000
H	41.318210000000	36.798188000000	39.681085000000
C	39.881628000000	38.202192000000	38.882037000000
H	39.657503000000	39.278895000000	38.994251000000
C	40.233773000000	37.926027000000	37.417273000000
H	40.510007000000	36.873123000000	37.289845000000
H	39.378983000000	38.149870000000	36.768236000000
H	41.079169000000	38.546622000000	37.093171000000
O	38.746013000000	37.441379000000	39.292841000000
H	38.016402000000	37.631625000000	38.662966000000
C	40.272134000000	33.400468000000	39.775984000000
H	40.148476000000	32.372229000000	40.146600000000
C	38.957535000000	33.897829000000	39.140453000000
H	39.102845000000	34.949130000000	38.870413000000
C	38.599794000000	33.106219000000	37.874865000000
H	39.369915000000	33.219013000000	37.104526000000
H	38.489219000000	32.034154000000	38.086505000000
H	37.653348000000	33.465481000000	37.454081000000
C	37.817824000000	33.837454000000	40.166444000000
H	38.089068000000	34.363153000000	41.090718000000
H	36.917972000000	34.313610000000	39.761310000000
H	37.570156000000	32.800004000000	40.432097000000
C	41.467763000000	33.482948000000	38.834219000000
O	41.653906000000	34.421714000000	38.066764000000
N	42.342507000000	32.420044000000	38.901552000000
H	42.185856000000	31.709872000000	39.602807000000
C	43.545345000000	32.356300000000	38.091856000000
H	43.740724000000	33.363319000000	37.715341000000
C	43.483876000000	31.425640000000	36.869685000000
O	44.440879000000	31.332377000000	36.106263000000
N	42.324757000000	30.741577000000	36.712950000000
H	41.538149000000	30.917379000000	37.326994000000
C	42.032924000000	29.962135000000	35.532377000000
H	42.482415000000	30.433696000000	34.652523000000
C	40.512024000000	29.850749000000	35.411895000000
O	39.788535000000	29.936247000000	36.407166000000
N	40.027957000000	29.643320000000	34.166859000000
H	40.628244000000	29.566888000000	33.352656000000
C	38.611278000000	29.447320000000	33.925898000000
H	38.228831000000	28.733603000000	34.664443000000

C	37.794514000000	30.777101000000	34.068780000000
H	38.294680000000	31.351102000000	34.853506000000
H	37.856094000000	31.355948000000	33.141260000000
C	36.352007000000	30.554140000000	34.475182000000
C	35.295800000000	30.688664000000	33.560417000000
H	35.512079000000	30.954637000000	32.528996000000
C	33.973397000000	30.478574000000	33.969186000000
H	33.165328000000	30.595170000000	33.251654000000
C	33.690950000000	30.134432000000	35.291773000000
H	32.663322000000	29.977629000000	35.608735000000
C	34.738118000000	29.996813000000	36.208982000000
H	34.525728000000	29.733617000000	37.241937000000
C	36.056265000000	30.203165000000	35.803665000000
H	36.872620000000	30.102056000000	36.515306000000
C	38.478099000000	28.859525000000	32.517269000000
O	39.418403000000	28.851451000000	31.722643000000
N	37.255041000000	28.345676000000	32.208507000000
H	36.475668000000	28.605031000000	32.802652000000
C	36.961716000000	28.006549000000	30.832539000000
H	37.716717000000	27.301455000000	30.472211000000
C	36.901006000000	29.253584000000	29.929081000000
O	36.512172000000	30.337231000000	30.352142000000
N	37.258859000000	29.032968000000	28.635253000000
H	37.673897000000	28.141916000000	28.397710000000
C	37.286389000000	30.088581000000	27.630467000000
H	36.743892000000	30.932645000000	28.061678000000
C	38.708467000000	30.490255000000	27.210752000000
H	39.218296000000	29.607873000000	26.799084000000
H	38.620722000000	31.204523000000	26.380432000000
C	39.592961000000	31.099130000000	28.311130000000
H	39.738245000000	30.382117000000	29.128448000000
