Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

Unusual Catalytic Strategy by Non-Heme Fe(II)/2-Oxoglutarate-Dependent Aspartyl Hydroxylase AspH

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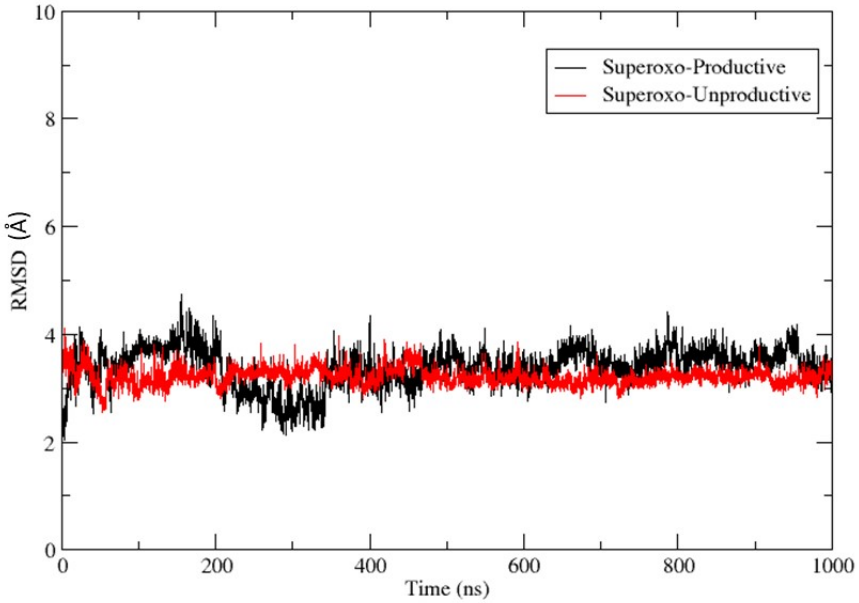


Figure S1. RMSD plot for Ferric-superoxo binding modes: A (productive, black) and B (unproductive, red) obtained from 1μs MD simulations.

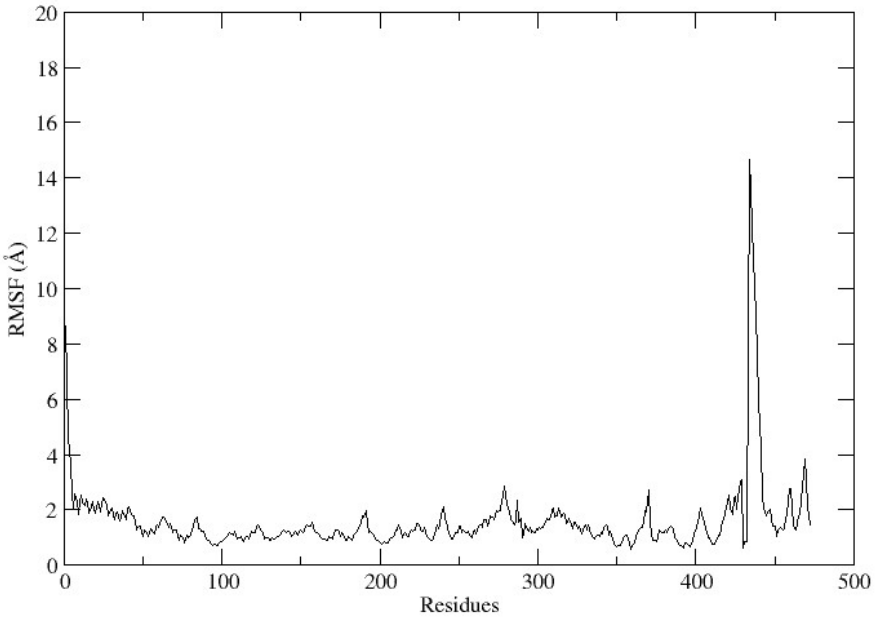


Figure S2. RMSF plot for ferric-superoxo binding mode A. Residues 1-429 are AspH protein residues; 430-Fe, 431-O_2, 432-2OG, 433-W1. Residues 434-472 are EGFD substrate residues; 451-Asp103$_{hFX}$.

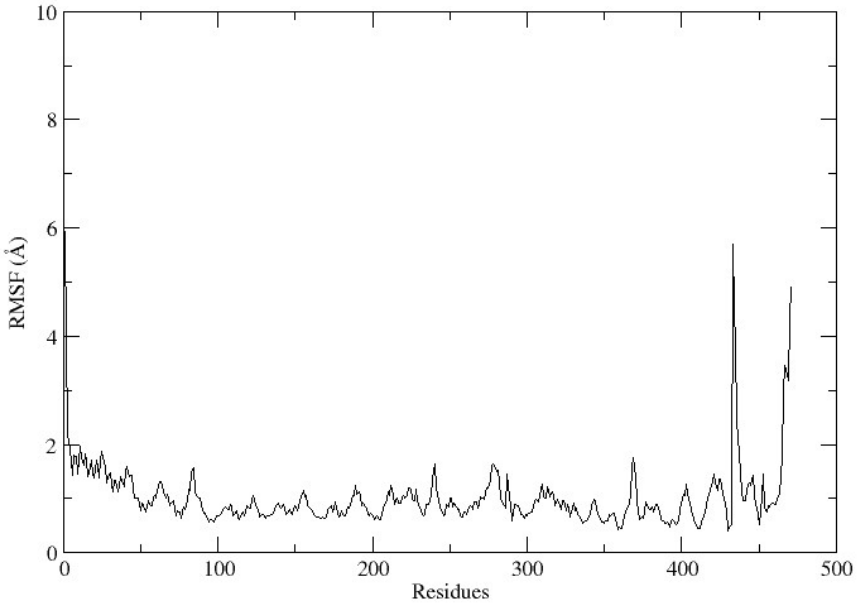


Figure S3. RMSF plot for ferric-superoxo bonding mode B. Residues 1-429 are AspH protein residues; 430-Fe, 431-O_2, 432-2OG. Residues 433-471 are EGFD substrate residues; 450-Asp103$_{hFX}$.

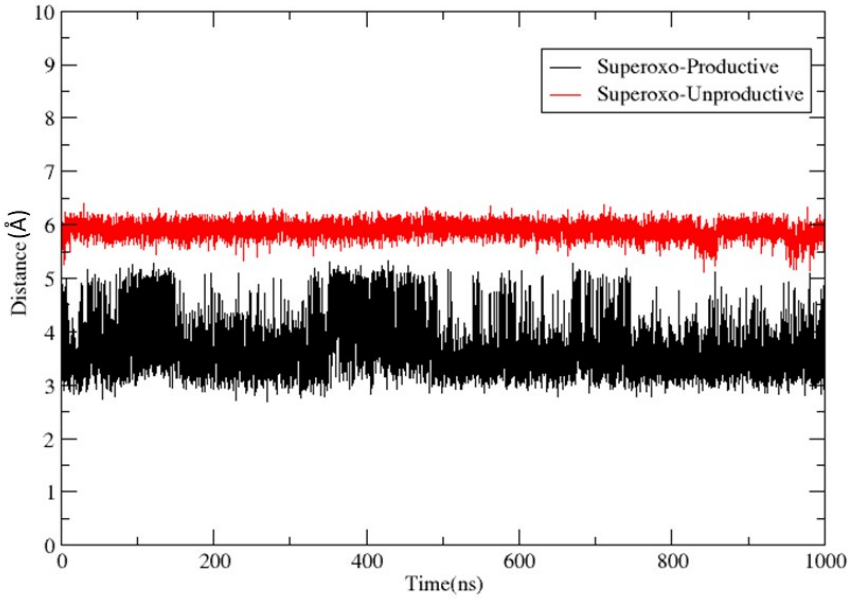


Figure S4. Plot of distance the between the superoxide distal oxygen (O_d) and C2 of 2OG in superoxo binding modes: A (productive, black) and B (unproductive, red) obtained from 1µs MD simulations.

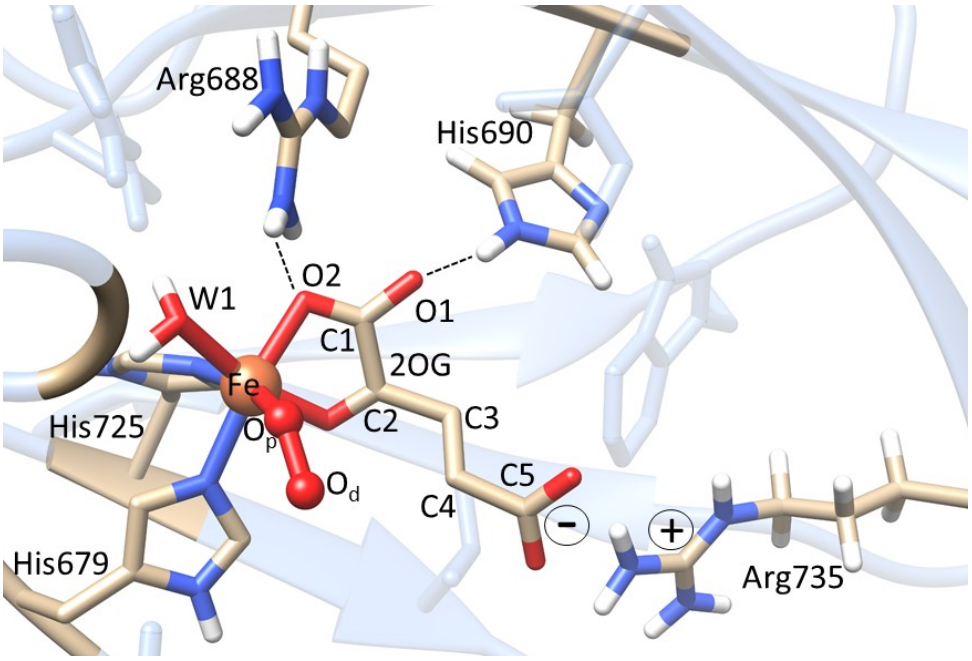


Figure S5. Protein interactions stabilizing the 2-oxoglutarate (2OG) cosubstrate in the AspH active site.

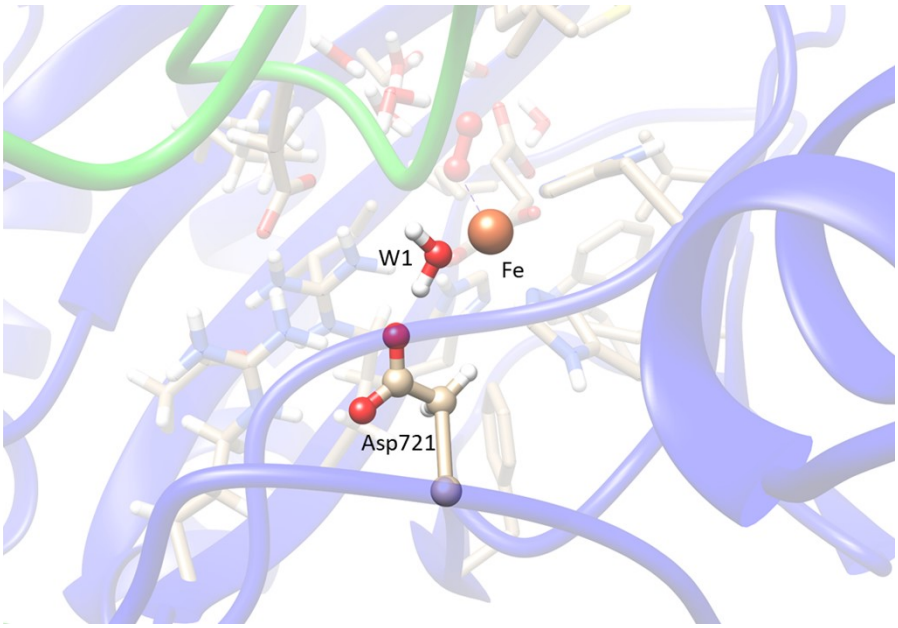


Figure S6. Hydrogen bond between the Fe coordinated water (W1) and the side chain carboxylate of Asp721.

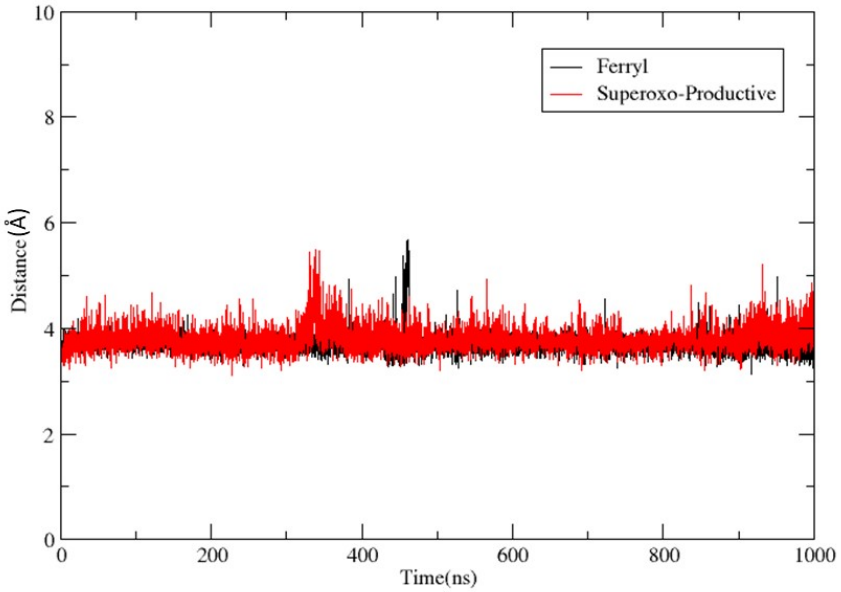


Figure S7. Hydrogen bond between Asp721 side chain carboxylate and Fe coordinated water (W1) in the ferryl (black) and superoxo (red) complexes obtained from 1μs MD simulations.

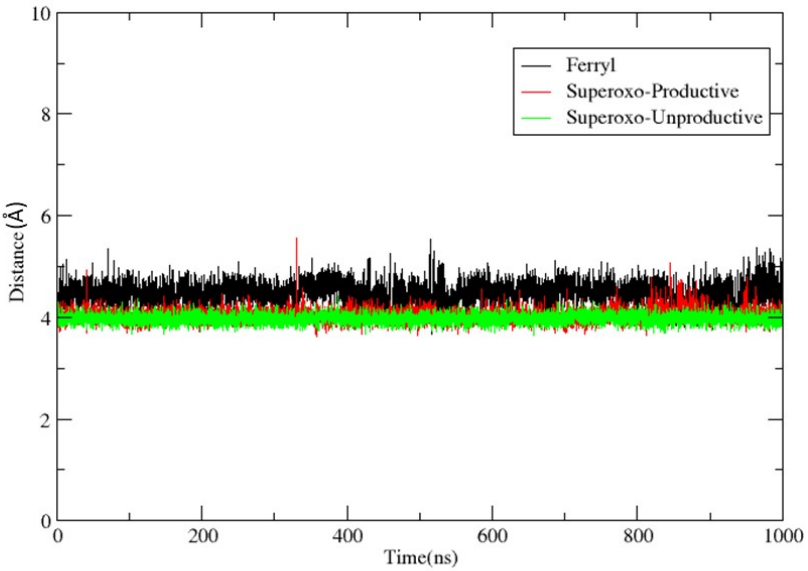


Figure S8. Salt bridge between the Arg686 side chain guanidium group and the Asp721 side chain carboxylate in the binding mode A (productive, red), binding mode B (unproductive, green) superoxo and ferryl (black) complexes obtained from 1µs MD simulations.

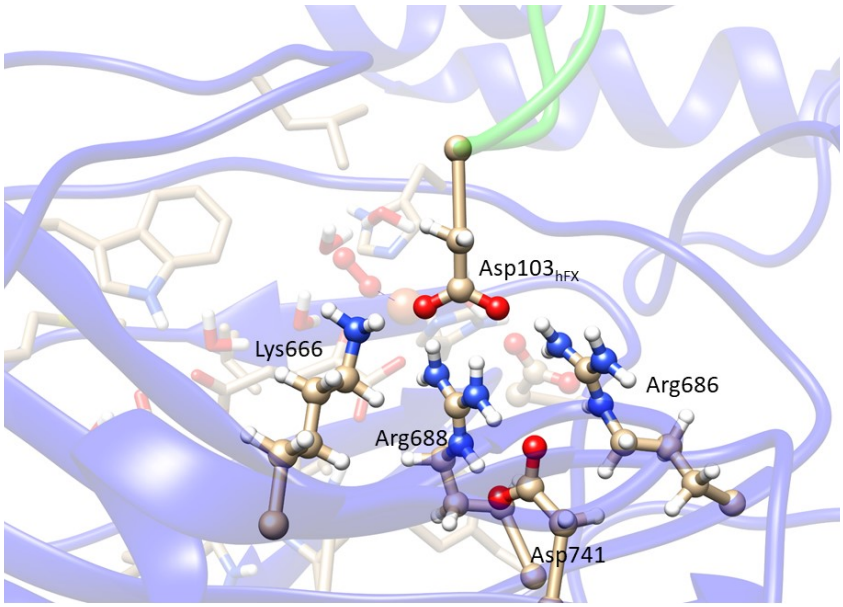


Figure S9. Salt bridge interactions stabilizing substrate ($Asp103_{hFX}$) positioning in the AspH active site.

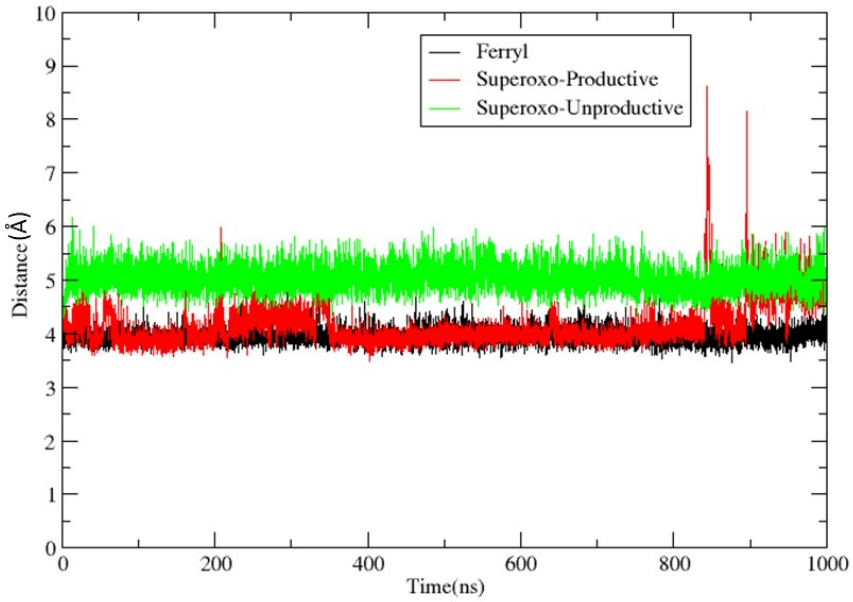


Figure S10. Salt bridge between the Arg688 guanidium group and the Asp103$_{hFX}$ carboxylate in the binding mode A (productive, red), binding mode B (unproductive, green) superoxo and ferryl (black) complexes obtained from 1μs MD simulations.

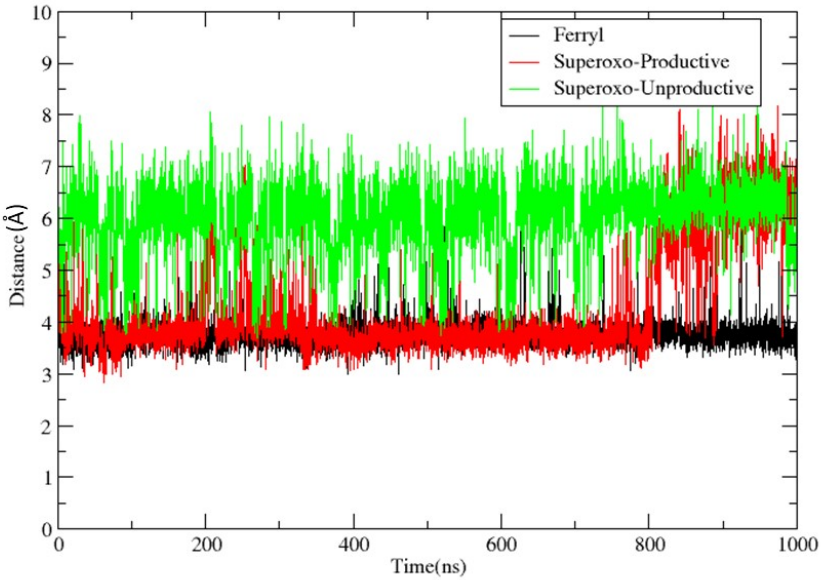


Figure S11. Salt bridge between the Lys666 side chain amine and the Asp103$_{hFX}$ carboxylate in the binding mode A (productive, red), binding mode B (unproductive, green) superoxo and ferryl (black) complexes obtained from 1μs MD simulations.

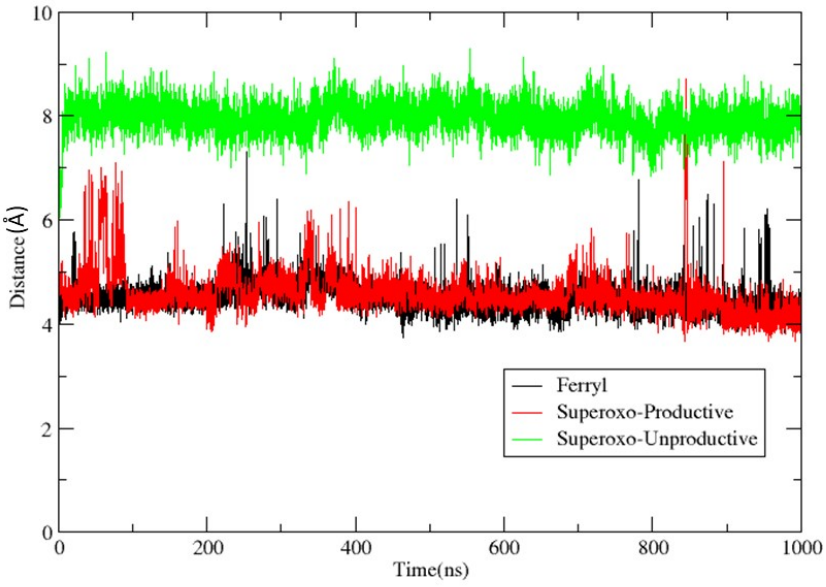


Figure S12. Electrostatic interaction between the Arg686 guanidium group and the $Asp103_{hFX}$ carboxylate in the binding mode A (productive, red), binding mode B (unproductive, green) superoxo and ferryl (black) complexes from 1μs MD simulations.

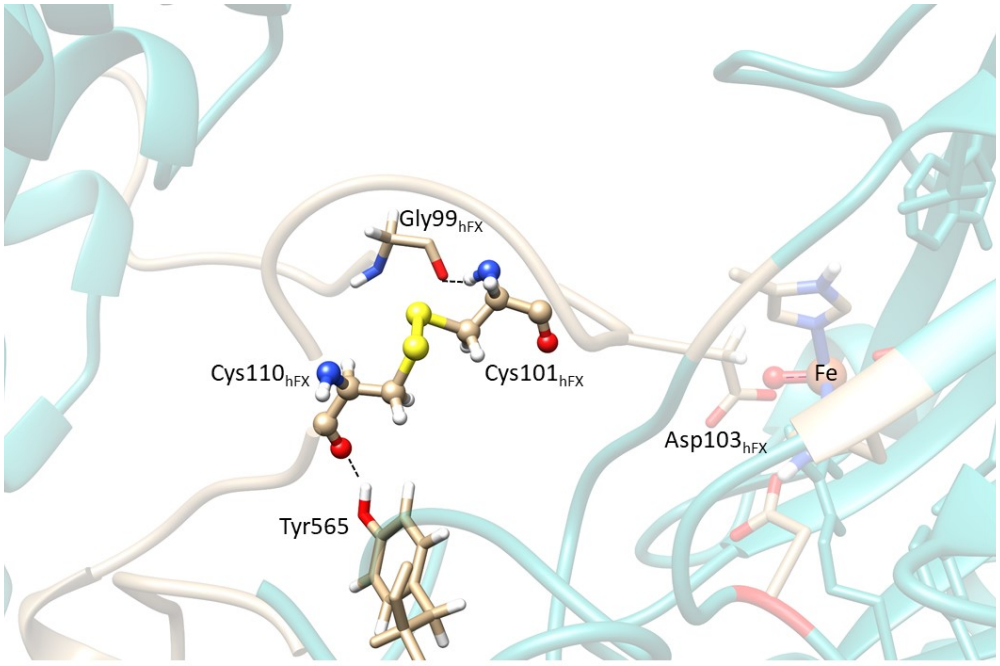


Figure S13. Protein residues stabilizing the Cys 3-4 disulfide bridge in the AspH -EGFD ES complex.

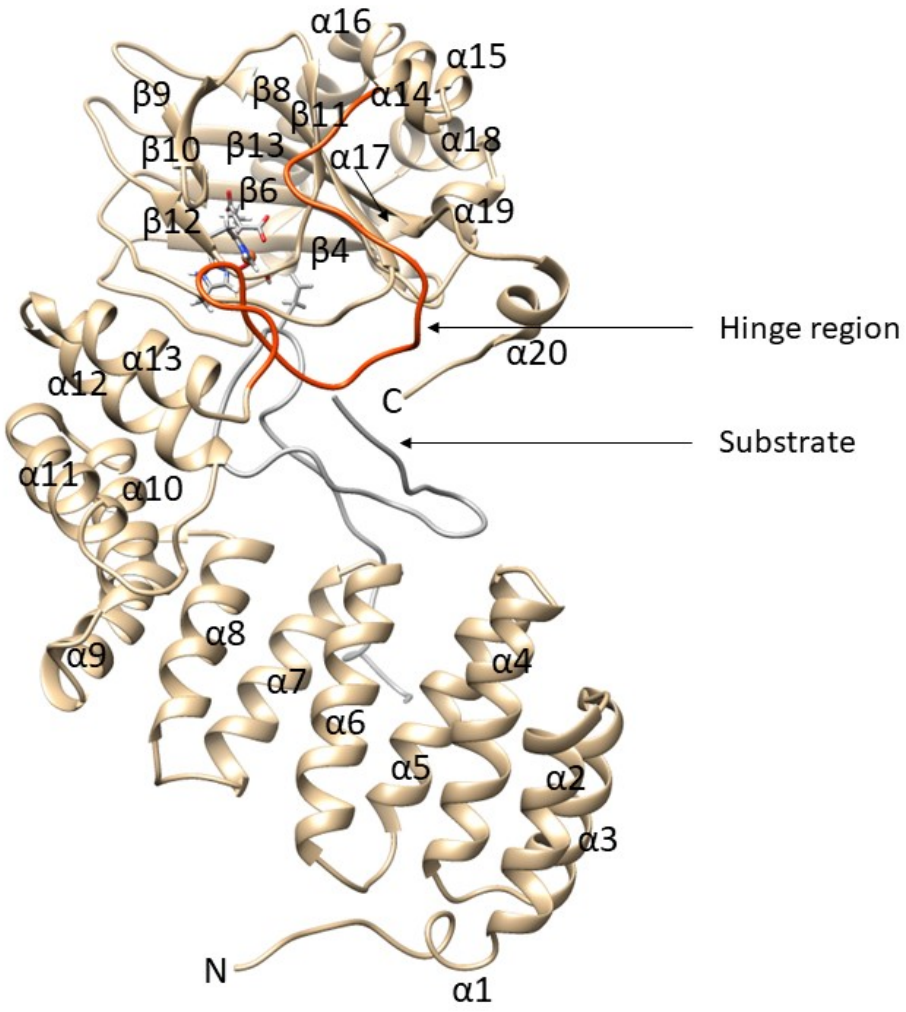
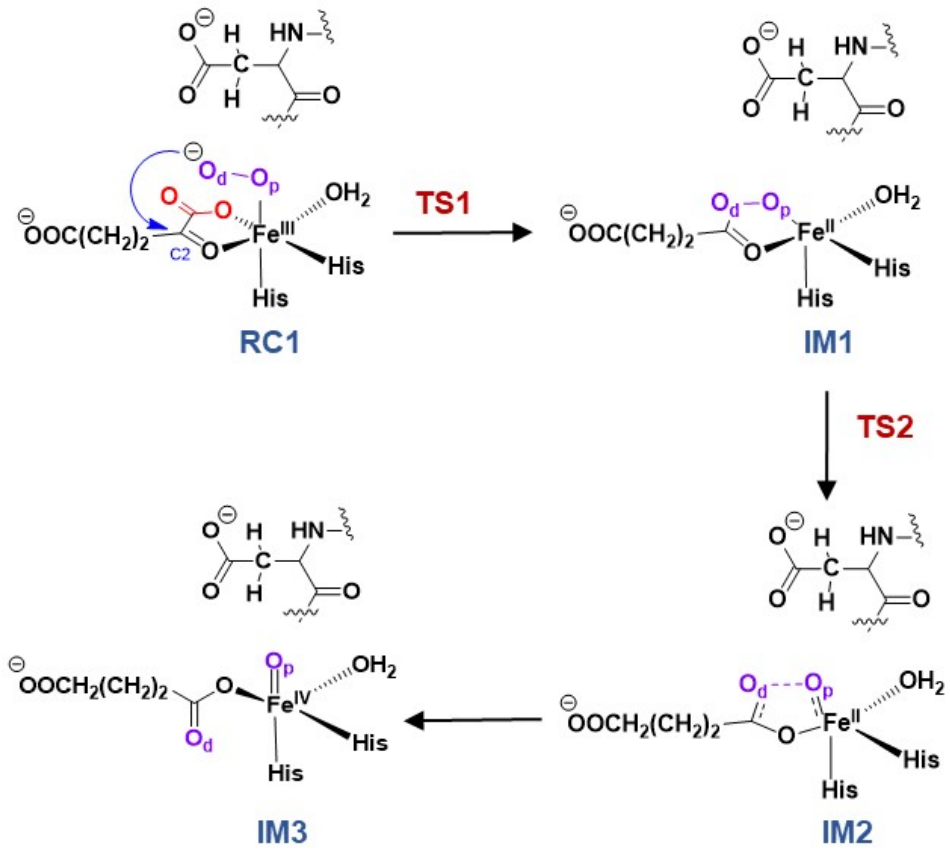


Figure S14. The AspH secondary structure based on PDB:5JZ8.



Scheme S1. Mechanism of dioxygen activation in non-heme Fe(II)/2OG oxygenases.

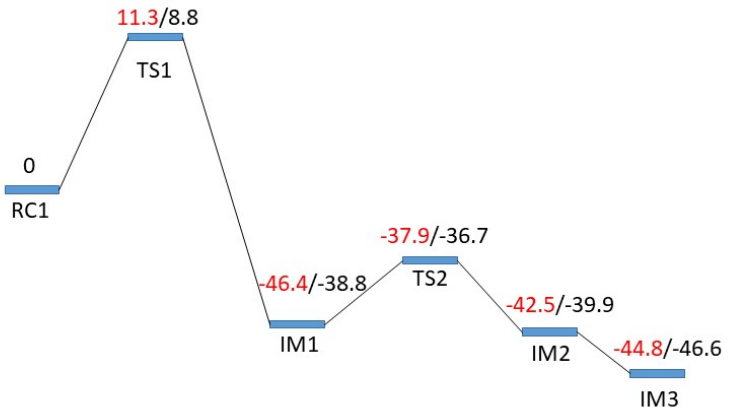


Figure S15. Energy profile for dioxygen activation in superoxo binding mode A.

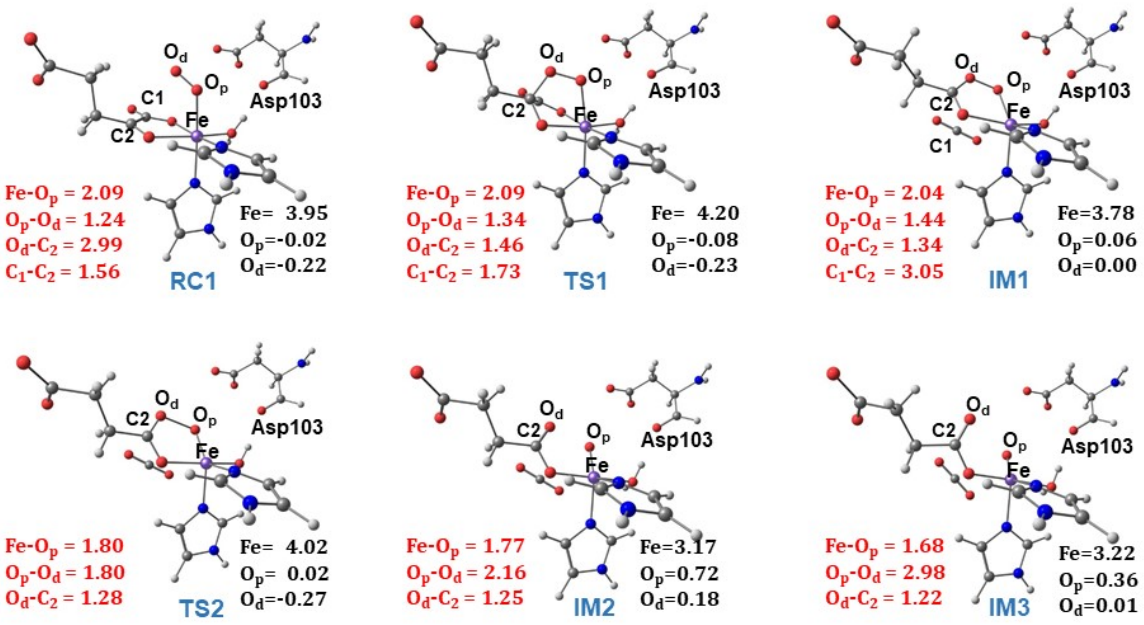


Figure S16. Optimized geometries for stationary points involved in dioxygen activation in the productive superoxo conformation. Asp103 is the hFX substrate residue undergoing hydroxylation.

Conformational Dynamics of AspH Fe(III)-$OO^{\cdot-}$ ES complex (binding mode A)-additional details

In superoxo binding mode A, the $Tyr108_{hFX}$ side chain of the substrate is positioned for cation-pi/pi-pi stacking with the sidechains of AspH TPR residues Arg526/Phe496. Other interactions involve hydrogen bonding of the $Tyr108_{hFX}$ side chain hydroxyl with His493 side chain imidazole nitrogen. The hydrophobic residues Tyr565, Pro682, and Ile758 stabilize the $Cys101_{hFX}$-$Cys110_{hFX}$ disulfide bridge and help position $Asp103_{hFX}$ in the active site.

Fe(III)-$OO^{\cdot-}$ DCCA-additional details

$Tyr108_{hFX}$ showed a positive correlation with TPR α6 and α7 helices, suggesting their potential importance for AspH reactivity through long-range interactions. A strong anti-correlated motion was observed between α1-α5 helices of the TPR domain and α17-α19 helices and β4-

β6 β-sheets of the OXY domain. Lys666 showed anticorrelation with the TPR α6 and α7 helices, suggesting a potential role in fine-tuning the substrate conformation for catalysis.

Mechanism of Dioxygen Activation (binding mode A)-additional details

The geometric parameters and spin densities of the stationary points involved in dioxygen activation for binding mode A are provided in **Figure S16**. The reactant complex (RC1) is characterized by the following bond distances: Fe-O_p, O_p-O_d, O_d-C2, and C1-C2 bond distances are 2.09 Å, 1.24 Å, 2.99 Å and 1.56 Å, respectively. The calculated iron spin density is 3.95, indicating the Fe(III) oxidation state with four unpaired electrons on iron and the remaining one electron antiferromagnetically coupled to the superoxide radical.

The distal oxygen (O_d) of the Fe(III)-O-$O^{\cdot-}$ moiety attacks the C2 of 2OG, resulting in CO_2 release and C1-C2 bond cleavage, forming Fe(II)-peroxysuccinic intermediate IM1 via TS1. The decarboxylation step has a calculated energy barrier of 8.86 kcal/mol relative to the Fe(III)-O-$O^{\cdot-}$ intermediate (RC1). In TS1, the O_d-C2 distance decreases to 1.46 Å, and the O_p-O_d and C1-C2 bonds increase to 1.34 Å and 1.73 Å, respectively, indicating the formation of a partial bond between O_d and C2 and weakening of the existing O_p-O_d and C1-C2 bonds. The TS1 spin density for iron slightly increases to 4.20, with O_p and O_d showing -0.08 and -0.23 spin densities, respectively. TS1 leads to a relatively stable peroxysuccinic intermediate (IM1) and CO_2 release. The Fe-O_p and O_p-O_d bond distances elongate to 2.04 Å and 1.44 Å in IM1, respectively, while the O_d-C2 distance reduces to 1.34 Å. The Fe spin density in IM1 changes to 3.78, indicating the Fe(II) character of the peroxysuccinic intermediate, where the spin densities of O_p and O_d are 0.06 and 0.00, respectively. TS1 is stabilized by a network of water-mediated hydrogen bonding interactions between (i) O_p and the $Asp103_{hFX}$ side chain carboxylate, (ii) the Asp721 side chain carboxylate and $Asp103_{hfX}$ backbone carbonyl oxygen

(mediated by the Fe coordinated water), (iii) a hydrogen bond between 2OG C1 carboxylate and a Arg688 guanidium NH and, (iv) a salt bridge interaction between the Arg735 side chain guanidium and the 2OG C5 carboxylate. IM1 is exothermic, with an energy change of -38.92 kcal/mol relative to RC1 (**Figure S15).**

Following decarboxylation, the Fe(II)-peroxysuccinic intermediate IM1 converts to IM2 through homolytic O_p-O_d bond cleavage. The process is exothermic (relative to IM1) with a 2.04 kcal/mol activation energy barrier at the B3 level. In TS2, for the O_p-O_d bond cleavage step, the Fe-O_p and O_d-C2 distances are 1.80 Å and 1.28 Å, respectively, and the O_p-O_d distance is 1.80 Å. The Fe-O_p bond becomes stronger with a partial double bond character in TS2. IM2 displays partial bonding between O_d and O_p (2.16 Å), which cleaves to form a more stable IM3. In IM3, the O_p-O_d bond is completely broken, and the Fe-O_p double bond is formed with bond distances of 1.68 Å, 1.22 Å, and 3.22 Å for Fe-O_p, O_d-C2, and O_p-O_d, respectively.

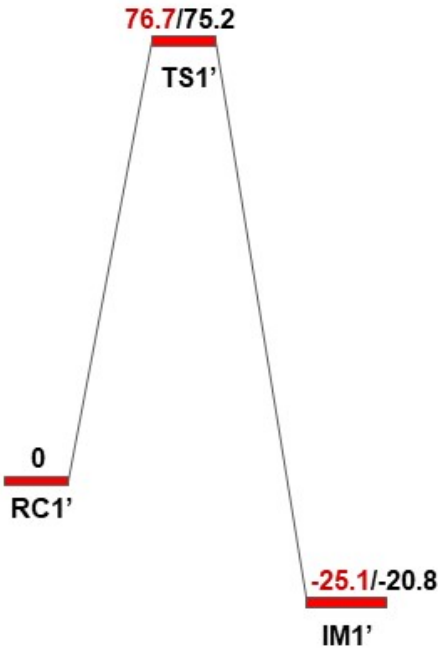


Figure S17. Energy profile for the dioxygen activation step in binding mode B.

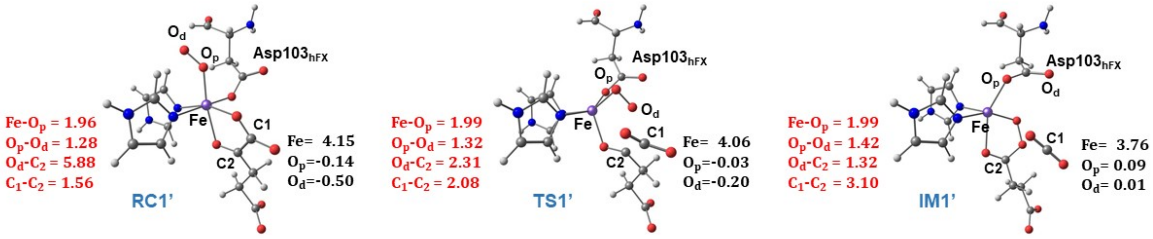


Figure S18. Optimized geometries for stationary points involved in dioxygen activation in the binding mode B.

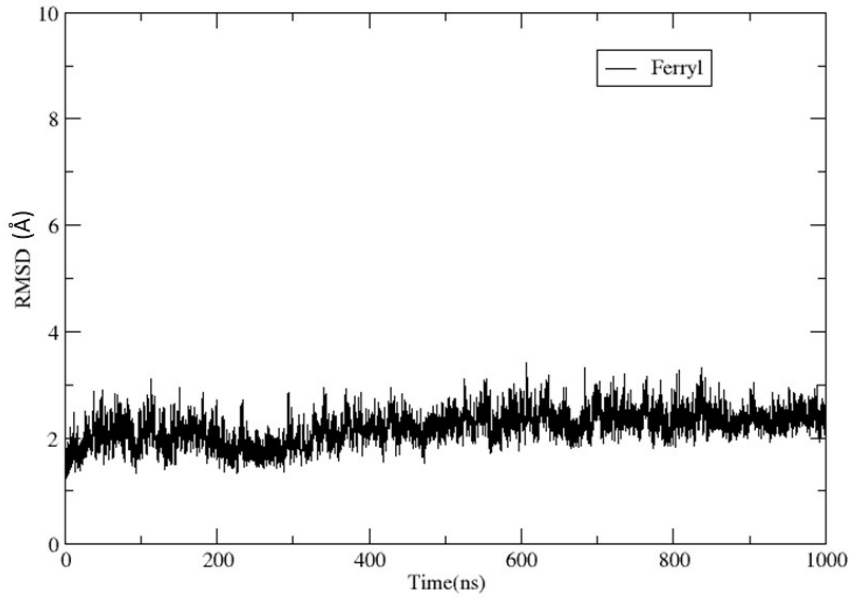


Figure S19. RMSD plot for the AspH WT ferryl complex obtained from 1µs MD simulation.

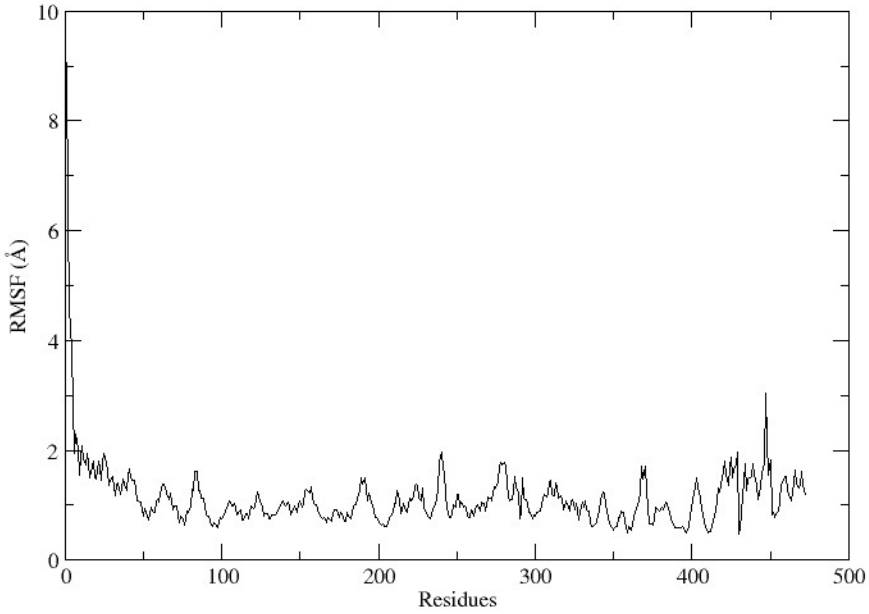


Figure S20. RMSF plot for the ferryl complex. Residues 1-429 are AspH protein residues; 430-Fe, 431-O_P, 432-SC, 433-W1. Residues 434-472 are EGFD substrate residues; 451-$Asp103_{hFX}$.

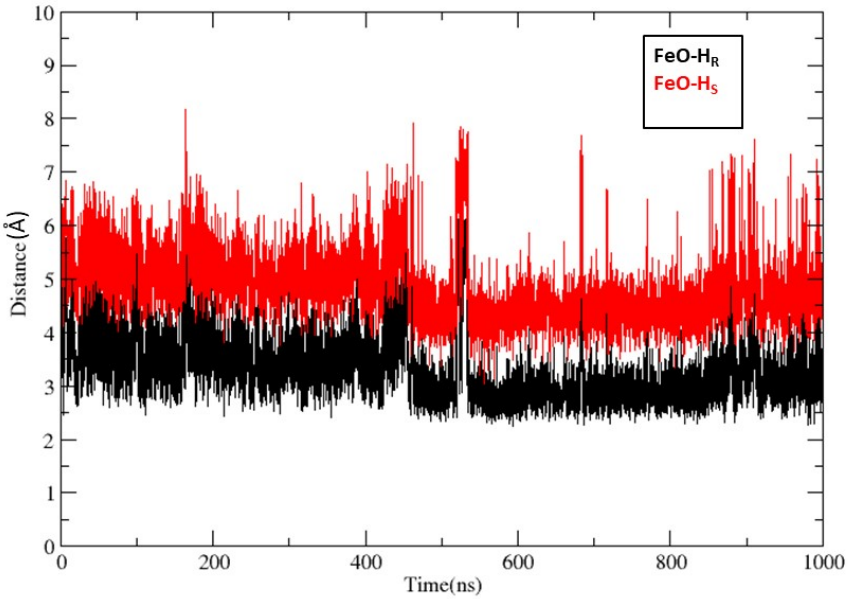


Figure S21. Plot of the distance between the ferryl O_p and the *pro*-chiral hydrogen atoms (H_R and H_S) of C3 of $Asp103_{hFX}$ in the ferryl complex obtained from 1µs MD.