H	40.581243000000	31.274374000000	27.862615000000
C	39.057762000000	32.428386000000	28.872608000000
H	38.517898000000	32.983541000000	28.092865000000
H	38.356192000000	32.241329000000	29.691694000000
N	40.173408000000	33.264923000000	29.337383000000
H	41.106081000000	32.890108000000	29.238734000000
C	40.075984000000	34.602938000000	29.547625000000
N	38.891065000000	35.141430000000	29.836003000000
H	38.214917000000	34.576166000000	30.354041000000
H	38.842796000000	36.185908000000	29.922292000000
N	41.161310000000	35.373799000000	29.452283000000
H	41.974531000000	35.032937000000	28.960695000000
H	41.129256000000	36.395581000000	29.747375000000
C	44.956675000000	34.581774000000	33.921747000000
H	45.171761000000	34.181573000000	32.921853000000
C	43.685576000000	35.441347000000	33.909198000000
H	43.486364000000	35.816275000000	34.924019000000
H	43.860600000000	36.328667000000	33.284857000000
C	42.420669000000	34.726007000000	33.392169000000
H	42.648450000000	34.332050000000	32.388031000000
C	42.017004000000	33.546655000000	34.288661000000
H	42.816778000000	32.802530000000	34.361076000000
H	41.790141000000	33.893026000000	35.305597000000
H	41.121796000000	33.044758000000	33.896399000000
C	41.259531000000	35.720462000000	33.249605000000
H	40.356036000000	35.219872000000	32.874292000000
H	41.010497000000	36.167738000000	34.221115000000
H	41.501543000000	36.527434000000	32.549342000000
S	33.827630000000	41.912475000000	33.317468000000
C	35.831750000000	36.060543000000	42.898917000000
H	34.875430000000	36.465363000000	43.248525000000
H	35.618227000000	35.237413000000	42.209304000000
C	36.674255000000	37.138267000000	42.212999000000
H	37.632980000000	36.727717000000	41.878071000000
H	36.896019000000	37.958255000000	42.902602000000
N	36.031300000000	37.696779000000	41.025743000000
H	36.000265000000	37.124652000000	40.153814000000
C	35.621861000000	38.951201000000	40.884165000000
N	35.558008000000	39.492568000000	39.670644000000
H	34.949297000000	40.277955000000	39.472150000000

H	35.962659000000	38.982231000000	38.856996000000
N	35.322397000000	39.707270000000	41.988949000000
H	34.970511000000	40.635457000000	41.794545000000
H	34.781220000000	39.233433000000	42.703351000000
O	34.304976000000	38.115496000000	35.178862000000
Fe	34.206939000000	39.789741000000	34.309398000000
N	36.200105000000	40.010196000000	34.173377000000
N	34.179552000000	40.744170000000	36.099652000000
N	32.189219000000	39.596335000000	34.433821000000
N	34.194201000000	39.040987000000	32.447695000000
C	37.042119000000	39.567860000000	33.175826000000
C	38.436179000000	39.839178000000	33.519928000000
C	38.387817000000	40.513024000000	34.704236000000
C	37.005519000000	40.617799000000	35.101241000000
C	35.249149000000	41.351835000000	36.690115000000
C	34.827875000000	42.073951000000	37.869408000000
C	33.483218000000	41.865395000000	37.992837000000
C	33.093166000000	41.033640000000	36.876985000000
C	31.374131000000	39.938868000000	35.478507000000
C	30.002889000000	39.581662000000	35.188045000000
C	30.001264000000	39.039929000000	33.940635000000
C	31.372217000000	39.066080000000	33.477621000000
C	33.080948000000	38.678627000000	31.724363000000
C	33.466782000000	38.280026000000	30.390781000000
C	34.824605000000	38.386583000000	30.323865000000
C	35.265276000000	38.858242000000	31.615814000000
C	36.604168000000	39.032023000000	31.971180000000
H	37.347802000000	38.730036000000	31.235299000000
C	36.566949000000	41.267828000000	36.246715000000
H	37.323975000000	41.756166000000	36.853356000000