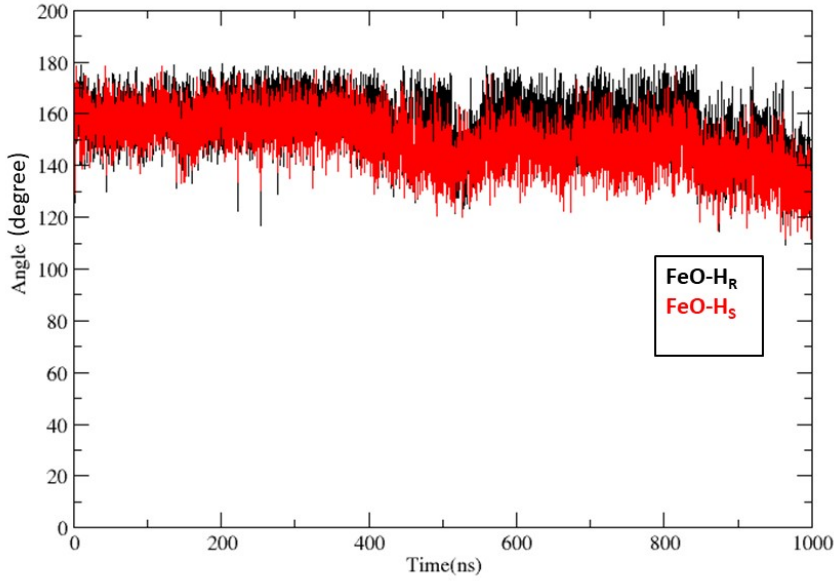


Figure S22. Plot of the Fe-O_p-H angle for the *pro*-chiral hydrogen atoms (H_R and H_S) of C3 of $Asp103_{hFX}$ in ferryl obtained from 1µs MD simulations.

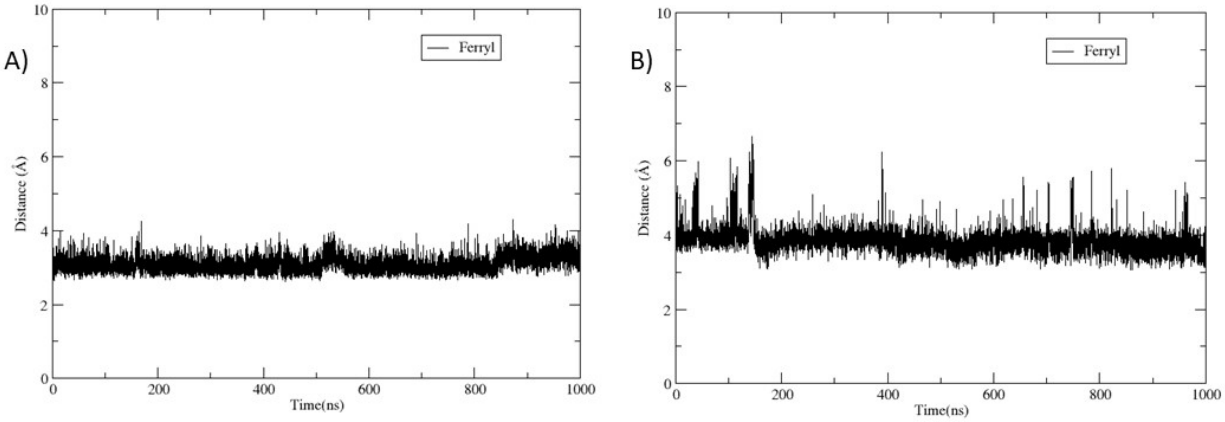


Figure S23. Plots for hydrogen bonds between: A) Arg688 guanidium NH and the Fe coordinated water (W1), B) the Ser668 side chain hydroxyl and succinate C4 carboxylate oxygen in the ferryl complex, obtained from 1μs MD simulation.

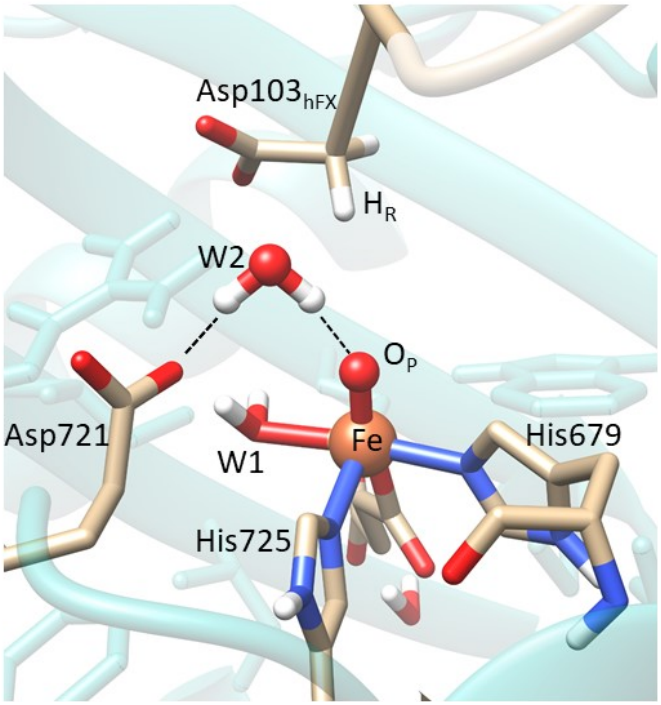


Figure S24. Solvent-mediated (W2) bridging hydrogen bonding interaction between SCS residue Asp721 and the Fe(IV)=O (O_p).

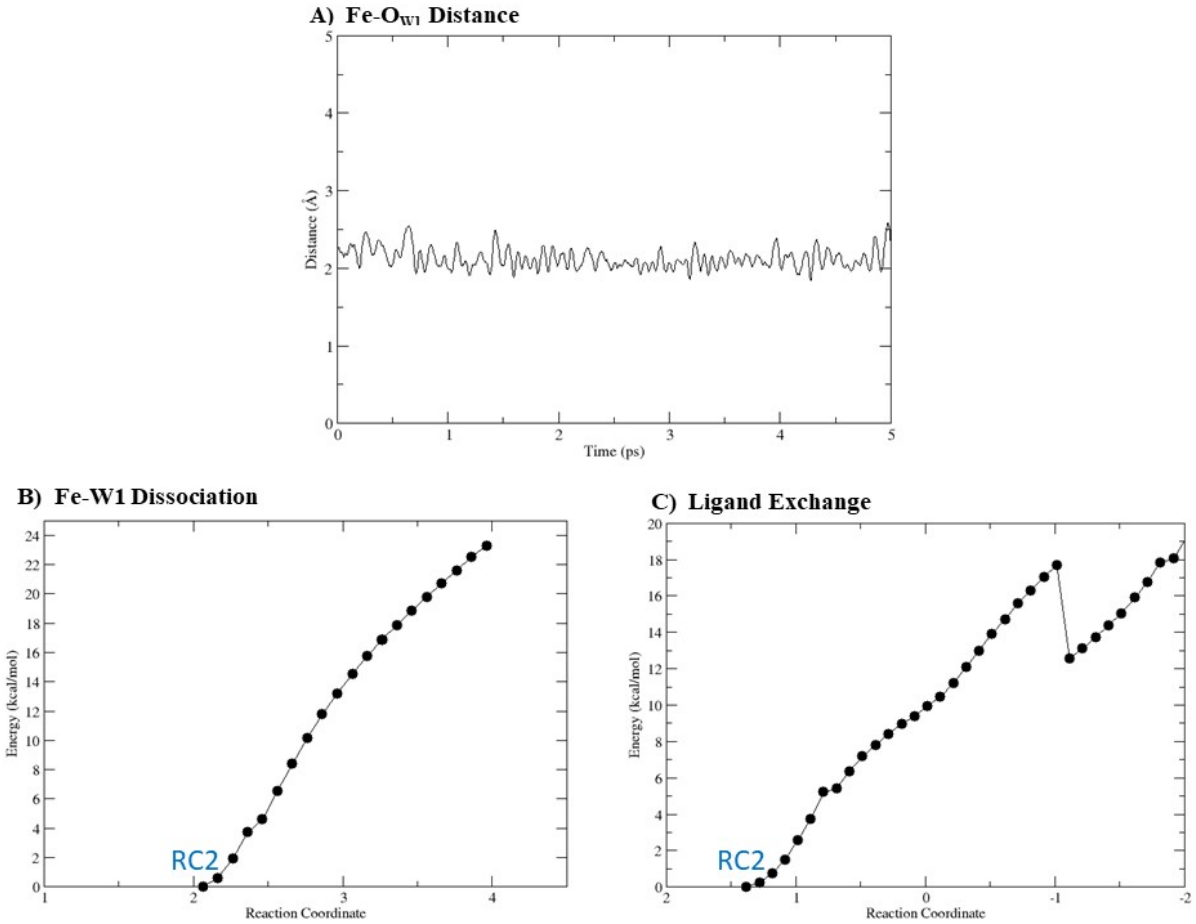


Figure S25. A) Plot for distance between Fe and O atom of W1 obtained from 5 ps QM/MM MD simulation. QM/MM energy scans for B) Fe-W1 bond dissociation. C) ligand exchange of W1 with other solvent water molecule (Ws). Reaction coordinate for B) is the distance between Fe and O_{W1}. Reaction coordinate for C) is the difference between the Fe-O_{W1} and Fe-O_{Ws} distances (d1(Fe-O_{W1}) — d2(Fe-O_{Ws})).

Table S1. Spin densities of stationary points involved in the HAT step.

		Fe	**O_P**	**C_B**
Snapshot 1	RC2	3.26	0.57	0
	TS_{ProR}	4.06	0.13	-0.34
	TS_{ProS}	4.05	0.07	-0.35
Snapshot 2	RC2	3.40	0.48	0
	TS_{ProR}	4.11	0.18	-0.31
	TS_{ProS}	4.07	0.14	-0.22
Snapshot 3	RC2	3.62	0.54	0
	TS_{ProR}	4.15	0.27	-0.29
	TS_{ProS}	4.13	0.30	-0.21
Snapshot 4	RC2	3.13	0.65	0
	TS_{ProR}	4.05	0.17	-0.37
	TS_{ProS}	4.04	0.06	-0.34
Snapshot 5	RC2	3.96	0.66	0
	TS_{ProR}	4.12	0.32	-0.31
	TS_{ProS}	4.13	0.23	-0.34

Table S2.Geometric features of stationary points involved in the HAT step.

AspH WT		**d(Fe-O_P) (Å)**	**d(O_P-H) (Å)**	**d(C_B-H) (Å)**	**<(Fe-O_P-H) (deg)**	**<(C_B-H-O_P) (deg)**	**φ(N-C_A-C_B-C_G) (deg)**
Snapshot 1	RC2	1.64	3.18(H_R) 4.81(H_S)	1.11(H_R) 1.10(H_S)	121.2(H_R) 114.4(H_S)	169.3(H_R) 55.03(H_S)	-76.09
	TS_{proR}	1.77	1.32	1.34	160.5	177.9	-74.96
	TS_{proS}	1.78	1.34	1.33	165.4	152.9	-27.10
Snapshot 2	RC2	1.65	2.80(H_R) 4.40(H_S)	1.10(H_R) 1.10(H_S)	129.4(H_R) 124.5(H_S)	170.6(H_R) 56.3(H_S)	-74.18
	TS_{proR}	1.79	1.29	1.39	156.6	175.9	-72.13
	TS_{proS}	1.78	1.41	1.31	159.7	152.7	-16.55
Snapshot 3	RC2	1.67	3.01(H_R) 4.51(H_S)	1.10(H_R) 1.10(H_S)	136.2(H_R) 128.8(H_S)	172.9(H_R) 61.5(H_S)	-74.51
	TS_{proR}	1.79	1.24	1.44	157.8	174.3	-83.33
	TS_{proS}	1.78	1.32	1.40	159.6	162.8	-23.19
Snapshot 4	RC2	1.62	3.27(H_R) 4.89(H_S)	1.10(H_R) 1.10(H_S)	117.3(H_R) 110.9(H_S)	170.0(H_R) 55.9(H_S)	-72.89
	TS_{proR}	1.76	1.31	1.34	158.2	177.5	-71.40
	TS_{proS}	1.76	1.34	1.31	160.4	153.3	-21.97
Snapshot 5	RC2	1.70	2.64(H_R) 4.14(H_S)	1.11(H_R) 1.10(H_S)	164.1(H_R) 149.9(H_S)	174.0(H_R) 61.8(H_S)	-76.77
	TS_{proR}	1.78	1.26	1.47	171.9	172.6	-74.73
	TS_{proS}	1.79	1.28	1.42	166.6	161.1	-29.71

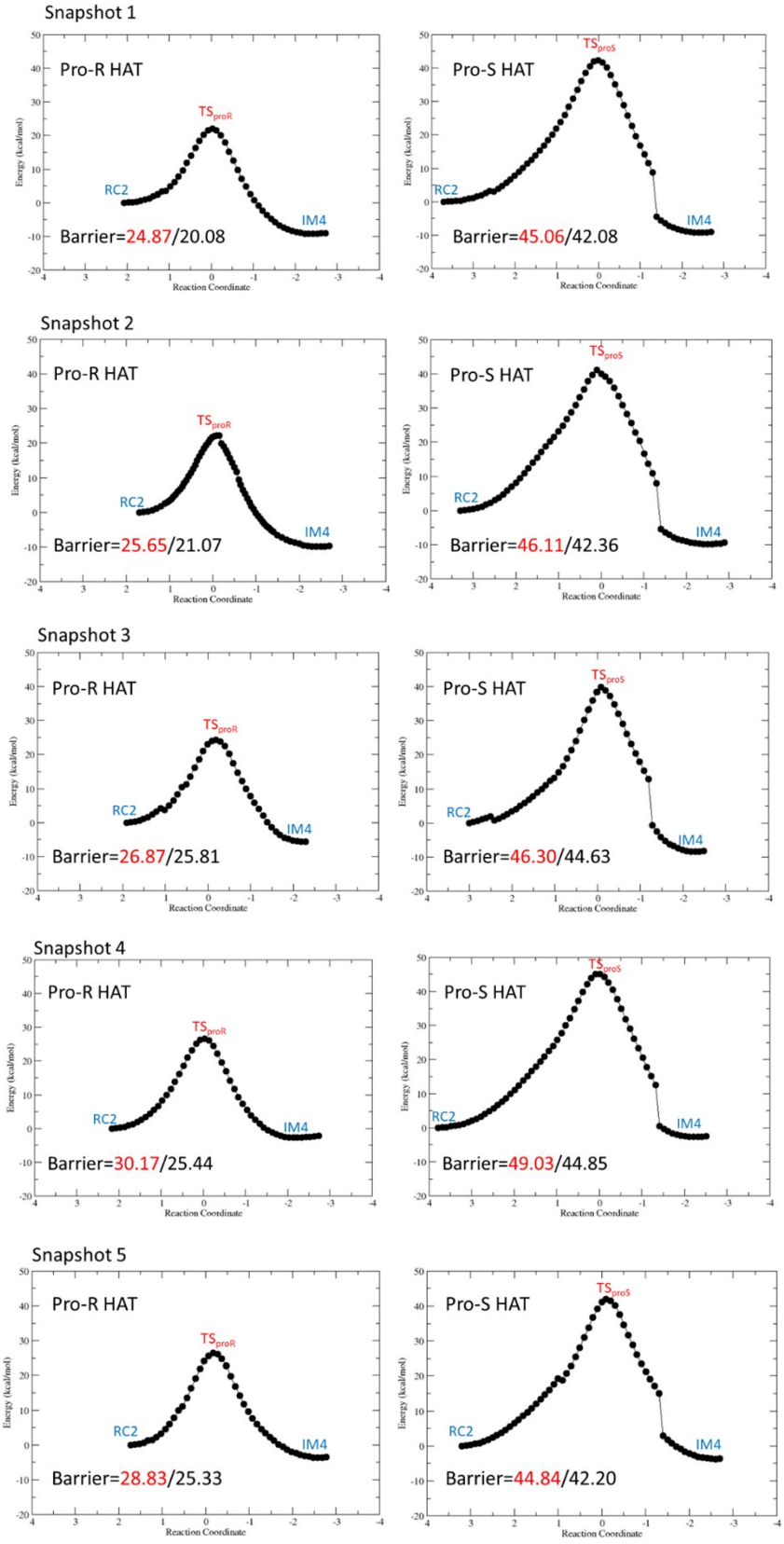


Figure S26. QM/MM energy scans (snapshots 1-5) *pro-R/S* HAT step, calculated at the UB3LYP/def2-SVP level. Energy barriers calculated at B2 (red) and B3 (black) levels are provided. Reaction coordinate is defined as the difference between the O_p-$H_{R/S}$ and C_B-$H_{R/S}$ distances (d1(O_p-$H_{R/S}$) — d2(C_B-$H_{R/S}$)).

Table S3. Computed energy barriers with dispersion corrections (D3-BJ) for representative snapshots in the *pro-(R)* HAT step.

	B2 (kcal/mol)	B3 (kcal/mol)
Snapshot 1	23.1	19.4
Snapshot 4	28.8	23.4

Table S4. Relationships between W2-Asp721-W1 hydrogen bond distances and the HAT barrier.

AspH WT	**$d(H_{W2}...O_p)$ (Å)**	**$<(O_{w2}-H_{W2}-O_p)$ (deg)**	**$d(H_{W1}...O_{Asp})$ (Å)**	**$<(O_{w1}-H_{W1}-O_{Asp})$ (deg)**	**ΔE_{HAT} B2/B3 (kcal/mol)**
Snapshot 1	1.59	177.0	1.51	176.9	24.9/20.8
Snapshot 2	1.64	175.2	1.49	175.7	25.7/21.1
Snapshot 3	1.70	163.7	1.40	173.1	26.9/25.8
Snapshot 4	1.70	160.3	1.37	175.9	30.2/25.4
Snapshot 5	1.77	157.83	1.36	175.3	28.8/27.3

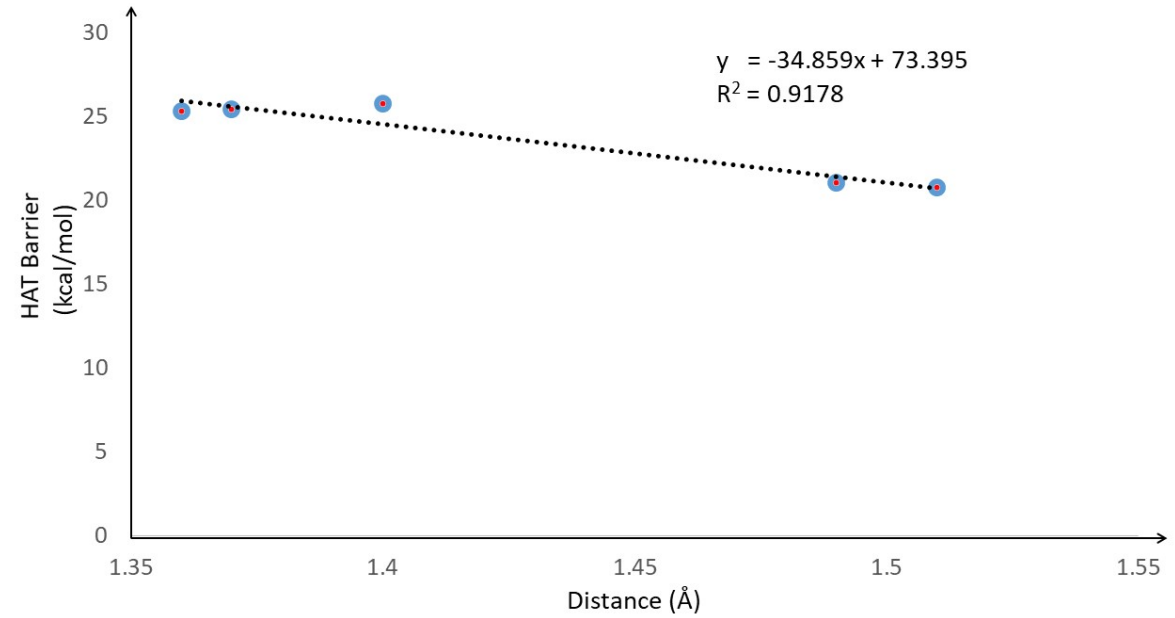


Figure S27. Correlation plot for the *pro*-(*R*) HAT barrier versus the W1-Asp721 hydrogen bond distance.

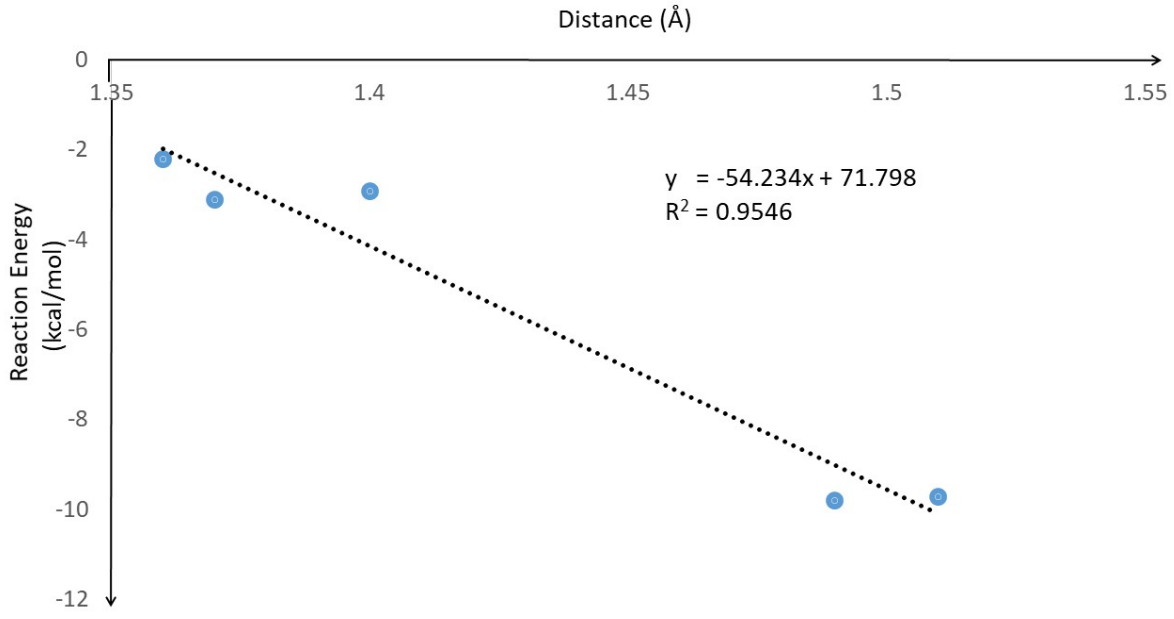


Figure S28. Correlation plot for the *pro*-(*R*) HAT reaction energy versus the W1-Asp721 hydrogen bond distance.

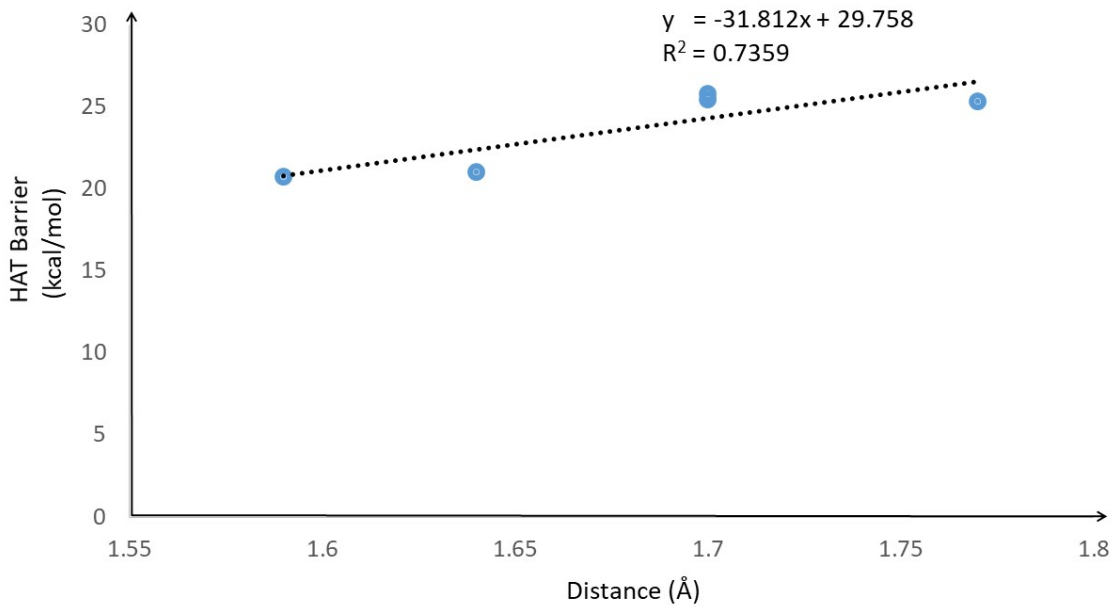


Figure S29. Correlation plot for the *pro*-(*R*) HAT barrier versus the W2-Asp721 hydrogen bond distance.

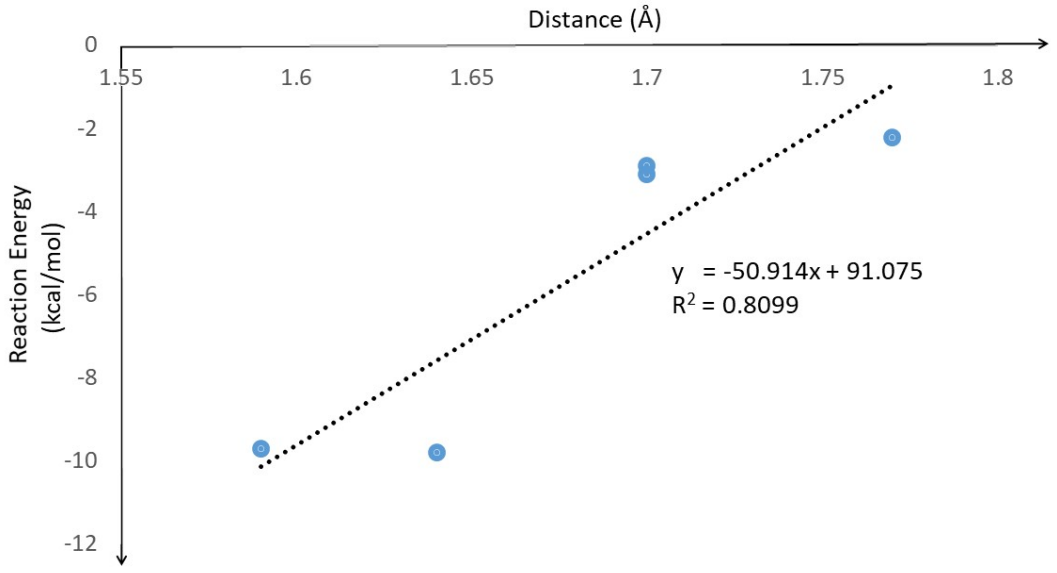


Figure S30. Correlation plot for the *pro*-(*R*) HAT reaction energy versus the W2-Asp721 hydrogen bond distance.

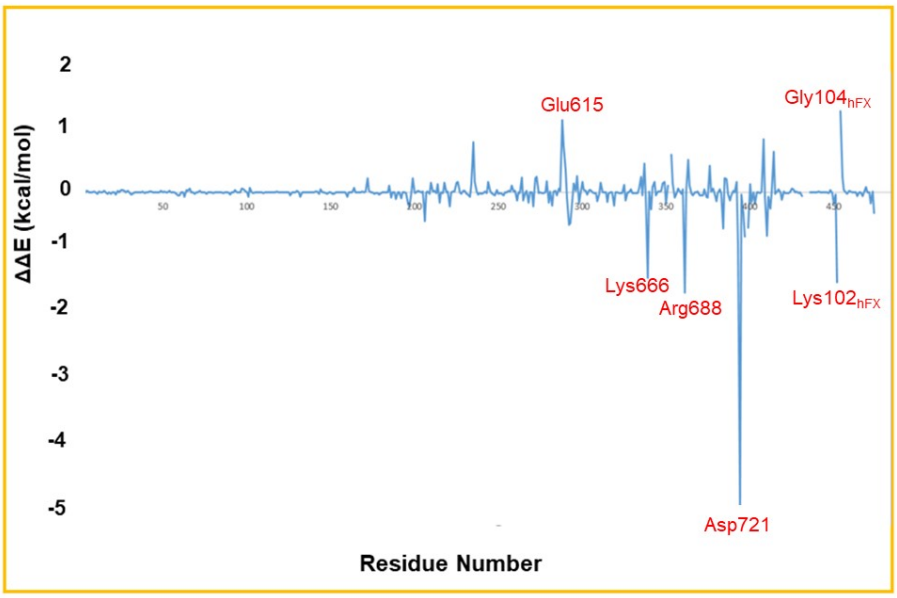


Figure S31. Energy Decomposition Analysis of the HAT step based on Snapshot 1. Residues stabilizing/destabilizing IM4 over RC2 are marked in red.

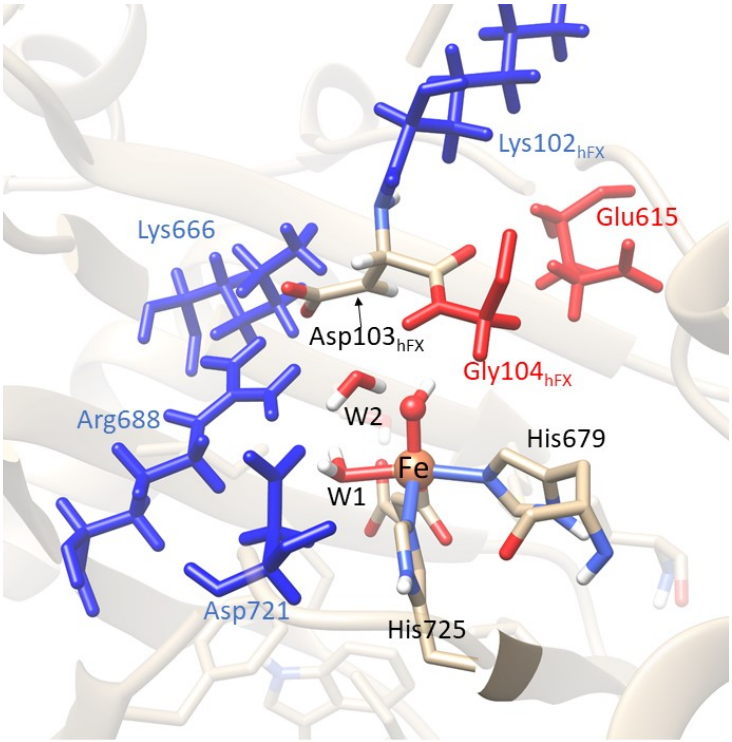


Figure S32. SCS residues stabilizing (blue) and destabilizing (red) the IM4 relative to RC2.

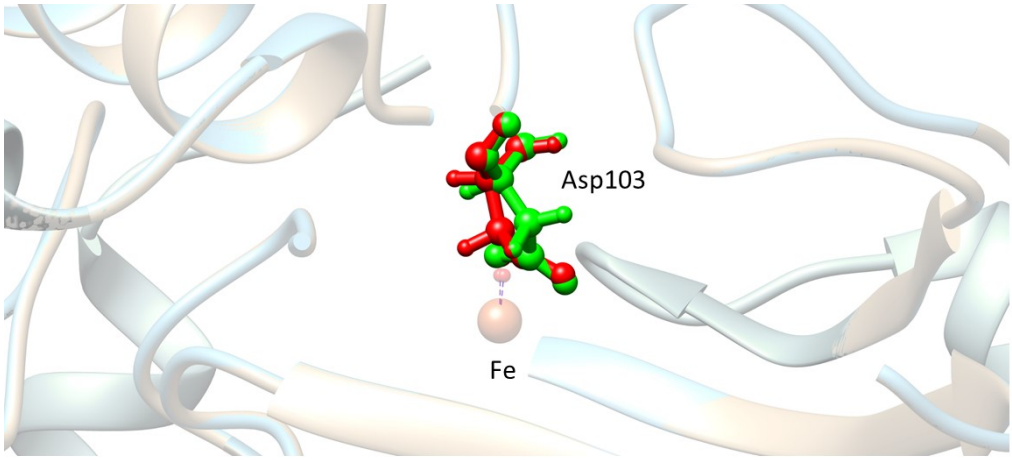


Figure S33. Superimposed structures of Fe center and $Asp103_{hFX}$ in TS_{proR} (green) and TS_{proS} (red)

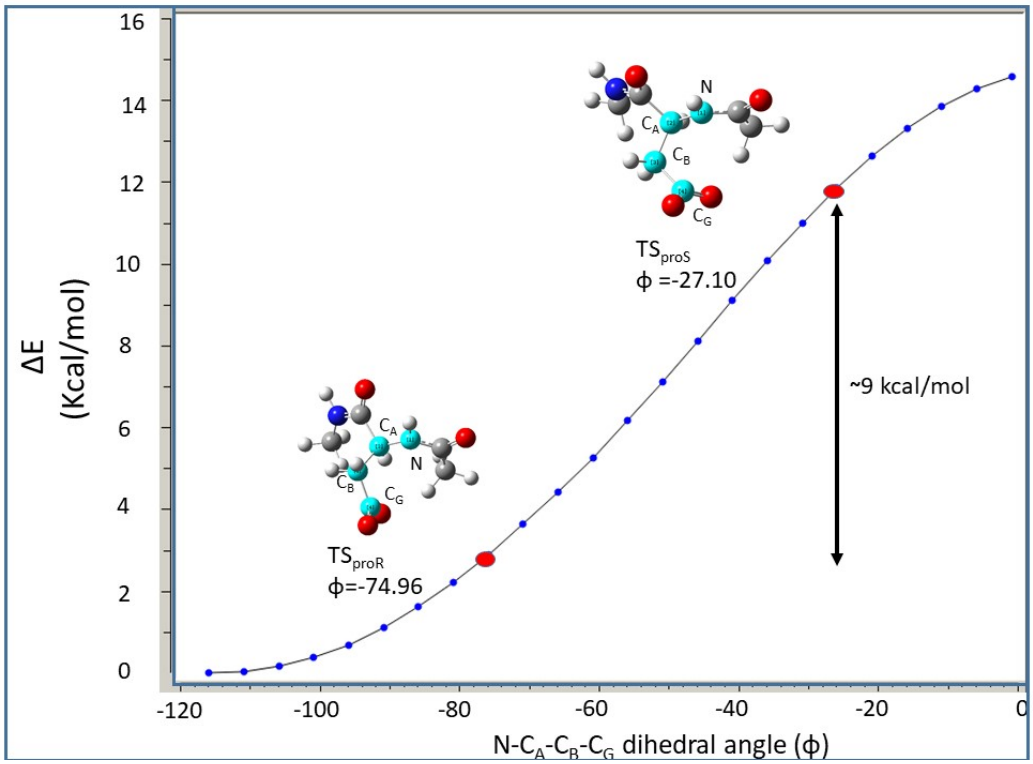


Figure S34. QM energy scan varying the $N\text{-}C_A\text{-}C_B\text{-}C_G$ dihedral angle, at the DFT/UB3LYP/def2-SVP level. Stationary points corresponding to TS_{proR} and TS_{proS} dihedral angles from snapshot 1 are marked in red.

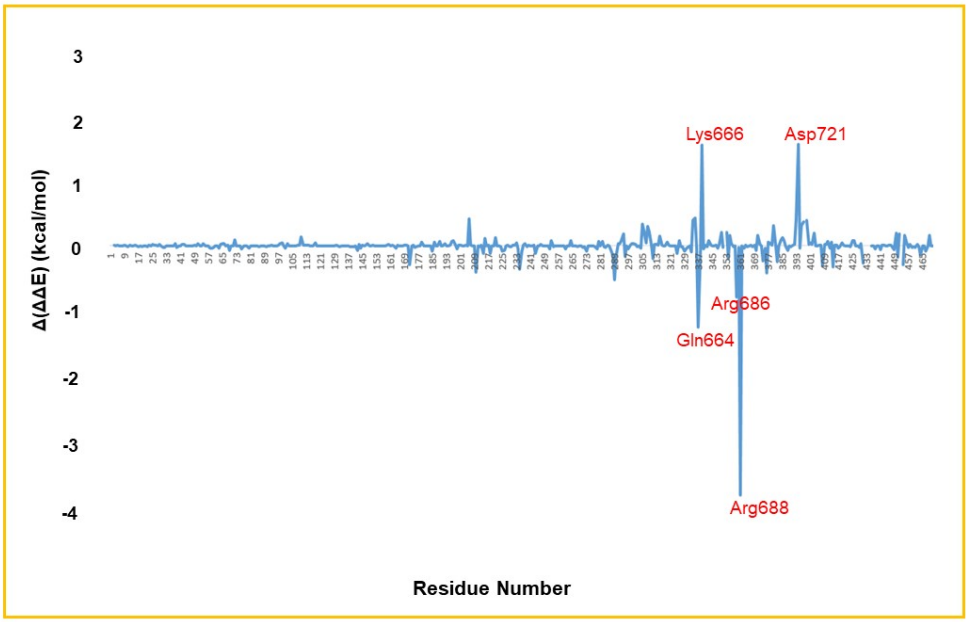


Figure S35. Energy Decomposition Analysis of HAT step. Residues stabilizing/destabilizing TS_{proR} over TS_{proS} are marked in red.

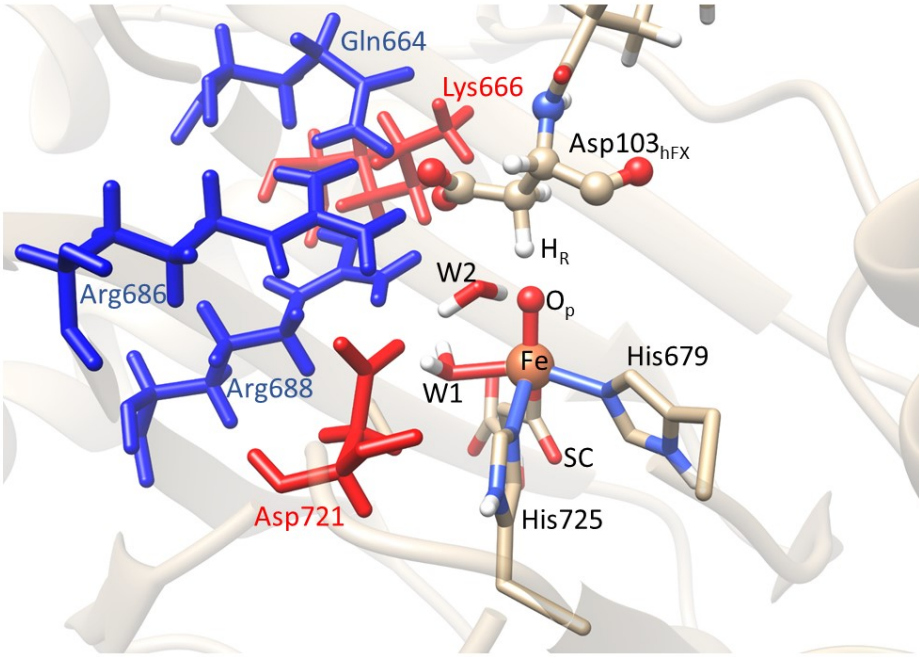


Figure S36. Second sphere residues contributing to stereoselectivity, as obtained from Energy Decomposition Analysis (EDA). Residues in blue stabilize, while residues in red destabilize TS_{proR} over TS_{proS}. SC-succinate

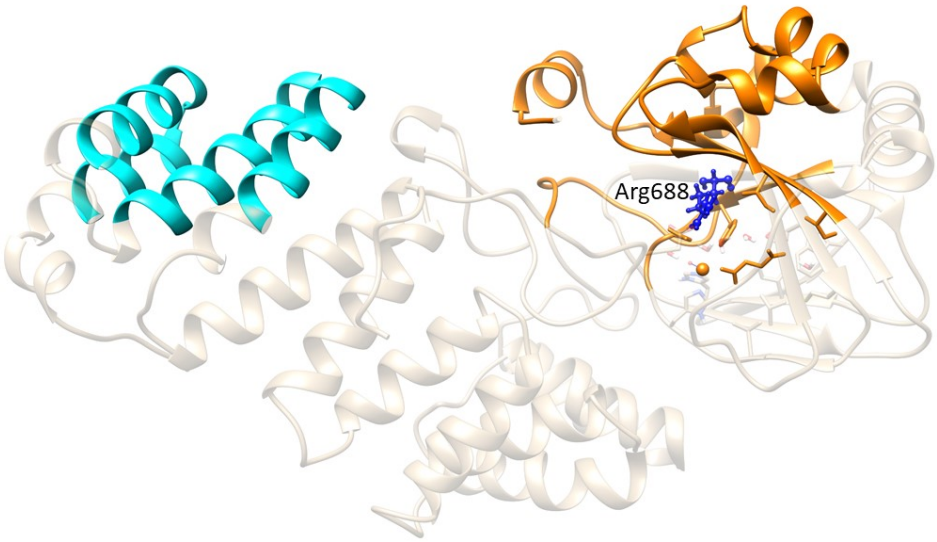


Figure S37. Residues showing positive (orange) and negative (cyan) correlated motion with Arg688 (blue).

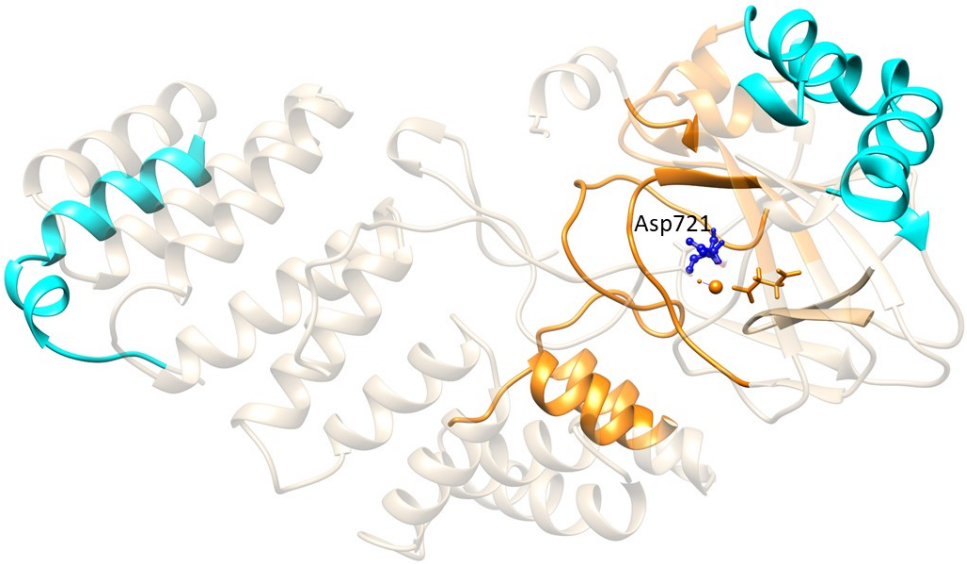


Figure S38. Residues showing positive (orange) and negative (cyan) correlated motion with Asp721 (blue).

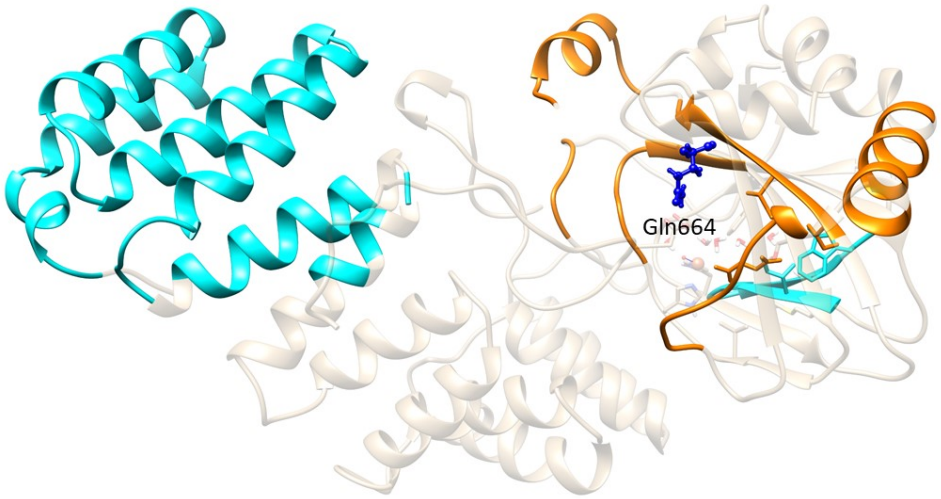


Figure S39. Residues showing positive (orange) and negative (cyan) correlated motions with Gln664 (blue).