C	31.788810000000	40.619891000000	36.616341000000
H	31.024623000000	40.894960000000	37.338173000000
C	31.780765000000	38.656770000000	32.210096000000
H	31.007518000000	38.304370000000	31.533028000000
C	39.679779000000	39.371518000000	32.812228000000
H	39.745198000000	38.282567000000	32.936089000000
H	40.537152000000	39.773234000000	33.362274000000
C	39.841863000000	39.710905000000	31.292593000000
H	40.761699000000	40.282429000000	31.144416000000
H	39.003407000000	40.317272000000	30.938519000000
C	39.931567000000	38.411026000000	30.480893000000
O	41.084895000000	37.934580000000	30.281368000000
O	38.836026000000	37.868783000000	30.132433000000
C	34.949736000000	34.993983000000	33.848838000000
C	35.196539000000	36.337838000000	33.816264000000
C	35.366069000000	37.163834000000	35.060460000000
C	35.382654000000	36.333375000000	36.314043000000
C	35.078138000000	34.985755000000	36.291238000000
C	34.860681000000	34.306587000000	35.085896000000
C	35.808069000000	36.946110000000	37.622458000000
O	36.538263000000	37.986984000000	37.565543000000
O	35.459530000000	36.353568000000	38.684275000000
O	34.768411000000	34.195958000000	32.727689000000
C	34.364627000000	34.853665000000	31.522730000000
H	35.228914000000	36.873031000000	32.881012000000
H	36.330901000000	37.700030000000	35.000979000000
H	35.033607000000	34.449291000000	37.232929000000
H	34.626521000000	33.246297000000	35.074896000000
H	34.093329000000	34.056863000000	30.827052000000
H	35.178829000000	35.448936000000	31.095696000000
H	33.504205000000	35.504452000000	31.707577000000
O	37.452736000000	33.608424000000	31.879719000000
H	36.514586000000	33.618043000000	32.161433000000
H	37.924948000000	34.042008000000	32.608183000000
H	36.370671000000	35.651665000000	43.761313000000
H	40.505337000000	34.025404000000	40.649784000000
H	44.404854000000	32.053252000000	38.699333000000
H	42.454898000000	28.948002000000	35.605166000000
H	35.988107000000	27.506340000000	30.802260000000
H	36.729367000000	29.752989000000	26.746703000000
H	31.522372000000	36.900848000000	39.166664000000

H	42.152090000000	37.845805000000	26.352305000000
H	40.768669000000	36.739760000000	26.374373000000
H	40.726165000000	37.990319000000	40.866914000000
H	41.903914000000	38.474232000000	39.625403000000
H	35.486909000000	38.181482000000	29.492292000000
H	32.775969000000	37.967977000000	29.617182000000
H	29.161793000000	38.665907000000	33.368070000000
H	29.165207000000	39.747635000000	35.853761000000
H	39.223674000000	40.889339000000	35.281635000000
H	35.481439000000	42.670440000000	38.494567000000
H	32.802154000000	42.265310000000	38.734371000000
H	34.829783000000	41.884397000000	32.409637000000
H	45.824546000000	35.177676000000	34.228843000000
H	44.882080000000	33.732508000000	34.609555000000

⁴Intermediate2_mut / HS_I2_mut

C	41.271072000000	37.731242000000	26.634833000000
H	41.027908000000	38.078666000000	27.643602000000
C	40.593809000000	38.565353000000	25.540752000000
H	40.898759000000	39.618007000000	25.640556000000
H	40.967331000000	38.234645000000	24.560477000000
C	39.053244000000	38.494608000000	25.523539000000
H	38.772043000000	37.429595000000	25.482252000000
C	38.420562000000	39.102879000000	26.784746000000
H	37.325173000000	39.057895000000	26.728426000000
H	38.724331000000	38.591525000000	27.703532000000
H	38.698408000000	40.161364000000	26.882667000000
C	38.499541000000	39.173259000000	24.260833000000
H	37.406442000000	39.095590000000	24.212777000000
H	38.755066000000	40.241183000000	24.247527000000
H	38.909766000000	38.722576000000	23.348357000000