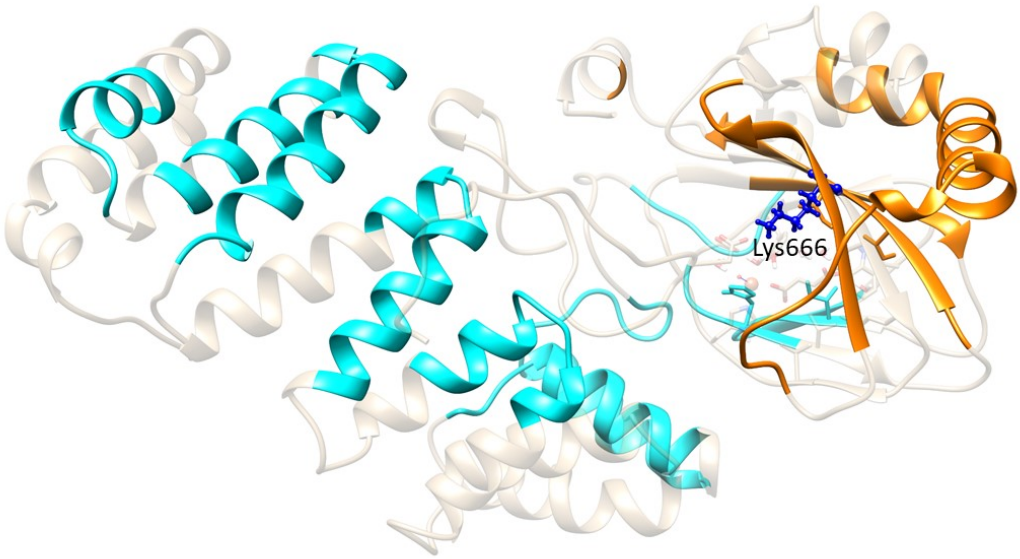


Figure S40. Residues showing positive (orange) and negative (cyan) correlated motion with Lys666 (blue).

Table S5. Internal Electric Field (IEF) (in atomic units) calculated along the Fe=O direction for *pro-R/S* HAT steps.

AspH Ferryl	RC2	TS_{proR}	TS_{proS}	ΔEF (TS_{proR} - RC2)	ΔEF (TS_{proS} - RC2)
Snapshot 1	-0.0038	-0.0211	-0.0229	-0.0173	-0.0191
Snapshot 2	-0.0143	-0.0298	-0.0305	-0.0155	-0.0162
Snapshot 3	-0.0146	-0.0301	-0.0340	-0.0155	-0.0194
Snapshot 4	0.0005	-0.0214	-0.0245	-0.0219	-0.0250
Snapshot 5	-0.0308	-0.0351	-0.0371	-0.0043	-0.0063

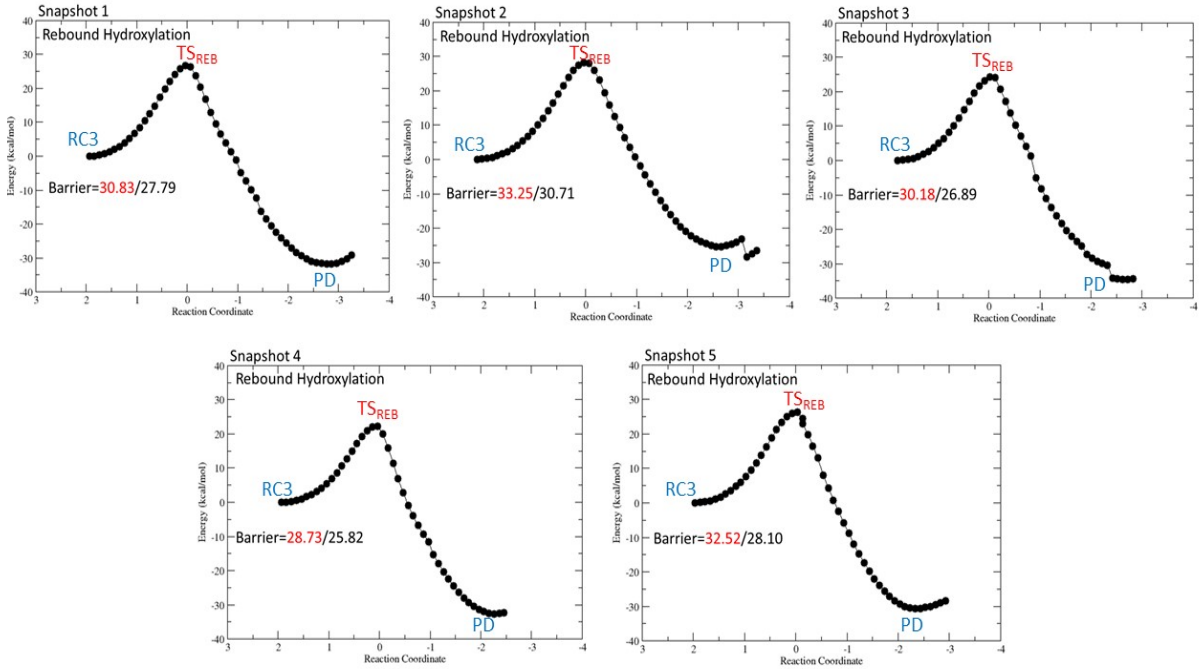


Figure S41. QM/MM energy scans (snapshots 1-5) for the rebound hydroxylation step, calculated at the UB3LYP/def2-SVP level. Energy barriers calculated at B2 (red) and B3 (black) are provided. Reaction coordinate is defined as the difference between the O_p-C_B and Fe-O_p distances (d1(O_p-C_B) — d2(Fe-O_p)).

Table S6. Computed energy barriers with dispersion corrections (D3-BJ) for representative snapshots in the rebound hydroxylation step.

	B2 (kcal/mol)	B3 (kcal/mol)
Snapshot 1	28.5	25.5
Snapshot 4	26.4	23.4

Table S7. Spin densities of stationary points involved in the rebound hydroxylation step.

		Fe	**O_p**	**C_B**
Snapshot 1	RC3/IM4	4.27	0.27	-0.90
	TS_{REB}	4.06	0.19	-0.57
	PD	3.82	0	0
Snapshot 2	RC3/IM4	4.24	0.28	-0.88
	TS_{REB}	4.03	0.18	-0.50
	PD	3.78	0	0
Snapshot 3	RC3/IM4	4.23	0.23	-0.88
	TS_{REB}	3.96	0.11	-0.47
	PD	3.79	0	0
Snapshot 4	RC3/IM4	4.23	0.29	-0.89
	TS_{REB}	4.07	0.18	-0.54
	PD	3.81	0	0
Snapshot 5	RC3/IM4	4.22	0.25	-0.89
	TS_{REB}	3.98	0.14	-0.46
	PD	3.81	0	0

Table S8. Geometric parameters for stationary points involved in the rebound hydroxylation step.

AspH WT		**d(Fe-O_P) (Å)**	**d(O_P-C_B) (Å)**	**<(Fe-O_P-C) (deg)**	**φ(N-C_A-C_B-C_G) (deg)**
Snapshot 1	RC3/IM4	1.85	3.78	151.5	-87.70
	TS_{REB}	2.20	2.23	165.5	-79.55
	PD	4.21	1.44	-	-76.05
Snapshot 2	RC3/IM4	1.84	3.97	130.3	-90.60
	TS_{REB}	2.17	2.17	160.9	-74.54
	PD	4.01	1.44	-	-68.46
Snapshot 3	RC3/IM4	1.87	3.65	171.1	-110.13
	TS_{REB}	2.34	2.19	175.0	-88.93
	PD	4.10	1.42	-	-80.80
Snapshot 4	RC3/IM4	1.83	3.77	151.5	-86.08
	TS_{REB}	2.11	2.18	173.1	-76.35
	PD	3.70	1.43	-	-63.00
Snapshot 5	RC3/IM4	1.87	3.83	167.6	-88.51
	TS_{REB}	2.30	2.27	174.1	-82.26
	PD	3.82	1.45	-	-74.01

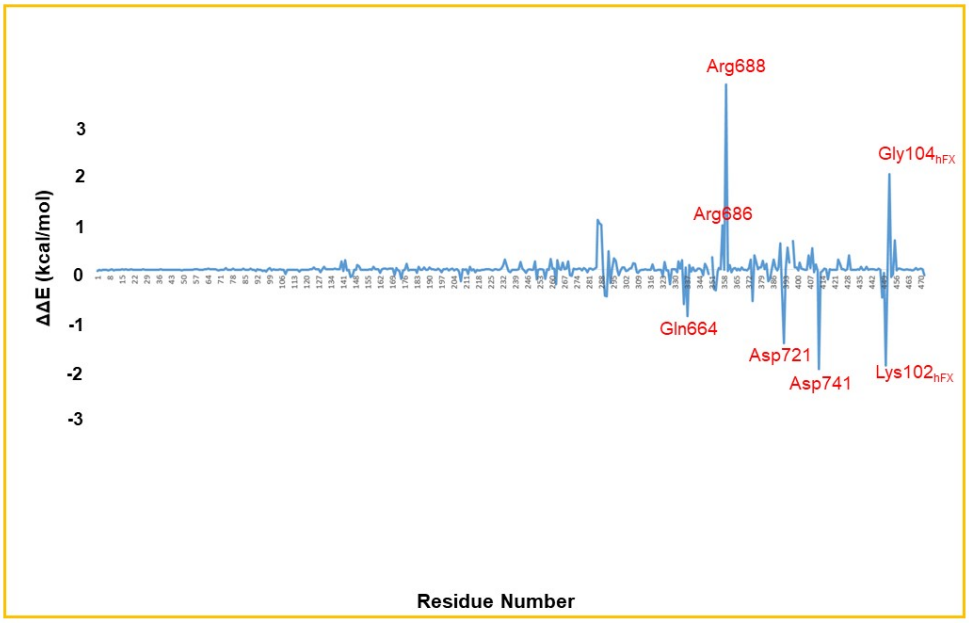


Figure S42. Energy Decomposition Analysis of the rebound step based on Snapshot 1. Residues stabilizing/destabilizing TS_{REB} are marked in red.

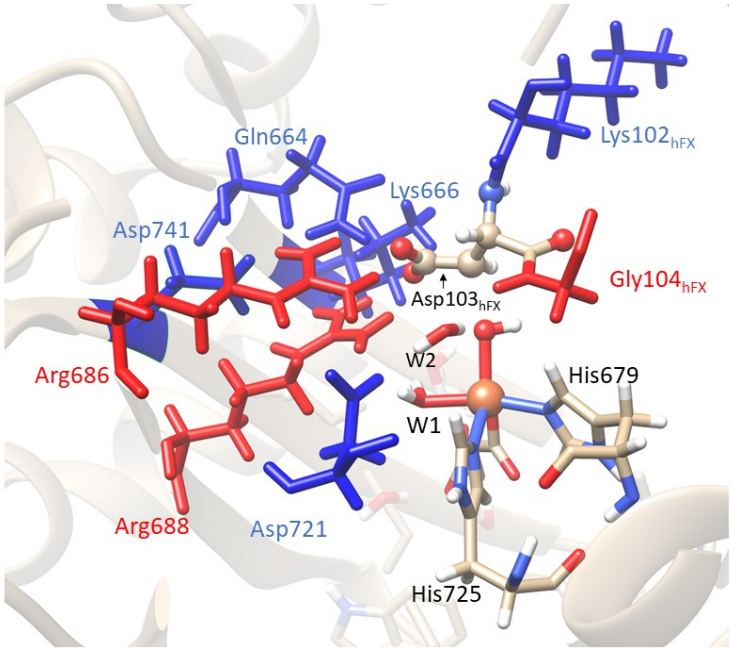


Figure S43. Second sphere residues involved in rebound hydroxylation, obtained from Energy Decomposition Analysis (EDA). Residues in blue stabilize, while residues in red destabilizes TS_{REB}.

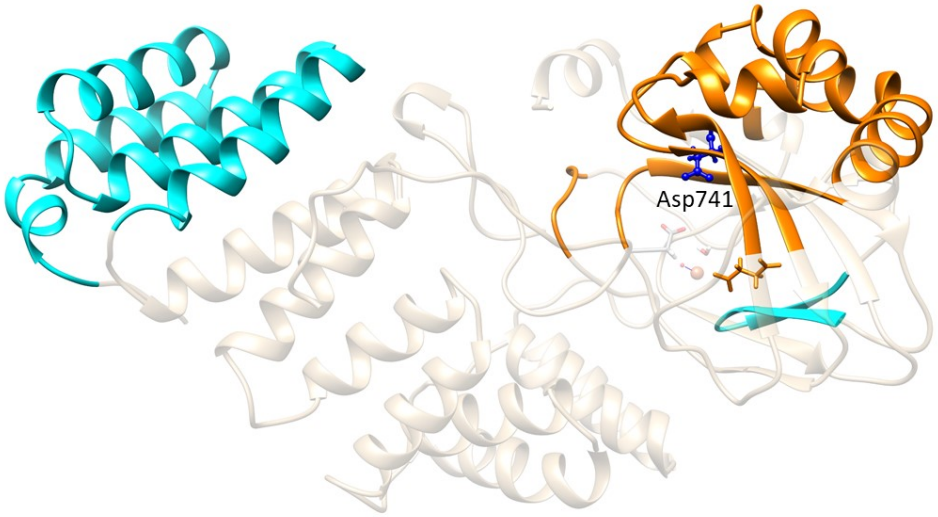


Figure S44. Residues showing negative (cyan) and positive correlated motions (orange) with Asp741 (yellow).

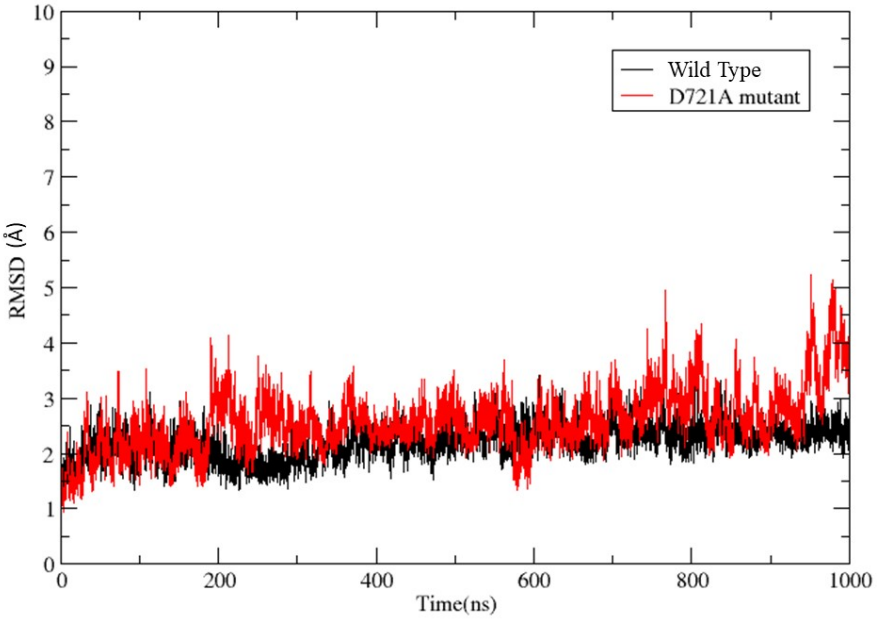


Figure S45. RMSD plot for AspH WT and the D721A mutant Fe(IV)=O complexes obtained from 1μs MD.

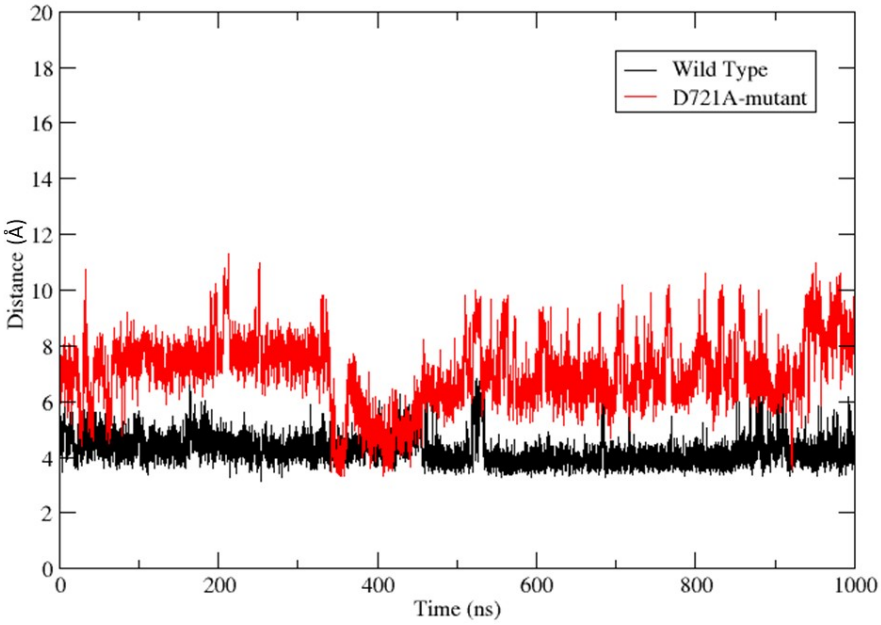


Figure S46. O_P-C_B distance plot for AspH WT and the D721A mutant Fe(IV)=O complexes obtained from 1µs MD.

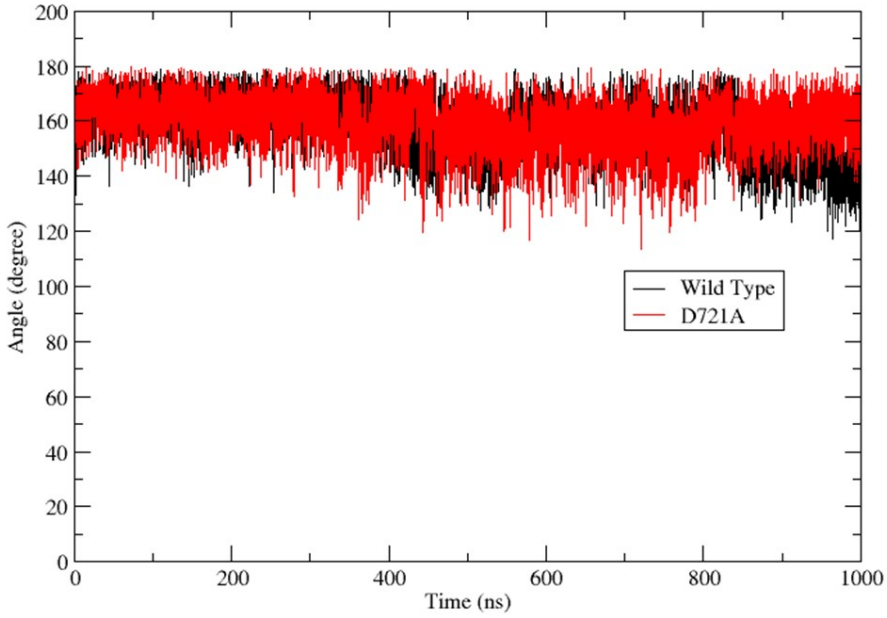


Figure S47. Fe-O_p-C_B angle plot for AspH WT and the D721A mutant Fe(IV)=O complexes obtained from 1µs MD.

Table S9. Key geometric parameters of the Fe(IV)=O intermediate for AspH WT and the D721A mutant, from 1μs MD simulations.

AspH - Ferryl	**Average-RMSD (Å)**	**Average $d(O_p\text{-}H_R)$ (Å)**	**Average $<(Fe\text{-}O_p\text{-}H_R)$ (Å)**	**Average $d(O_p\text{-}C_B)$ (Å)**	**Average $<(Fe\text{-}O_p\text{-}C_B)$ (Å)**
Wild type	2.53	3.34	154.6	4.25	157.7
D721A	2.31	6.43	157.3	7.03	159.2

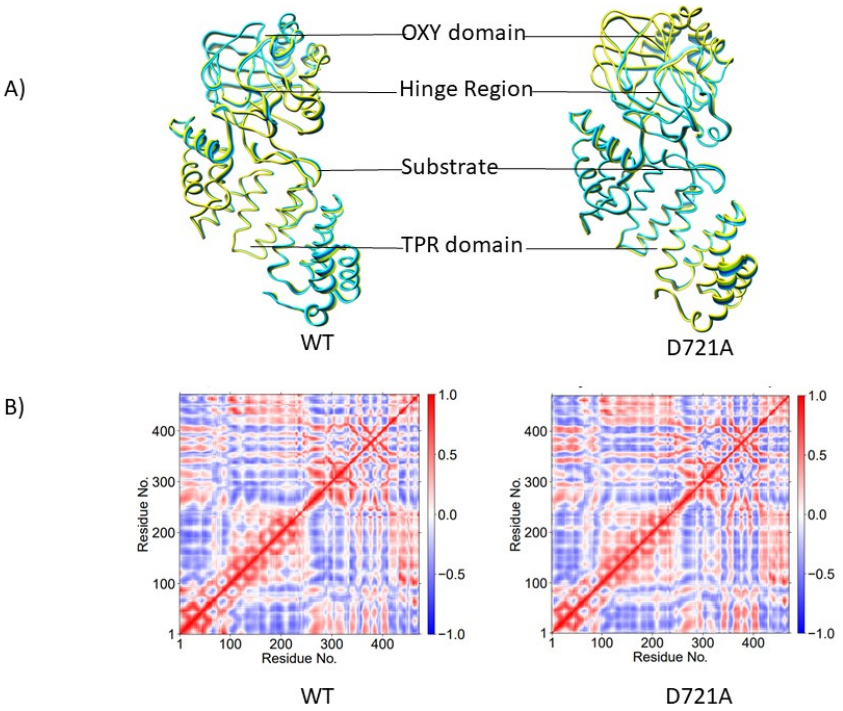


Figure S48. A) PCA and B) DCCA plots for AspH WT and the D721A mutant ferryl complexes. Residues 1-429 are AspH protein residues; 430-Fe, 431-O_p, 432- succinate, 433-W1, and 434-472 are EGFD substrate residues; 451-$Asp103_{hFX}$. The motion of the residues in PCA (part A) is indicated by the color change from yellow to blue.