C	32.372890000000	36.553926000000	39.988107000000
H	32.171340000000	35.590729000000	40.469058000000
H	33.395631000000	36.517425000000	39.588764000000
C	32.188986000000	37.696645000000	40.958608000000
C	31.956539000000	39.002804000000	40.498297000000
H	31.897742000000	39.183131000000	39.427131000000
C	31.795415000000	40.065982000000	41.389767000000
H	31.597596000000	41.065138000000	41.007754000000
C	31.865405000000	39.848231000000	42.769146000000
H	31.723701000000	40.671662000000	43.464450000000
C	32.096670000000	38.554321000000	43.243966000000
H	32.133009000000	38.364928000000	44.314273000000
C	32.253179000000	37.493721000000	42.345745000000
H	32.413073000000	36.487409000000	42.726533000000
C	41.082174000000	37.988947000000	39.588824000000
H	41.374310000000	36.936400000000	39.502727000000
C	39.909498000000	38.283614000000	38.657935000000
H	39.683267000000	39.365034000000	38.708893000000
C	40.225575000000	37.919170000000	37.204123000000
H	40.512336000000	36.863641000000	37.136773000000
H	39.349110000000	38.090633000000	36.568535000000
H	41.053483000000	38.527341000000	36.816810000000
O	38.789445000000	37.546070000000	39.142192000000
H	38.037435000000	37.703714000000	38.527856000000
C	40.341346000000	33.432460000000	39.749243000000
H	40.199513000000	32.399301000000	40.098880000000
C	39.041448000000	33.951717000000	39.098050000000
H	39.187330000000	35.013522000000	38.871538000000
C	38.717100000000	33.211967000000	37.792281000000
H	39.502810000000	33.363462000000	37.044172000000
H	38.608015000000	32.131002000000	37.955010000000
H	37.777879000000	33.584922000000	37.367664000000
C	37.876193000000	33.843709000000	40.090953000000
H	38.121915000000	34.328560000000	41.044727000000
H	36.985757000000	34.333202000000	39.681757000000
H	37.628450000000	32.794473000000	40.305653000000
C	41.553258000000	33.519034000000	38.830147000000
O	41.793743000000	34.495121000000	38.126995000000
N	42.373078000000	32.410953000000	38.835394000000
H	42.171104000000	31.664910000000	39.485893000000

C	43.565061000000	32.323124000000	38.012879000000
H	43.804397000000	33.334903000000	37.676287000000
C	43.446354000000	31.443900000000	36.757293000000
O	44.399424000000	31.305465000000	35.995183000000
N	42.240670000000	30.859016000000	36.566099000000
H	41.474466000000	31.029124000000	37.206088000000
C	41.917460000000	30.103913000000	35.379120000000
H	42.286965000000	30.620731000000	34.486834000000
C	40.399311000000	29.921321000000	35.342544000000
O	39.730757000000	29.936957000000	36.378718000000
N	39.857584000000	29.735400000000	34.118248000000
H	40.418212000000	29.707849000000	33.273186000000
C	38.443583000000	29.466804000000	33.940123000000
H	38.141662000000	28.697030000000	34.659861000000
C	37.560004000000	30.735453000000	34.191639000000
H	38.048383000000	31.282539000000	35.002422000000
H	37.567873000000	31.378194000000	33.304799000000
C	36.143976000000	30.402378000000	34.616122000000
C	35.053978000000	30.554278000000	33.744706000000
H	35.222397000000	30.920464000000	32.735505000000
C	33.758164000000	30.236780000000	34.168186000000
H	32.923273000000	30.369403000000	33.484962000000
C	33.535666000000	29.765957000000	35.462711000000
H	32.528119000000	29.525966000000	35.791840000000
C	34.616120000000	29.611010000000	36.336916000000
H	34.450128000000	29.251626000000	37.349182000000
C	35.907818000000	29.925598000000	35.916959000000
H	36.748701000000	29.815439000000	36.598251000000
C	38.274246000000	28.932400000000	32.513373000000
O	39.185387000000	28.982733000000	31.685959000000