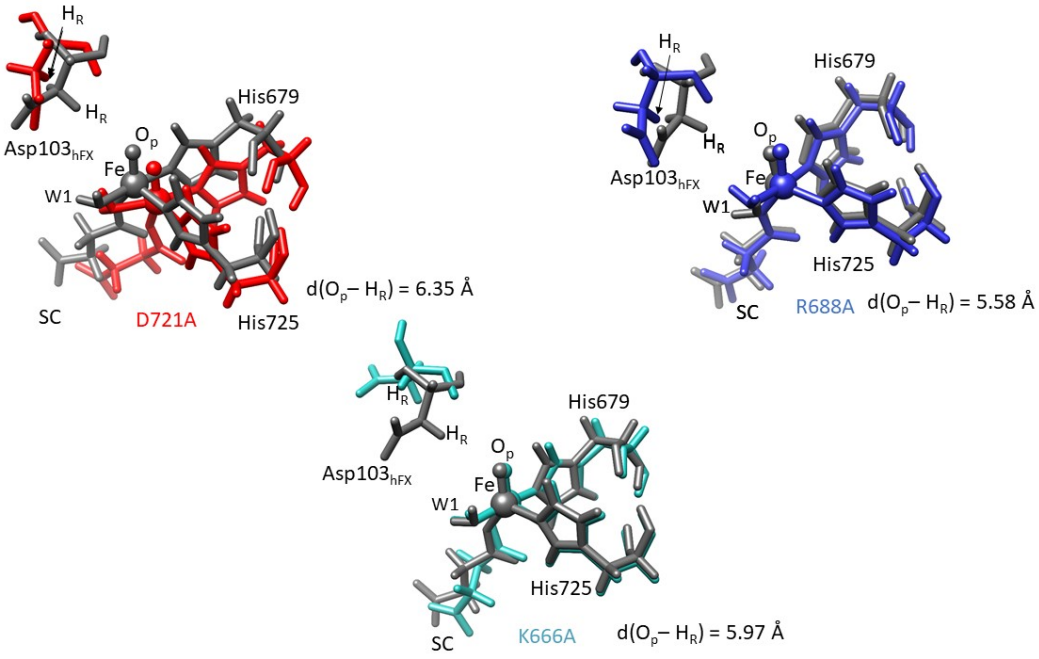


Figure S49. QM/MM optimized structures of AspH WT (black), D721A (red), R688A (blue), K666A (cyan) mutants superimposed, showing Fe(IV)=O and hFX substrate positioning in the ferryl complex. SC-succinate.

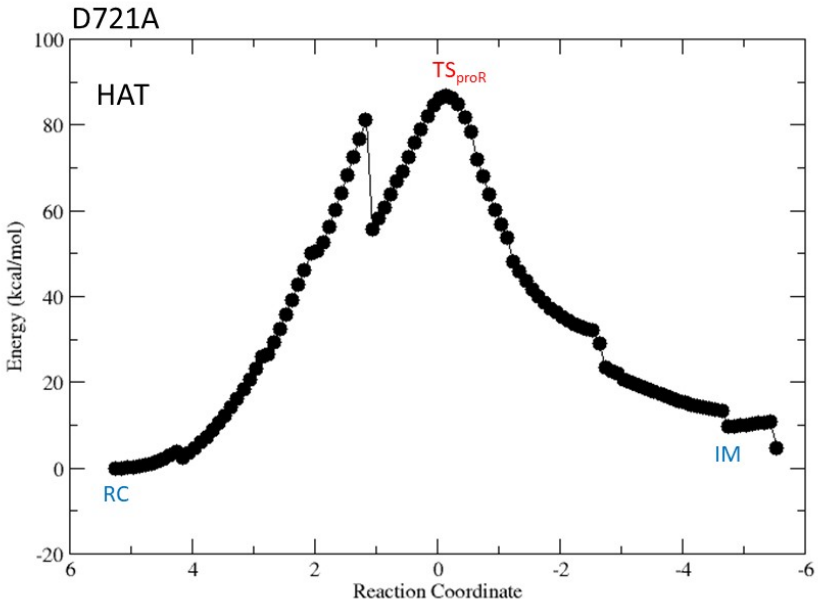


Figure S50. QM/MM energy scan for the HAT step for the D721A mutant calculated at the UB3LYP/def2-SVP level. Reaction coordinate is defined as the difference between the O_p-H_R and C_B-H_R distances (d1(O_p-H_R) — d2(C_B-H_R)).

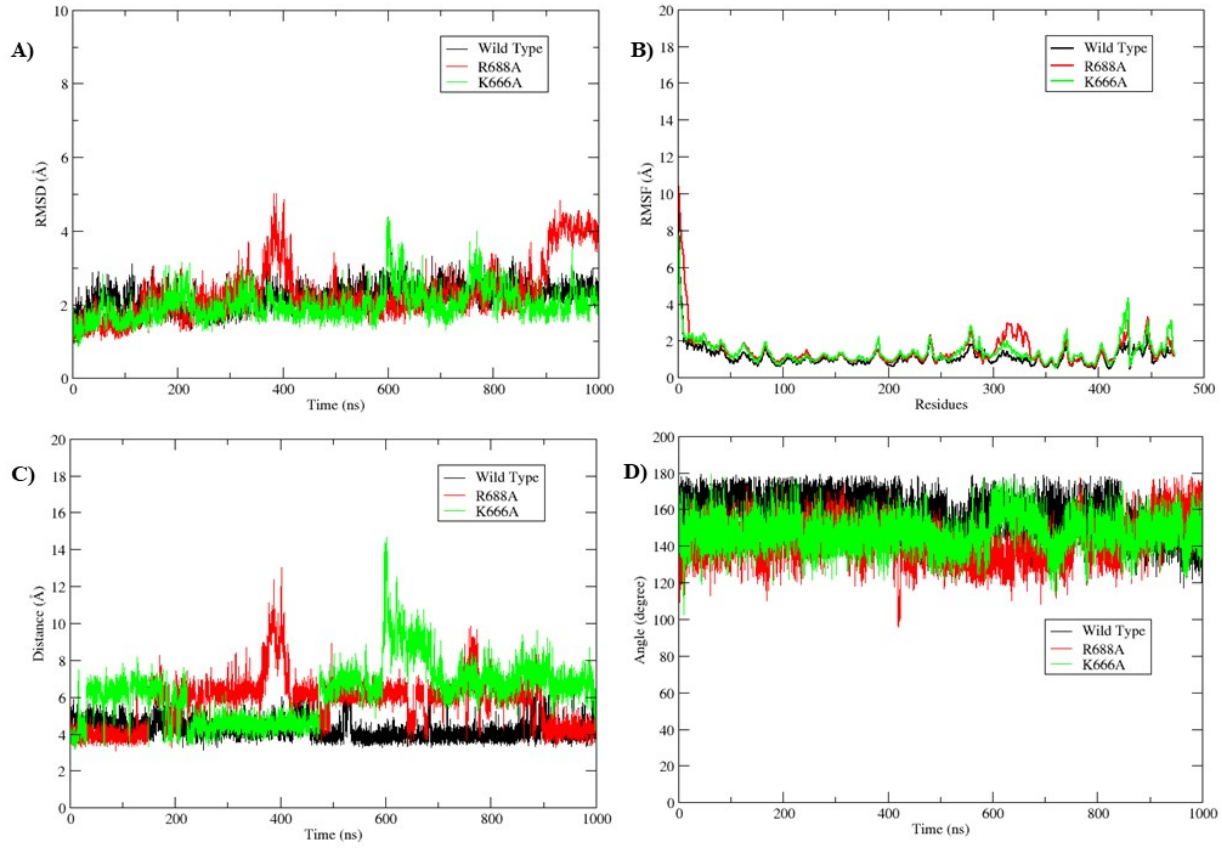


Figure S51. A) RMSD. B) RMSF. C) O_p-C_B Distance. D) Fe-O_P-C_B angle plots for AspH WT and mutants - R688A, K666A from 1 µs MD simulation.

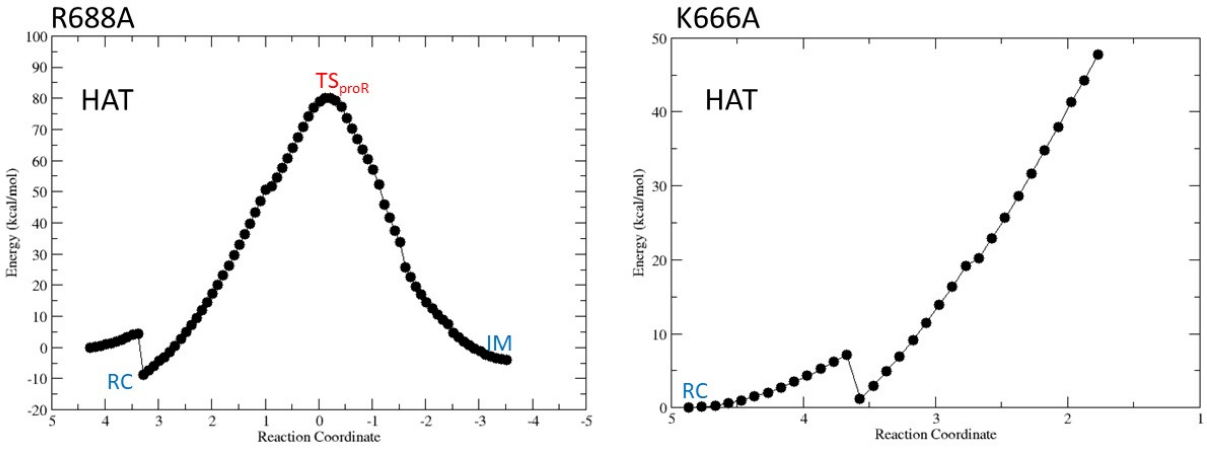


Figure S52. QM/MM energy scans for the HAT step for mutants A) R688A. B) K666A calculated at the UB3LYP/def2SVP level. Reaction coordinate is defined as the difference between the O_p-H_R and C_B-H_R distances (d1(O_p-H_R) — d2(C_B-H_R)).

Cartesian Coordinates for the QM/MM Optimized Structures

Dioxygen Activation Step – Substrate Binding Mode A (productive)

RC1

C	34.8345976	55.6945873	45.6068694
N	34.2171102	56.8845582	45.2892055
H	34.5617768	57.8197429	45.5467335
C	33.0763701	56.6013984	44.6296960
H	32.3902635	57.3533602	44.2447791
N	32.9284246	55.2845000	44.4998130
C	34.0217785	54.7052499	45.1064475
H	34.1603835	53.6255654	45.1341864
C	34.4087979	55.1108885	40.1261753
N	34.8903588	53.9372664	40.6618611
H	35.7508963	53.4356111	40.3930443
C	34.0204268	53.5228390	41.5999934
H	34.1370230	52.6023174	42.1651910
N	32.9953574	54.3656523	41.6984711
C	33.2336058	55.3713463	40.7847609
H	32.5632570	56.2186760	40.6702722
Fe	31.4797451	54.3528652	43.1809469
O	30.2073167	54.7940226	44.7732855
O	29.0270401	55.1642840	44.6744715
C	29.0681133	54.9566081	41.6878684
C	29.6908095	56.3459173	42.0109212
C	27.8921846	57.8616237	42.8316596
C	26.9264761	59.0211282	42.3936430
O	28.0218269	54.8808697	41.0602900
O	29.7752798	53.9710797	42.1334796
O	30.8160653	56.3299796	42.5246642
O	26.5210842	58.9811569	41.2101400
C	28.9340018	57.5814762	41.7218787
O	26.6528155	59.8493536	43.2823840
H	27.2638531	56.9696206	42.9916306
H	28.3752742	58.1188626	43.7844989
H	29.6389793	58.4208510	41.6458056
H	28.3637811	57.4774480	40.7886821
O	31.8105981	52.2936709	43.5848081
H	31.4844035	51.7510016	44.3271697
H	31.7916415	51.6689741	42.7617808
N	29.5638350	48.2807414	48.5733582
H	29.6274701	48.8864798	49.4018524
C	29.3577326	48.8803702	47.2482750
H	29.2453082	48.0796188	46.4917360
C	28.0648773	49.7093707	47.1127549
H	27.2606510	49.1629351	47.6335062
H	28.1452993	50.6947926	47.5889218
C	27.6487239	49.8560369	45.6444413
O	27.7542723	48.8231694	44.9291077
O	27.2011804	50.9560808	45.2297128
C	30.5989212	49.6574646	46.7345766
O	30.4936388	50.4164703	45.7752436
H	29.4575898	47.2992823	48.7327995
H	31.5348700	49.4648686	47.2589552
H	35.8262143	55.6444026	46.0565849
H	34.9266992	55.7052227	39.3734394

TS1

C	34.8719189	55.6912132	45.6253924
N	34.2542931	56.8782264	45.2949462
H	34.5920611	57.8162786	45.5504141
C	33.1208033	56.5882137	44.6272297
H	32.4319115	57.3321183	44.2325515
N	32.9780163	55.2708525	44.5044917
C	34.0648909	54.6967003	45.1253339
H	34.2033528	53.6173758	45.1620633
C	34.4022991	55.1048989	40.1076140
N	34.9114996	53.9449723	40.6512759
H	35.7789903	53.4570654	40.3798764
C	34.0565016	53.5167874	41.5939014
H	34.1930584	52.6046612	42.1681148
N	33.0120885	54.3367360	41.6827438
C	33.2201115	55.3433898	40.7617442
H	32.5156187	56.1639206	40.6506059
Fe	31.5365536	54.3929732	43.1703873
O	30.0732730	54.8301238	44.5917061
O	29.1404409	55.6566333	44.0879339
C	28.9242831	54.7853994	41.9082747
C	29.5238846	56.1611109	42.7694841
C	27.5990867	57.8526217	43.3029339
C	26.7697048	58.9790994	42.6359099
O	27.8465300	54.8648752	41.3598715
O	29.7626094	53.8510296	42.0328260
O	30.8160143	56.1462883	42.5899439
O	26.4959384	58.8686393	41.4197396
C	28.7682036	57.4465503	42.4119277
O	26.4139751	59.9197733	43.3854136
H	26.9083175	57.0066563	43.4478159
H	27.9362800	58.1833886	44.2951386
H	29.5331954	58.2388971	42.3998002
H	28.3875053	57.3395863	41.3865922
O	31.8224945	52.3174274	43.5922827
H	31.5053327	51.7911162	44.3512563
H	31.7797041	51.6856314	42.7767228
N	29.5912270	48.3070544	48.5683808
H	29.6533537	48.9094069	49.3996557
C	29.3734671	48.9186692	47.2493333
H	29.2758124	48.1219540	46.4864556
C	28.0712080	49.7316230	47.1188711
H	27.2752248	49.1817372	47.6488930
H	28.1469791	50.7231159	47.5832122
C	27.6442060	49.8628904	45.6533531
O	27.7658321	48.8292776	44.9399810
O	27.1734227	50.9514097	45.2359491
C	30.6040884	49.7200676	46.7425802
O	30.4856188	50.5004690	45.8032710
H	29.4684438	47.3271188	48.7252954
H	31.5436772	49.5159288	47.2559675
H	35.8659131	55.6458366	46.0703449
H	34.9158963	55.7058234	39.3571649

IM1

C	34.9116621	55.7373829	45.7925667
N	34.2738321	56.9173660	45.4771223
H	34.6264145	57.8603582	45.6906909
C	33.0957472	56.6139291	44.8972616
H	32.3872951	57.3557582	44.5321904
N	32.9403816	55.2944845	44.8198282
C	34.0689058	54.7344640	45.3785262
H	34.2095941	53.6557877	45.4279800
C	34.4674400	55.1406582	40.2329231
N	34.9646314	53.9475424	40.7090788
H	35.7932038	53.4358434	40.3698204
C	34.1732087	53.5435549	41.7191838
H	34.3067138	52.6097643	42.2570337
N	33.1891133	54.4111071	41.9237061
C	33.3667086	55.4227918	41.0042803
H	32.7071552	56.2879267	40.9689693
Fe	31.6992250	54.3009382	43.4194921
O	29.7343305	53.7812078	43.5498607
O	28.7957630	54.8443738	43.3051206
C	29.7527327	54.3262603	40.4033417
C	29.3590409	55.9947316	42.9256989
C	27.9817512	58.1230126	43.4208829
C	26.9231312	59.0777883	42.7744954
O	28.8259916	54.9866207	40.1561002
O	30.6551743	53.6422020	40.6459080
O	30.5863262	56.1145471	42.9063506
O	26.4664809	58.7356307	41.6554059
C	28.3634491	57.0041547	42.4474851
O	26.6403488	60.0846913	43.4494371
H	27.5442227	57.7122524	44.3442817
H	28.8563060	58.7201265	43.7246625
H	28.7912315	57.4569671	41.5404695
H	27.4427411	56.4937817	42.1353581
O	32.0546236	52.1780076	43.6689333
H	31.7223256	51.6158318	44.3911581
H	31.9467829	51.6162723	42.8191280
N	29.5744212	48.2196654	48.5974277
H	29.6418677	48.8315932	49.4208706
C	29.3600572	48.8121306	47.2732006
H	29.2092730	48.0138595	46.5223693
C	28.0837595	49.6696288	47.1776501
H	27.2829551	49.1402171	47.7209100
H	28.2006771	50.6509196	47.6534561
C	27.6232511	49.8330828	45.7296248
O	27.7043601	48.8115708	44.9948383
O	27.1637323	50.9425679	45.3515716
C	30.6023464	49.5699033	46.7360837
O	30.5071519	50.2520394	45.7205071
H	29.4639744	47.2388054	48.7576982
H	31.5295413	49.4372920	47.2935692
H	35.9271970	55.6943795	46.1861473
H	34.9433302	55.7268479	39.4468084

TS2

C	34.9140708	55.6841777	45.7945220
N	34.2792526	56.8648542	45.4739644
H	34.6313670	57.8084070	45.6883554
C	33.1071848	56.5659688	44.8856253
H	32.4071752	57.3066877	44.5046142
N	32.9501798	55.2443811	44.8103040
C	34.0747594	54.6800654	45.3762261
H	34.2146731	53.6013440	45.4229019
C	34.4545497	55.1280680	40.2240503
N	34.9569120	53.9396636	40.7078474
H	35.7939607	53.4349078	40.3786308
C	34.1557177	53.5246346	41.7032458
H	34.2969936	52.5966835	42.2479646
N	33.1563522	54.3820816	41.8904201
C	33.3380642	55.3988126	40.9750030
H	32.6691244	56.2555048	40.9353225
Fe	31.6810009	54.3142068	43.4013194
O	29.9648228	53.8471306	43.6774973
O	28.9008033	55.2899760	43.4888471
C	29.6522704	54.3852921	40.5225243
C	29.5976129	56.2471843	42.9961697
C	27.8568004	58.1080758	43.5304582
C	26.8612319	59.0460243	42.7776102
O	28.7185255	55.0511806	40.3251026
O	30.5614499	53.6876893	40.7019555
O	30.8453949	56.1467102	42.8026966
O	26.5444128	58.7013966	41.6098178
C	28.8572959	57.4858817	42.5583296
O	26.4557720	60.0350117	43.4187667
H	27.2480986	57.3187836	44.0011171
H	28.3457453	58.6697844	44.3400214
H	29.6191491	58.2104135	42.2342025
H	28.2611698	57.2140914	41.6667501
O	32.2839424	52.1841265	43.6602929
H	31.8382014	51.6754144	44.3614155
H	32.1131634	51.6272028	42.8108620
N	29.5676675	48.2290571	48.5898280
H	29.6401306	48.8420469	49.4121427
C	29.3614261	48.8186889	47.2624104
H	29.1995173	48.0193581	46.5154460
C	28.0954434	49.6920641	47.1634329
H	27.2882947	49.1756528	47.7097303
H	28.2259616	50.6744946	47.6340108
C	27.6370980	49.8530080	45.7135178
O	27.6980034	48.8241125	44.9878321
O	27.1992081	50.9685532	45.3264882
C	30.6103382	49.5645564	46.7226965
O	30.5260851	50.2282886	45.6937874
H	29.4618535	47.2478626	48.7511737
H	31.5316470	49.4423762	47.2921948
H	35.9298598	55.6487549	46.1882023
H	34.9363837	55.7170576	39.4436699

IM2

C	34.8778964	55.6789647	45.7678580
N	34.2393698	56.8602913	45.4540368
H	34.5892139	57.8036045	45.6755853
C	33.0725427	56.5627004	44.8563886
H	32.3681425	57.3008975	44.4789672
N	32.9234531	55.2395614	44.7686038
C	34.0472513	54.6737610	45.3366969
H	34.1908321	53.5952640	45.3741270
C	34.4398806	55.1341351	40.1973146
N	34.9528694	53.9539211	40.6912191
H	35.7962893	53.4546841	40.3679002
C	34.1556084	53.5344886	41.6846215
H	34.3065691	52.6141298	42.2385704
N	33.1440024	54.3827955	41.8595587
C	33.3155612	55.3974867	40.9379999
H	32.6347274	56.2443000	40.8894638
Fe	31.6688828	54.3251041	43.3460563
O	30.0805343	53.5790550	43.6053227
O	28.8449847	55.3543605	43.5582292
C	29.5978713	54.4214932	40.5316433
C	29.5622798	56.2423257	43.0572205
C	27.8988484	58.1619580	43.5295834
C	26.9209035	59.0933906	42.7542930
O	28.6459964	55.0712187	40.3742789
O	30.5291592	53.7417965	40.6637838
O	30.8325511	56.0671661	42.8344917
O	26.6737579	58.7834456	41.5598296
C	28.9507284	57.5512393	42.6081037
O	26.4440248	60.0460147	43.4035340
H	27.2797827	57.3580328	43.9597109
H	28.3397231	58.7172248	44.3707160
H	29.7658195	58.2521474	42.3732136
H	28.4158769	57.3420326	41.6604045
O	32.4082740	52.1956204	43.6647144
H	31.9233400	51.7281622	44.3685060
H	32.1993542	51.6341068	42.8237670
N	29.5547365	48.2137618	48.5991253
H	29.6296842	48.8279661	49.4200717
C	29.3562344	48.7995590	47.2696690
H	29.1822138	48.0006156	46.5251495
C	28.0997499	49.6865605	47.1702770
H	27.2904856	49.1835009	47.7258306
H	28.2427863	50.6715351	47.6320573
C	27.6321931	49.8417484	45.7223786
O	27.6895604	48.8111171	44.9990688
O	27.1892512	50.9549592	45.3362941
C	30.6115743	49.5307867	46.7287519
O	30.5371942	50.1799566	45.6897710
H	29.4566106	47.2316555	48.7597806
H	31.5300382	49.4176175	47.3046711
H	35.8909829	55.6423721	46.1683364
H	34.9263226	55.7255946	39.4216754

IM3

C	34.8651383	55.6135232	45.7504965
N	34.2197950	56.7895756	45.4315652
H	34.5603458	57.7346455	45.6529035
C	33.0571390	56.4750279	44.8280156
H	32.3519551	57.2091793	44.4478361
N	32.9169010	55.1540283	44.7390499
C	34.0426198	54.6024587	45.3132448
H	34.1956014	53.5254081	45.3470565
C	34.4222544	55.1460171	40.1730379
N	34.9543817	53.9816146	40.6839248
H	35.8082202	53.4946955	40.3723512
C	34.1470402	53.5530791	41.6672013
H	34.3185434	52.6444516	42.2338099
N	33.1106445	54.3731910	41.8169182
C	33.2769421	55.3835985	40.8927406
H	32.5732054	56.2094148	40.8203922
Fe	31.5951782	54.2156294	43.3136464
O	30.1651474	53.3393680	43.3149435
O	29.0982422	55.9047255	44.3905977
C	29.4334789	54.5285458	40.6501158
C	29.6632125	56.4120765	43.4343534
C	28.1361777	58.4479563	43.6022095
C	27.0336362	59.1587866	42.8208365
O	28.3895370	55.0384962	40.7539903
O	30.4448813	53.9895808	40.4801916
O	30.7773398	55.9810115	42.8970173
O	26.7256463	58.8229483	41.6585124
C	29.0898900	57.6509644	42.7204988
O	26.4262216	60.0765285	43.4407355
H	27.6197638	57.7577947	44.2851535
H	28.6550098	59.1744859	44.2464856
H	29.9143082	58.2611935	42.3226539
H	28.5286220	57.2728773	41.8485192
O	32.5452252	52.2061696	43.7035028
H	31.9968747	51.7854456	44.3887617
H	32.3068509	51.6528023	42.8687962
N	29.5297197	48.1941849	48.6049237
H	29.6104886	48.8112319	49.4230235
C	29.3358581	48.7730995	47.2722148
H	29.1629540	47.9705686	46.5315810
C	28.0782965	49.6579907	47.1683871
H	27.2706982	49.1558185	47.7271168
H	28.2194873	50.6459998	47.6234733
C	27.6075658	49.8053088	45.7210338
O	27.6665422	48.7738665	45.0005434
O	27.1575494	50.9146481	45.3318675
C	30.5917756	49.5042104	46.7312928
O	30.5206105	50.1358518	45.6828610
H	29.4459917	47.2109737	48.7669635
H	31.5069362	49.4049439	47.3149823
H	35.8755732	55.5904254	46.1586068
H	34.9139930	55.7389989	39.4019141

Dioxygen Activation – Substrate Binding Mode B (unproductive)

RC1'

C	28.8801502	55.5051573	56.9429404
N	28.4123123	56.4912684	57.7802388
H	27.9052470	57.3344730	57.4872973
C	28.7022043	56.1252998	59.0489537
H	28.4450901	56.7147690	59.9265070
N	29.3307173	54.9521527	59.0668326
C	29.4464309	54.5563559	57.7535125
H	29.9063120	53.6146337	57.4657657
C	25.3096956	53.5861503	60.0166560
N	25.6626134	52.4664386	59.2964650
H	25.0408278	51.8803188	58.7186491
C	26.9784471	52.2499709	59.4736062
H	27.5308722	51.4501289	58.9848564
N	27.4963990	53.1679617	60.2879965
C	26.4610614	54.0102948	60.6337320
H	26.6063213	54.8602714	61.2965589
Fe	29.5956034	53.5021677	60.6796117
O	30.1254183	51.9384290	59.6319450
O	29.8655560	51.4782241	58.4613098
C	29.4600220	53.3181103	63.5631190
C	29.4769343	54.8454211	63.2680688
C	29.4562888	57.2543853	64.1930213
C	29.5376252	58.0112907	65.5488570
O	29.4591090	52.9253992	64.7224055
O	29.4004564	52.5966192	62.5032408
O	29.2549690	55.1890522	62.1061827
O	30.4851804	58.8257104	65.6734880
C	29.7514367	55.7739732	64.3948847
O	28.6580098	57.7327055	66.3964766
H	30.1473545	57.7083786	63.4710120
H	28.4304633	57.3424096	63.8014439
H	29.2163217	55.3919514	65.2765282
H	30.8160884	55.5923065	64.6547502
N	34.7938944	51.3796143	59.1947463
H	35.5370779	52.0724414	59.1515533
C	33.4702184	51.7967264	58.7480764
H	32.7339251	51.0449094	59.0798296
C	33.0982582	53.1340756	59.4283944
H	33.9943032	53.7781447	59.4886952
H	32.3723953	53.6716600	58.8052510
C	32.4856293	53.0295020	60.8248140
O	32.9162215	52.2448753	61.6663203
O	31.4962679	53.8456907	61.0395801
C	33.3248480	51.9833184	57.2157410
O	34.3092080	52.2543075	56.5500932
H	35.1241220	50.4670616	58.9535643
H	32.3232096	51.8399282	56.8104930
H	28.7928693	55.4924892	55.8565299
H	24.3084136	54.0164108	60.0360585

TS1'

C	28.8581627	55.7598789	56.8132057
N	28.2880427	56.7682135	57.5530668
H	27.7460272	57.5616909	57.1883087
C	28.5687276	56.5377942	58.8527560
H	28.2282214	57.1773976	59.6644816
N	29.2956911	55.4360306	58.9864594
C	29.4861609	54.9435496	57.7174282
H	30.0651875	54.0429007	57.5282485
C	25.4827619	53.6667934	59.9082510
N	25.8517755	52.5162295	59.2461876
H	25.2294941	51.8831318	58.7211320
C	27.1851566	52.3647782	59.3894562
H	27.7295465	51.5228473	58.9663371
N	27.7014488	53.3578129	60.1097761
C	26.6405661	54.1742430	60.4429461
H	26.7725767	55.0627561	61.0557200
Fe	29.7345691	54.0650710	60.5981394
O	30.2457143	52.2651867	61.2863098
O	30.6803354	53.0453405	62.2613302
C	29.0399688	52.8113746	63.9812630
C	29.4606104	54.7260250	63.2774702
C	29.5589812	57.0935542	64.2445104
C	29.6727837	57.8763796	65.5813401
O	29.5569070	52.7901459	65.0703726
O	28.3424713	52.2029403	63.2201195
O	29.1913273	55.2008789	62.1722243
O	30.6144485	58.7041087	65.6634028
C	29.8957536	55.6090228	64.4078738
O	28.8061077	57.6247682	66.4503336
H	30.1925184	57.5614040	63.4800936
H	28.5091204	57.1572092	63.9149255
H	29.4650685	55.2093199	65.3339457
H	30.9828446	55.4149166	64.5233834
N	34.9008535	51.3920118	59.1506079
H	35.6619191	52.0635239	59.2051643
C	33.6540629	51.8240678	58.5529426
H	32.8302137	51.2137256	58.9761816
C	33.4026478	53.3004078	58.9108549
H	34.3637844	53.8383390	58.8961025
H	32.7599124	53.7325028	58.1337287
C	32.7002237	53.5531976	60.2383498
O	33.1637285	53.1132911	61.2832612
O	31.6179610	54.2594730	60.0822399
C	33.5736279	51.8002170	57.0081789
O	34.5807806	51.9347727	56.3387583
H	35.2101266	50.4574126	58.9749775
H	32.5617420	51.6998828	56.6156408
H	28.7898935	55.6500350	55.7309212
H	24.4664443	54.0563586	59.9665917

IM1'

C	28.8076471	55.6395288	56.7569011
N	28.2723405	56.6511928	57.5194333
H	27.7559424	57.4689010	57.1732490
C	28.5317624	56.3706214	58.8144467
H	28.2058561	56.9903665	59.6469468
N	29.2110189	55.2359077	58.9241184
C	29.3902092	54.7699450	57.6442243
H	29.9210435	53.8428531	57.4399427
C	25.2774977	53.5709348	59.9259743
N	25.6715303	52.4578035	59.2173436
H	25.0736901	51.8553217	58.6325077
C	26.9909448	52.2744663	59.4353541
H	27.5564980	51.4609563	58.9850125
N	27.4715042	53.2043103	60.2573106
C	26.4021501	54.0202325	60.5702050
H	26.5213159	54.8752146	61.2293674
Fe	29.4716269	53.9714003	60.6326561
O	30.9116278	54.6186683	61.8421301
O	30.5039733	55.3534368	62.9899894
C	29.7132863	53.0113193	64.2418631
C	29.2558296	55.7857042	62.9465819
C	29.7867257	57.6639716	64.5534292
C	29.4940308	58.3439652	65.9052836
O	30.0927412	53.4457753	65.2492568
O	29.2643267	52.5309925	63.2818622
O	28.5245824	55.5637206	61.9813670
O	30.3649747	59.1793028	66.2547919
C	28.8609045	56.4985190	64.2097498
O	28.4503466	58.0342148	66.5202546
H	30.8313318	57.3269636	64.5814239
H	29.7446768	58.4373408	63.7672460
H	27.8136684	56.8070044	64.1207875
H	28.9132422	55.7730958	65.0365436
N	34.7509628	51.3077738	59.1445185
H	35.4732916	52.0226881	59.1928888
C	33.4494027	51.7108752	58.6321857
H	32.7558470	50.8589898	58.7704151
C	32.9093083	52.8784222	59.5125706
H	33.7571314	53.4078976	59.9728153
H	32.3478359	53.5970001	58.8994727
C	31.9709111	52.3135190	60.5852691
O	32.4650669	51.7858831	61.5955033
O	30.7211073	52.3491169	60.2993601
C	33.3986345	52.0587336	57.1265368
O	34.4161228	52.3045433	56.5056264
H	35.1187169	50.4160326	58.8808404
H	32.4012000	52.0005055	56.6908762
H	28.7396016	55.5704090	55.6712407
H	24.2722946	53.9921697	59.9399007

HAT step

Snapshot 1

RC2

C	41.3781687	30.9548196	36.4108864
N	40.4840320	29.9206676	36.2423965
H	39.8064033	29.8384323	35.4713626
C	40.6282029	29.0697149	37.2724611
H	40.0661946	28.1476938	37.4285143
N	41.5837625	29.5148170	38.0907741
C	42.0612593	30.6917763	37.5644997
H	42.8677195	31.2350658	38.0478101
C	43.7037094	26.4607112	35.6980298
N	44.7590544	27.3417400	35.7739789
H	45.4920803	27.5020208	35.0655642
C	44.6592807	27.9991676	36.9422687
H	45.3588814	28.7627434	37.2726633
N	43.6034643	27.5678944	37.6276859
C	42.9908475	26.6030527	36.8610934
H	42.0853727	26.0927422	37.1876901
Fe	42.7717553	28.4395783	39.3552864
O	43.7721169	29.7236937	39.5129509
O	39.8672642	26.4747553	39.0241205
C	40.4108326	26.6605571	40.0974263
C	38.8764227	25.0325337	41.4582539
C	38.5023307	24.5762085	42.9075251
O	41.3902281	27.5445834	40.2619681
O	37.8163631	23.5378885	42.9717765
C	40.1003602	25.9348977	41.4003462
O	38.8860966	25.2862100	43.8739570
H	37.9950801	25.5632957	41.0569800
H	39.0014934	24.1320650	40.8389524
H	41.0156047	25.3691144	41.6565075
H	40.0126713	26.6959211	42.1885645
O	44.0005042	27.2198370	40.4816875
H	44.9611332	27.5206366	40.4587365
H	43.6712642	27.2916866	41.4240379
N	45.1251217	33.9593263	43.9730477
H	44.2821321	34.0105185	44.5509915
C	45.0652349	33.0874580	42.7968468
H	46.1003942	32.8635846	42.4798582
C	44.4463859	31.7511044	43.2131450
H	43.5182484	31.9229477	43.7797293
H	44.1430530	31.1914110	42.3097522
C	45.3670612	30.8008746	43.9981923
O	44.7739875	29.8911059	44.6489069
O	46.6110232	30.9161904	43.8930985
C	44.2681240	33.6854330	41.6127087
O	43.3913168	34.5011318	41.8426265
H	45.5249056	34.8614540	43.8108415
H	44.5676669	33.3751532	40.6116754
H	41.5373561	31.7740197	35.7097177
H	43.4829856	25.8239293	34.8413752

TS_{proR}

C	41.5806719	31.2200481	36.6388110
N	40.6413687	30.2172826	36.5473018
H	39.9654882	30.0975216	35.7799264
C	40.7384995	29.4574353	37.6560420
H	40.1572049	28.5580571	37.8646223
N	41.6942848	29.9306937	38.4538073
C	42.2295336	31.0316677	37.8316824
H	43.0364461	31.5964634	38.2889448

C	43.7168140	26.8432008	36.1256949
N	44.8164861	27.6735001	36.1330063
H	45.5409439	27.7544098	35.4052639
C	44.7777127	28.3982713	37.2706822
H	45.5378363	29.1309740	37.5344920
N	43.7213874	28.0691307	38.0099096
C	43.0466455	27.0915718	37.3017588
H	42.1298429	26.6393285	37.6803592
Fe	42.7993840	28.8736007	39.9147927
O	43.5387221	30.1806879	40.8461088
O	40.1356508	26.7624133	39.2953483
C	40.5563948	26.9393124	40.4294244
C	39.1014916	25.0508134	41.5320717
C	38.7244887	24.4751917	42.9222418
O	41.3334220	27.9624685	40.7629189
O	38.3035903	23.2894206	42.9451673
C	40.2728118	26.0241272	41.6102197
O	38.8382674	25.2162782	43.9293873
H	38.2031700	25.5678518	41.1485224
H	39.3073261	24.2135723	40.8513357
H	41.2098064	25.4680061	41.8015548
H	40.1331266	26.6679141	42.4860565
O	43.9566447	27.2782899	40.6890138
H	44.9408448	27.4520236	40.5814888
H	43.7430790	27.2760609	41.6589775
N	44.9472221	33.8953172	43.7216391
H	44.1316128	33.9320951	44.3369228
C	44.9047092	33.0004321	42.5439390
H	45.9496633	32.7833985	42.2579516
C	44.2984167	31.6559633	42.9298277
H	43.3012076	31.7594929	43.3866210
H	43.9378033	30.9044545	41.8757342
C	45.2356143	30.7479543	43.7431337
O	44.6744227	29.8891592	44.4816596
O	46.4746120	30.9042814	43.6233133
C	44.1521178	33.6167216	41.3328241
O	43.2635757	34.4200096	41.5395152
H	45.3969827	34.7805122	43.6028220
H	44.5118503	33.3333862	40.3436928
H	41.7372256	31.9896682	35.8830049
H	43.4965154	26.1291416	35.3321867

TS_{proS}

C	41.5707676	31.2131989	36.6155027
N	40.6203191	30.2200729	36.5346831
H	39.9344762	30.1074223	35.7751344
C	40.7240512	29.4568173	37.6396552
H	40.1369061	28.5630001	37.8576476
N	41.6960362	29.9198401	38.4237505
C	42.2362060	31.0152106	37.7970073
H	43.0632073	31.5640750	38.2370880
C	43.6678958	26.7515291	36.0752770
N	44.7579280	27.5918494	36.0537252
H	45.4687916	27.6761782	35.3131300
C	44.7257382	28.3363895	37.1757230
H	45.4767372	29.0906022	37.3914580
N	43.6848411	28.0091894	37.9399789
C	43.0109788	27.0122759	37.2565406
H	42.1023041	26.5581651	37.6514958
Fe	42.7653178	28.8505751	39.8778880
O	43.4306872	30.1590245	40.8771083
O	40.0714507	26.7826597	39.2838986
C	40.5187135	26.9329646	40.4105922
C	39.0747818	25.0506000	41.5411901
C	38.7248479	24.4757858	42.9465902
O	41.3206244	27.9481828	40.7332852

O	38.3268207	23.2870939	42.9839042
C	40.2538835	26.0155780	41.5904057
O	38.8480682	25.2470102	43.9344205
H	38.1742989	25.5773300	41.1753918
H	39.2608732	24.2098512	40.8587694
H	41.1920164	25.4543766	41.7634121
H	40.1359038	26.6556206	42.4731299
O	43.9605575	27.2789353	40.6433436
H	44.9324525	27.5003058	40.5422682
H	43.7348019	27.2677724	41.6104310
N	45.0322781	33.8504916	43.5975498
H	44.1807205	33.8337715	44.1625333
C	45.1106521	33.0593240	42.3520887
H	46.1447997	33.1798443	41.9786628
C	44.9992853	31.5143548	42.4429743
H	43.9765242	30.8944023	41.8540137
H	45.7114202	31.1414380	41.6967833
C	45.4319100	30.8058757	43.7379689
O	44.6469053	30.0992558	44.3941223
O	46.6702016	30.9384037	43.9506494
C	44.2047046	33.6288123	41.2110771
O	43.3387178	34.4240805	41.5093943
H	45.4546262	34.7553383	43.5441937
H	44.4578949	33.3503679	40.1881253
H	41.7257416	31.9819724	35.8585103
H	43.4408088	26.0478344	35.2744572

IM4

C	41.4037891	30.9494948	36.4521268
N	40.4942266	29.9439450	36.2230842
H	39.8357550	29.8951678	35.4335322
C	40.5847436	29.0615517	37.2340233
H	39.9980694	28.1480075	37.3272461
N	41.5107988	29.4555342	38.1015490
C	42.0355118	30.6343438	37.6262960
H	42.8234555	31.1540873	38.1655925
C	43.7020021	26.5275024	35.8081260
N	44.7587545	27.4070735	35.8815221
H	45.4918045	27.5627784	35.1717821
C	44.6705216	28.0564375	37.0568399
H	45.3874749	28.8079944	37.3804549
N	43.6181657	27.6264287	37.7515114
C	42.9995357	26.6652822	36.9784449
H	42.0969609	26.1523444	37.3114171
Fe	42.6482888	28.3435554	39.5122103
O	43.3060774	29.8733761	40.3154334
O	40.1023117	26.2832054	39.0868098
C	40.4494725	26.5361944	40.2264190
C	38.9378843	24.8020788	41.5112045
C	38.6371914	24.3191358	42.9690381
O	41.2399457	27.5879152	40.4965488
O	38.2886005	23.1262246	43.1034141
C	40.1261567	25.7541201	41.4801825
O	38.7629733	25.1811434	43.8805780
H	38.0331339	25.3192479	41.1427507
H	39.0979498	23.9198947	40.8762106
H	41.0512766	25.1986038	41.7295260
H	39.9982733	26.4782379	42.2948584
O	43.9500300	27.0144883	40.5354561
H	44.9036601	27.3247194	40.4660676
H	43.6724603	27.0993083	41.4892529
N	45.0962547	33.9927822	44.0017009
H	44.2540423	34.0405224	44.5809972
C	45.0660670	33.0671693	42.8592178

H	46.1100000	32.8433415	42.5742404
C	44.4789648	31.7892097	43.3612715
H	43.3907253	31.7053571	43.4448682
H	42.6825668	30.3895829	40.8470816
C	45.3209777	30.7308446	43.9724780
O	44.7019324	29.7917052	44.5599352
O	46.5757757	30.8223853	43.8716915
C	44.2711657	33.6122377	41.6372311
O	43.3565185	34.3895759	41.8433730
H	45.4996598	34.8905634	43.8249929
H	44.6075632	33.3084294	40.6459671
H	41.5901993	31.7820572	35.7737771
H	43.4868184	25.8799838	34.9581362

TS_{REB}

C	41.6202821	31.2851478	36.6461466
N	40.6325057	30.3270169	36.6278076
H	39.9308939	30.2065216	35.8833143
C	40.7362882	29.6039882	37.7606346
H	40.1346208	28.7294328	38.0185880
N	41.7446466	30.0582126	38.5061424
C	42.3088711	31.1044404	37.8172048
H	43.1734710	31.6349111	38.2043633
C	43.6967776	26.8512246	36.1362379
N	44.8023828	27.6732209	36.1501736
H	45.5293069	27.7526429	35.4249791
C	44.7611133	28.3993453	37.2862601
H	45.5251001	29.1268536	37.5536757
N	43.6972364	28.0790377	38.0197804
C	43.0196255	27.1062678	37.3068814
H	42.0959542	26.6635518	37.6799726
Fe	42.7965539	28.8660101	39.9127741
O	43.5091715	30.4687778	41.2380542
O	40.1185300	26.8968815	39.3337221
C	40.5521630	27.0148318	40.4714262
C	39.1072966	25.0899749	41.5387841
C	38.7353347	24.4881931	42.9331762
O	41.3462193	28.0253709	40.8287584
O	38.3482662	23.2993647	42.9426434
C	40.2800019	26.0601197	41.6181795
O	38.8369827	25.2605331	43.9262149
H	38.2107010	25.6189024	41.1670355
H	39.3075434	24.2603936	40.8469365
H	41.2208173	25.4999075	41.7796440
H	40.1520875	26.6731239	42.5186798
O	44.0418098	27.4679057	40.7931702
H	45.0339078	27.5800078	40.6732182
H	43.8150732	27.4020501	41.7580537
N	44.8807075	33.9052382	43.6730537
H	44.0690820	33.9461675	44.2932291
C	44.8502878	32.9966244	42.5019617
H	45.8978500	32.7721168	42.2338183
C	44.2657428	31.6764992	42.9596283
H	43.2265193	31.6831632	43.2970978
H	42.8045049	31.1216039	41.0971774
C	45.2065265	30.7435004	43.6970551
O	44.6720733	29.8740045	44.4407522
O	46.4433121	30.9130337	43.5421690
C	44.1021602	33.5942761	41.2808741
O	43.1742511	34.3548019	41.4786421
H	45.3552284	34.7790269	43.5667733
H	44.4956375	33.3402406	40.2966441
H	41.7693144	32.0347383	35.8689911
H	43.4814527	26.1340593	35.3441671

PD

C	41.4453300	30.9360990	36.4701812
N	40.5233130	29.9394127	36.2589741
H	39.8456910	29.9024114	35.4858824
C	40.6482010	29.0488312	37.2625235
H	40.0551726	28.1405713	37.3550646
N	41.6032222	29.4214668	38.1059725
C	42.1131726	30.6010965	37.6218016
H	42.9230583	31.1243883	38.1261781
C	43.7649339	26.3781075	35.5862504
N	44.7745957	27.3080788	35.6565568
H	45.4827261	27.5208757	34.9390541
C	44.6861241	27.9104656	36.8565932
H	45.3657810	28.6936036	37.1822836
N	43.6860865	27.4007682	37.5656752
C	43.0963839	26.4366119	36.7818731
H	42.2401783	25.8614897	37.1319942
Fe	42.6706758	28.0214401	39.3213880
O	43.8629561	30.9781446	42.0714900
O	40.9452911	26.4861511	39.4603230
C	40.9685565	26.7625794	40.6790295
C	39.1996666	25.0026937	41.5902310
C	38.7295937	24.4064718	42.9591816
O	41.6434698	27.8088557	41.0680250
O	38.3159220	23.2269069	42.9492942
C	40.3966538	25.9224251	41.7896171
O	38.8077293	25.1774106	43.9556484
H	38.3487256	25.5705456	41.1693670
H	39.4210320	24.1770784	40.8995285
H	41.2520288	25.3176378	42.1499890
H	40.1665465	26.6093132	42.6089747
O	44.0347406	26.5929416	40.4754216
H	44.9452712	26.9825147	40.3991472
H	43.7626552	26.7581203	41.3939401
N	45.0471785	33.9318792	43.8913894
H	44.2226521	33.9934325	44.4954830
C	44.9434092	33.0606954	42.7180977
H	45.9676916	32.8306163	42.3685153
C	44.3434465	31.7302645	43.2038353
H	43.4898361	31.9601255	43.8595596
H	43.0945087	30.4696977	42.3701822
C	45.3297742	30.8070154	43.9711486
O	44.7777040	29.9340773	44.6887209
O	46.5613844	30.9266472	43.7556221
C	44.1064774	33.6774497	41.5581356
O	43.2302500	34.4728242	41.8401655
H	45.4668251	34.8261098	43.7357594
H	44.3964414	33.4214082	40.5391014
H	41.6041462	31.7687436	35.7849458
H	43.5315528	25.7723838	34.7106368