N	37.056932000000	28.394834000000	32.226062000000
H	36.291544000000	28.609504000000	32.855497000000
C	36.725462000000	28.107041000000	30.846817000000
H	37.465546000000	27.411982000000	30.438636000000
C	36.647506000000	29.389104000000	29.995291000000
O	36.251869000000	30.450486000000	30.465263000000
N	37.000738000000	29.224469000000	28.691499000000
H	37.425018000000	28.348031000000	28.418466000000
C	37.041837000000	30.326210000000	27.738401000000
H	36.535845000000	31.164465000000	28.222391000000
C	38.469017000000	30.701322000000	27.311622000000
H	38.938359000000	29.827429000000	26.837863000000
H	38.390878000000	31.465640000000	26.526045000000
C	39.396728000000	31.212569000000	28.426321000000
H	39.540441000000	30.439470000000	29.191082000000
H	40.378032000000	31.392752000000	27.965514000000
C	38.911181000000	32.514579000000	29.089377000000
H	38.341706000000	33.120411000000	28.371949000000
H	38.248975000000	32.294608000000	29.932872000000
N	40.059109000000	33.318323000000	29.530598000000
H	40.975175000000	32.895358000000	29.491603000000
C	40.005251000000	34.654297000000	29.756357000000
N	38.837722000000	35.228959000000	30.041751000000
H	38.133109000000	34.682793000000	30.543642000000
H	38.815017000000	36.274462000000	30.099750000000
N	41.119370000000	35.388275000000	29.675275000000
H	41.910223000000	35.031706000000	29.158731000000
H	41.112610000000	36.414046000000	29.942697000000
C	45.175187000000	34.515481000000	33.909306000000
H	45.322425000000	34.149985000000	32.884035000000
C	44.004551000000	35.505432000000	33.977328000000
H	43.869404000000	35.843019000000	35.015578000000
H	44.260698000000	36.402760000000	33.396337000000
C	42.658636000000	34.959807000000	33.458798000000
H	42.819626000000	34.600735000000	32.428956000000
C	42.151476000000	33.780325000000	34.301506000000
H	42.871711000000	32.955865000000	34.317924000000
H	41.976336000000	34.091753000000	35.339783000000
H	41.202662000000	33.394420000000	33.904508000000
C	41.605816000000	36.075789000000	33.403136000000
H	40.641655000000	35.688929000000	33.047723000000

H	41.442526000000	36.504229000000	34.401036000000
H	41.903372000000	36.881087000000	32.722982000000
S	33.728816000000	41.834877000000	33.125902000000
C	36.045231000000	36.076479000000	42.856566000000
H	35.095562000000	36.478103000000	43.228496000000
H	35.818456000000	35.235882000000	42.193051000000
C	36.853340000000	37.146678000000	42.118231000000
H	37.804406000000	36.737838000000	41.761520000000
H	37.089682000000	37.984057000000	42.782258000000
N	36.169023000000	37.670874000000	40.939745000000
H	36.149661000000	37.096750000000	40.062689000000
C	35.671487000000	38.892726000000	40.815604000000
N	35.531400000000	39.429334000000	39.605053000000
H	34.856932000000	40.165102000000	39.437033000000
H	35.933602000000	38.937631000000	38.772679000000
N	35.361235000000	39.630024000000	41.932019000000
H	34.927790000000	40.525576000000	41.749268000000
H	34.883321000000	39.118925000000	42.665222000000
O	34.320602000000	38.112891000000	35.121791000000
Fe	34.170641000000	39.734762000000	34.279194000000
N	36.165981000000	40.060237000000	34.173951000000
N	34.077328000000	40.718610000000	36.051255000000
N	32.157414000000	39.547822000000	34.310517000000
N	34.217043000000	39.044216000000	32.393063000000
C	37.040145000000	39.637753000000	33.206109000000
C	38.420803000000	39.934720000000	33.581312000000
C	38.327116000000	40.598355000000	34.770259000000
C	36.933574000000	40.666193000000	35.130409000000
C	35.118031000000	41.334845000000	36.683355000000
C	34.650624000000	42.033254000000	37.858164000000
C	33.305208000000	41.807556000000	37.933612000000
C	32.964390000000	40.989024000000	36.793539000000
C	31.300455000000	39.895074000000	35.323838000000
C	29.946937000000	39.512080000000	34.993915000000
C	29.995154000000	38.939387000000	33.761209000000
C	31.377693000000	38.976727000000	33.340939000000
C	33.145829000000	38.613392000000	31.646037000000
C	33.587557000000	38.204964000000	30.333533000000
C	34.940550000000	38.365869000000	30.303016000000
C	35.326026000000	38.878206000000	31.595943000000
C	36.642490000000	39.090265000000	31.986791000000
H	37.412627000000	38.798555000000	31.272901000000
C	36.449266000000	41.290342000000	36.272772000000
H	37.177886000000	41.784165000000	36.908952000000
C	31.671252000000	40.571676000000	36.477865000000
H	30.880584000000	40.830928000000	37.176575000000
C	31.835075000000	38.542464000000	32.100585000000
H	31.094851000000	38.141591000000	31.413878000000
C	39.698272000000	39.506117000000	32.906862000000
H	39.817632000000	38.426366000000	33.066759000000
H	40.521678000000	39.966489000000	33.462903000000
C	39.881897000000	39.809055000000	31.382190000000
H	40.813997000000	40.360960000000	31.236174000000
H	39.059822000000	40.425377000000	31.006240000000
C	39.964505000000	38.495359000000	30.589207000000
O	41.110616000000	37.997665000000	30.414882000000
O	38.865676000000	37.967069000000	30.225841000000
C	34.805438000000	34.919506000000	33.861862000000
C	35.101522000000	36.246181000000	33.780140000000
C	35.338573000000	37.108470000000	34.998516000000
C	35.380300000000	36.291726000000	36.277423000000
C	35.038294000000	34.953311000000	36.286639000000
C	34.740204000000	34.244691000000	35.114277000000
C	35.865719000000	36.913145000000	37.549883000000
O	36.518835000000	38.009100000000	37.471442000000
O	35.631934000000	36.302249000000	38.637699000000
O	34.576294000000	34.098668000000	32.758070000000
C	34.134715000000	34.732931000000	31.558201000000
H	35.139486000000	36.745702000000	32.823689000000
H	36.311827000000	37.611747000000	34.893301000000
H	35.033175000000	34.439840000000	37.242799000000

H	34.473917000000	33.193542000000	35.134305000000
H	33.823388000000	33.926019000000	30.890588000000
H	34.937943000000	35.307209000000	31.082231000000
H	33.292386000000	35.402170000000	31.762556000000
O	37.300218000000	33.679526000000	32.000526000000
H	36.343445000000	33.609647000000	32.202151000000
H	37.661250000000	34.140428000000	32.774615000000
H	36.615610000000	35.693785000000	43.710824000000
H	40.563077000000	34.040059000000	40.637812000000
H	44.415092000000	31.955184000000	38.597479000000
H	42.393982000000	29.111886000000	35.394577000000
H	35.748366000000	27.613497000000	30.825632000000
H	36.457611000000	30.054659000000	26.849989000000
H	31.698050000000	36.652458000000	39.130582000000
H	42.362412000000	37.769154000000	26.530535000000
H	40.967838000000	36.677663000000	26.565315000000
H	40.805687000000	38.196342000000	40.629010000000
H	41.949144000000	38.608374000000	39.330626000000
H	35.636296000000	38.167637000000	29.497746000000
H	32.933193000000	37.846905000000	29.548458000000
H	29.180934000000	38.537380000000	33.171692000000
H	29.085224000000	39.678590000000	35.627862000000
H	39.138951000000	40.986665000000	35.373158000000
H	35.276411000000	42.626020000000	38.514151000000
H	32.595320000000	42.186252000000	38.658709000000
H	34.881974000000	41.919125000000	32.424972000000
H	46.109665000000	34.996921000000	34.221956000000
H	45.024126000000	33.642703000000	34.554020000000