Snapshot 2

RC2

C	44.1603082	29.1870617	46.0861427
N	43.7165102	28.0520229	46.7288429
H	42.7329661	27.7853546	46.8845941
C	44.7878752	27.3429821	47.1185381
H	44.7442960	26.3829712	47.6304311
N	45.9034969	27.9746567	46.7530445
C	45.5285500	29.1288564	46.1070407
H	46.2716156	29.8085606	45.7011317
C	45.6876912	25.0116873	43.4857742
N	46.1271582	26.0608186	42.7096400
H	45.9301013	26.2175127	41.7091361
C	46.9062727	26.8421346	43.4777339
H	47.4110867	27.7340341	43.1147015
N	47.0019525	26.3370214	44.7068487
C	46.2386263	25.1875465	44.7296723
H	46.1438303	24.5830280	45.6327895
Fe	47.7655009	27.1680585	46.4934340
O	48.4266513	28.6325610	46.1082791
O	46.7373529	24.2878461	48.0410016
C	47.5297703	25.0379718	48.5796838
C	47.9876074	23.4936563	50.6175934
C	48.9538558	23.2064818	51.8055229
O	47.7291532	26.2852218	48.1614942
O	49.9305261	23.9745421	51.9861519
C	48.4215915	24.6745961	49.7571829
O	48.6546094	22.2161265	52.5102002
H	46.9898646	23.6730666	51.0512263
H	47.8807336	22.5757801	50.0171436
H	49.4187397	24.4774059	49.3245976
H	48.5587234	25.5722433	50.3717927
O	49.5368984	26.1132062	46.1660261
H	49.9731271	26.3822954	45.2888180
H	50.1783840	26.3462613	46.9062396
N	52.4182029	32.8097480	47.3038120
H	52.6689407	32.7412714	48.2908640
C	51.4720755	31.8642903	46.7249745
H	51.8044233	31.6103153	45.7015750
C	51.4886220	30.5676387	47.5457742
H	51.3290333	30.7907650	48.6118323
H	50.6246666	29.9487289	47.2480498
C	52.7013200	29.6496301	47.3726214
O	52.7991257	28.6883384	48.1850311
O	53.4642944	29.8465966	46.3955560
C	49.9976544	32.3398716	46.7068536
O	49.6178135	33.0944431	47.5807857
H	52.3913535	33.7547135	46.9777879
H	49.3740938	31.9664043	45.8945966
H	43.514767	29.9164894	45.5978935
H	44.997468	24.2364940	43.1483203

TS_{proR}

C	44.2863086	29.3867120	46.0536540
N	43.9145276	28.2519972	46.7397568
H	42.9492866	27.9258638	46.8964356
C	45.0373123	27.6361075	47.1601792
H	45.0568132	26.6872851	47.6962240
N	46.1143308	28.3223135	46.7769868
C	45.6569961	29.4169666	46.0857000
H	46.3427681	30.1386373	45.6559702
C	45.8638748	25.3036531	43.6233799

N	46.2998752	26.2942925	42.7703087
H	46.0904709	26.3850465	41.7654403
C	47.0975444	27.1221504	43.4723460
H	47.6030422	27.9778622	43.0312989
N	47.2112563	26.7126714	44.7345061
C	46.4376356	25.5693854	44.8436785
H	46.3476856	25.0290115	45.7871459
Fe	48.0989276	27.5384369	46.5584211
O	49.1762029	28.9684913	46.6155152
O	46.6929844	24.7559341	48.0963121
C	47.6159702	25.3750708	48.6014568
C	47.9689873	23.6517570	50.5118196
C	48.8821807	23.2398254	51.6931250
O	47.9638147	26.5939333	48.2220846
O	49.8635706	23.9575995	52.0060386
C	48.5027477	24.8309031	49.7104413
O	48.5483270	22.1870342	52.2908214
H	46.9800250	23.8901544	50.9386633
H	47.8019344	22.7714494	49.8710891
H	49.4582983	24.5590263	49.2286747
H	48.7528708	25.6667277	50.3733024
O	49.6763275	26.1616696	46.1164239
H	50.1095981	26.4071869	45.2359339
H	50.3348524	26.3346109	46.8490235
N	52.2112288	32.7373027	47.2909478
H	52.4818033	32.6393140	48.2681106
C	51.2813619	31.7891451	46.6619774
H	51.6516227	31.5589582	45.6475196
C	51.2268363	30.4827738	47.4372162
H	50.8957459	30.6251571	48.4767817
H	50.1946449	29.6708110	46.9872896
C	52.4488502	29.5882957	47.3288306
O	52.6226132	28.7234960	48.2294444
O	53.2119482	29.7544964	46.3371215
C	49.8094561	32.3046082	46.5926696
O	49.4130593	33.0369377	47.4712296
H	52.2543512	33.6792131	46.9579048
H	49.2181877	31.9693310	45.7405792
H	43.5973724	30.0706141	45.5579605
H	45.2135702	24.4818452	43.3237088

TS_{proS}

C	44.2305003	29.3736512	46.0408426
N	43.8396204	28.2534569	46.7405815
H	42.8704992	27.9389679	46.8961997
C	44.9498116	27.6298754	47.1796073
H	44.9554354	26.6889630	47.7294611
N	46.0363820	28.2986643	46.7956607
C	45.6007064	29.3877089	46.0837197
H	46.3036292	30.0864985	45.6456682
C	45.8183783	25.2677360	43.6213732
N	46.2403416	26.2767453	42.7830411
H	46.0325981	26.3778322	41.7791972
C	47.0202607	27.1099976	43.4974139
H	47.5053005	27.9846359	43.0695905
N	47.1370710	26.6838716	44.7551975
C	46.3827284	25.5266668	44.8469460
H	46.2966025	24.9746898	45.7841160
Fe	47.9886669	27.4924206	46.6050345
O	49.0741297	28.8972700	46.6573208
O	46.6461826	24.7245196	48.1426086
C	47.5532868	25.3591626	48.6573567
C	47.9697432	23.6299766	50.5598997
C	48.9037960	23.2489806	51.7381294
O	47.8632264	26.5959741	48.2980107
O	49.8851390	23.9865823	52.0104145
C	48.4649516	24.8192553	49.7476158

O	48.5907338	22.2113537	52.3685364
H	46.9777500	23.8441925	50.9920360
H	47.8205230	22.7407764	49.9264090
H	49.4146423	24.5615393	49.2458979
H	48.7197200	25.6550125	50.4081714
O	49.5508524	26.0725917	46.1947044
H	49.9826361	26.3175522	45.3137616
H	50.1928026	26.2997023	46.9278060
N	52.1401079	32.6669034	47.1457585
H	52.2301231	32.5427003	48.1512563
C	51.2312848	31.8241551	46.3573615
H	51.4806294	32.0170183	45.2994313
C	51.3442863	30.2806828	46.5242919
H	50.2470129	29.6516451	46.8473376
H	51.3771807	29.8789103	45.5000257
C	52.6025260	29.6800437	47.1749688
O	52.5213722	28.8277794	48.0929237
O	53.6517296	30.0291889	46.5825581
C	49.7235960	32.2397318	46.4953374
O	49.4122425	32.9522140	47.4214336
H	52.2289568	33.6218172	46.8625312
H	49.0476686	31.9055373	45.7082521
H	43.5540612	30.0627755	45.5352685
H	45.1704305	24.4477671	43.3117252

IM4

C	44.0874513	29.2381849	46.0418018
N	43.6399515	28.1256406	46.7162850
H	42.6576862	27.8638596	46.8813492
C	44.7118010	27.4157580	47.1091757
H	44.6666703	26.4673951	47.6431252
N	45.8302649	28.0204776	46.7180747
C	45.4553804	29.1602113	46.0457275
H	46.1955955	29.8197010	45.6015047
C	45.6723631	25.0316369	43.4761199
N	46.1221905	26.0713787	42.6930226
H	45.9319441	26.2212301	41.6897898
C	46.9029583	26.8535934	43.4568331
H	47.4168712	27.7373399	43.0863325
N	46.9886795	26.3590221	44.6926678
C	46.2163791	25.2155146	44.7210258
H	46.1095837	24.6248666	45.6302752
Fe	47.7804020	27.2027851	46.4404097
O	48.5335903	28.8424815	46.0657701
O	46.7333109	24.7763630	48.0027597
C	47.6199822	25.3780070	48.5914296
C	47.9759436	23.6284287	50.4919635
C	48.8955949	23.1991674	51.6770123
O	47.9443327	26.6288020	48.2528548
O	49.8449642	23.9644030	52.0037665
C	48.4915929	24.8133293	49.6895396
O	48.5779166	22.1227302	52.2240955
H	46.9900740	23.8638964	50.9292397
H	47.8043274	22.7500892	49.8494680
H	49.4405490	24.5411067	49.1919521
H	48.7635018	25.6380084	50.3569867
O	49.5707904	26.0871048	46.1095770
H	50.0280141	26.3499945	45.2453658
H	50.1927883	26.3048224	46.8648476
N	52.4712509	32.8678607	47.3506963
H	52.7926762	32.7916354	48.3169543
C	51.5875715	31.8489943	46.7887880
H	51.9579993	31.5624676	45.7887562
C	51.6860746	30.6488867	47.6781638
H	51.0775881	30.6152947	48.5848741
H	48.5464123	29.4950789	46.7819331

C	52.6775416	29.5814865	47.4354451
O	52.7320086	28.6214003	48.2572102
O	53.4067516	29.6912219	46.4066008
C	50.0848146	32.2625116	46.7319117
O	49.6393611	32.9320405	47.6415443
H	52.4050357	33.8082077	47.0170266
H	49.5140732	31.9331770	45.8636606
H	43.4439458	29.9628851	45.5430259
H	44.9882083	24.2520451	43.1411036

TS_{REB}

C	44.3054809	29.4797776	46.0328910
N	43.9806441	28.3762869	46.7883883
H	43.0278477	28.0216291	46.9616473
C	45.1302596	27.8253543	47.2308857
H	45.1953027	26.9008348	47.8082347
N	46.1831595	28.5243877	46.7959718
C	45.6740520	29.5538975	46.0412955
H	46.3170095	30.2648753	45.5358647
C	45.8877629	25.3607770	43.6797994
N	46.3388110	26.3313913	42.8120647
H	46.1387021	26.4055311	41.8042231
C	47.1312039	27.1704970	43.5075633
H	47.6460891	28.0128413	43.0510916
N	47.2288902	26.7891369	44.7804120
C	46.4476198	25.6520905	44.9016196
H	46.3390002	25.1351679	45.8553691
Fe	48.1527366	27.6199291	46.5938738
O	49.5366782	29.2744383	46.7897062
O	46.6195845	25.1340489	48.2455605
C	47.6469285	25.6229090	48.6942046
C	48.0218182	23.7541232	50.4734682
C	48.9335499	23.2573239	51.6364837
O	48.0673509	26.8371094	48.3460401
O	49.8937600	23.9929402	52.0016485
C	48.5749666	24.9202100	49.6658374
O	48.5981029	22.1642585	52.1400521
H	47.0608378	24.0413359	50.9350373
H	47.7837548	22.8923855	49.8301767
H	49.4419720	24.5917662	49.0638099
H	48.9840525	25.6854897	50.3332133
O	49.7770774	26.3812793	46.1387759
H	50.2125570	26.5624825	45.2463864
H	50.4487419	26.4414317	46.8758886
N	52.1563494	32.7190449	47.3170132
H	52.4232732	32.6261257	48.2953675
C	51.2292079	31.7696227	46.6691794
H	51.6295356	31.5248235	45.6703118
C	51.2138795	30.4744282	47.4633386
H	50.7437205	30.5056603	48.4484758
H	48.9533022	29.8978450	47.2497873
C	52.4130524	29.5677653	47.3320894
O	52.6191746	28.7296855	48.2456910
O	53.1477082	29.7367501	46.3183970
C	49.7695888	32.2898378	46.5747534
O	49.3351104	32.9523594	47.4933392
H	52.2210126	33.6551918	46.9714414
H	49.2150332	32.0189125	45.6763467
H	43.5923820	30.1330663	45.5301277
H	45.2494500	24.5291667	43.3813900

PD

C	44.0823819	29.3468597	46.0000323
N	43.6560858	28.2673683	46.7365211
H	42.6786324	27.9942499	46.9152024
C	44.7436590	27.6021148	47.1646530

H	44.7164438	26.6788184	47.7446000
N	45.8546918	28.2018173	46.7365614
C	45.4528826	29.2934830	46.0038824
H	46.1629914	29.9585152	45.5186439
C	45.5989500	24.9724867	43.4178369
N	46.0573631	26.0175839	42.6510219
H	45.8788741	26.1788393	41.6478806
C	46.8180705	26.7986273	43.4374268
H	47.3351749	27.6835599	43.0722992
N	46.8829154	26.2992430	44.6716800
C	46.1152732	25.1528745	44.6744628
H	45.9838274	24.5554212	45.5768948
Fe	47.5700516	27.0080859	46.5160732
O	50.6483023	29.5538763	46.9141448
O	46.5554764	24.6395307	48.2298651
C	47.5084254	25.2363663	48.7159423
C	48.0167219	23.4783341	50.5785331
C	48.9769492	23.1120797	51.7482219
O	47.8306706	26.4671272	48.3433914
O	49.8946900	23.9284705	52.0433619
C	48.4672935	24.6608502	49.7375675
O	48.7243947	22.0318524	52.3231243
H	47.0354888	23.6952022	51.0353446
H	47.8485047	22.5777080	49.9661939
H	49.3850081	24.4057272	49.1746255
H	48.7781634	25.4843611	50.3887722
O	49.5852466	26.8809128	46.1552212
H	50.0606834	26.8672596	45.2675117
H	50.2313357	26.8537021	46.9155587
N	52.3932070	32.7855495	47.3146876
H	52.6850249	32.6994902	48.2887563
C	51.5026001	31.8187484	46.6964699
H	51.8553917	31.5976498	45.6719489
C	51.5799620	30.4885998	47.4762106
H	51.3390179	30.6737420	48.5358730
H	49.8402821	29.5299500	47.4382054
C	52.9132843	29.7142395	47.3738760
O	53.0544191	28.7725737	48.1971266
O	53.6594520	29.9796449	46.4054685
C	50.0050075	32.2537518	46.6727197
O	49.5918556	32.9155809	47.6045941
H	52.3716441	33.7295850	46.9855912
H	49.4054460	31.9503784	45.8144903
H	43.4206106	30.0403400	45.4811770
H	44.9124543	24.1995166	43.0724267

Snapshot 3

RC2

C	39.3395554	43.8467596	32.1884340
N	38.0800208	44.0399036	31.6674967
H	37.8251018	44.7287023	30.9460318
C	37.2425299	43.1749972	32.2661132
H	36.1788758	43.0987345	32.0515937
N	37.9042092	42.4326631	33.1469239
C	39.2177550	42.8384211	33.1098742
H	39.9625806	42.3495116	33.7322080
C	37.9804204	39.3661778	29.9099198
N	39.2260598	39.0571140	30.4118734
H	40.0525487	38.7392406	29.8856951
C	39.2018343	39.2792010	31.7389543
H	40.0436660	39.0990210	32.4027454
N	38.0023956	39.7137473	32.1135563
C	37.2255178	39.7722905	30.9784690
H	36.1857506	40.0906883	31.0018556
Fe	37.4222907	40.5531665	33.9607271
O	38.7971848	40.5782593	34.9088888
O	34.4044318	39.1124371	34.0149096
C	34.4322201	40.3556342	34.0565602
C	32.2069328	40.4139167	35.3159271
C	30.7377003	40.8682473	35.2343768
O	35.4978636	41.0528336	33.8269870
O	30.0353171	40.5713715	36.2440042
C	33.1604452	41.1437216	34.3677239
O	30.2959535	41.4183147	34.2131135
H	32.1903037	39.3436134	35.0575444
H	32.5376108	40.4714856	36.3635952
H	33.4330812	42.1413717	34.7383563
H	32.6320864	41.3050339	33.4129468
O	36.8934399	38.7225868	34.6672934
H	36.0393564	38.4883583	34.2284893
H	37.6692029	38.0584198	34.4726106
N	41.5842121	40.9151005	40.3476302
H	40.9500748	41.5416693	40.8374715
C	41.2381341	40.6113975	38.9577915
H	41.8280169	39.7369331	38.6354061
C	39.7531435	40.2164832	38.8839146
H	39.1371549	40.9787486	39.3925107
H	39.4245217	40.2464643	37.8330390
C	39.3346316	38.8223671	39.4002114
O	38.1089333	38.5726585	39.3348139
O	40.2185140	38.0278662	39.8248175
C	41.4754386	41.8092500	38.0069767
O	41.3813761	42.9373154	38.4625240
H	42.5303235	41.1788206	40.5355040
H	41.7385353	41.6106947	36.9680242
H	40.2276327	44.3763371	31.8435679
H	37.6908694	39.3237513	28.8599548

TS_{proR}

C	39.5780527	43.9127904	32.4939649
N	38.2805185	44.0933722	32.0705878
H	37.9728811	44.7247901	31.3155517
C	37.4886205	43.2994466	32.8180553
H	36.4103007	43.2259564	32.6952306
N	38.2096027	42.6182968	33.7052262
C	39.5183846	42.9922833	33.5106022
H	40.3124492	42.5493556	34.1031904
C	38.1580376	39.5477325	30.4519158

N	39.4142407	39.1514509	30.8579501
H	40.1641831	38.7532128	30.2752779
C	39.5302855	39.4159347	32.1736841
H	40.4151362	39.1687399	32.7564472
N	38.4127087	39.9641276	32.6453455
C	37.5438167	40.0487439	31.5732553
H	36.5369558	40.4467322	31.6726635
Fe	37.7907600	40.6849381	34.6303582
O	38.8516741	40.8563001	36.0576591
O	34.8068058	39.2282755	34.2725025
C	34.7800499	40.4624764	34.4454913
C	32.3934303	40.4047589	35.3376052
C	30.9429624	40.8832863	35.2501962
O	35.8472093	41.1899801	34.5415437
O	30.1868585	40.5821070	36.2165154
C	33.4310176	41.1772469	34.5143870
O	30.5112926	41.4838287	34.2455261
H	32.3804773	39.3580004	34.9934696
H	32.6649276	40.3708461	36.4031432
H	33.5692072	42.2009235	34.8843242
H	33.0595564	41.2661533	33.4789053
O	37.2596325	38.7399832	34.9761112
H	36.3870020	38.6035569	34.5245711
H	37.9820293	38.0540529	34.7012059
N	41.4348589	41.0912557	40.2649730
H	40.9324534	41.9343086	40.5521977
C	41.1619338	40.7550291	38.8261307
H	41.6896875	39.8165755	38.5901376
C	39.6749649	40.5212848	38.5820550
H	39.0542705	41.3439584	38.9660069
H	39.2716929	40.6517184	37.2047885
C	39.0553602	39.1568154	38.8747411
O	37.8093288	39.1557894	39.0113919
O	39.8040016	38.1441475	38.9334542
C	41.5972294	41.9107430	37.8918848
O	41.5890732	43.0435857	38.3430794
H	42.3945016	41.2380200	40.5048015
H	41.8903735	41.6763668	36.8685566
H	40.4392419	44.4165168	32.0550125
H	37.7740794	39.4346279	29.4380867

TS_{proS}

C	39.5821183	43.8676270	32.4568425
N	38.2775091	44.0711837	32.0668910
H	37.9622721	44.7212345	31.3309575
C	37.4954446	43.2594732	32.8075866
H	36.4139561	43.1983236	32.7089544
N	38.2309614	42.5455597	33.6552894
C	39.5372172	42.9136724	33.4430382
H	40.3400929	42.4360879	33.9947399
C	38.1010361	39.5175333	30.3684095
N	39.3817375	39.1743470	30.7395648
H	40.1352189	38.8136499	30.1377183
C	39.5180522	39.4299979	32.0532164
H	40.4387485	39.2298323	32.5930789
N	38.3880134	39.9154038	32.5643619
C	37.4906873	39.9735325	31.5123437
H	36.4685386	40.3230037	31.6389923
Fe	37.7860949	40.6410371	34.6030590
O	38.7408468	40.7700769	36.1022437
O	34.7906466	39.2218217	34.1769491
C	34.7791445	40.4482130	34.4048583
C	32.4079687	40.4115272	35.3311871
C	30.9627892	40.9044332	35.2581538
O	35.8532800	41.1559945	34.5490651
O	30.2138633	40.5975407	36.2297738
C	33.4410275	41.1786642	34.4964075

O	30.5276014	41.5167996	34.2635326
H	32.3785689	39.3667785	34.9834445
H	32.6944499	40.3677643	36.3928656
H	33.5994046	42.1969958	34.8732896
H	33.0549946	41.2747940	33.4673353
O	37.2123948	38.6397542	34.8254166
H	36.3658255	38.5685950	34.3074457
H	37.9693935	38.0195601	34.5298704
N	41.5917500	41.0376805	40.0093799
H	40.9499773	41.7476096	40.3564800
C	41.4517664	40.6719079	38.5819339
H	42.3087782	40.0220133	38.3428922
C	40.1977091	39.8295510	38.1562895
H	39.3275517	40.4145865	37.2268602
H	40.5806960	39.0888484	37.4346620
C	39.4577152	38.9658081	39.1926903
O	38.2143520	39.0093059	39.2640926
O	40.1952569	38.1632328	39.8437510
C	41.5851204	41.9203192	37.6663904
O	41.4317136	43.0220347	38.1591540
H	42.5179917	41.2256773	40.3360374
H	41.8651413	41.7724462	36.6234197
H	40.4376747	44.3851017	32.0228961
H	37.7225946	39.4203587	29.3508608

IM4

C	39.3563291	43.7662990	32.3485975
N	38.0941323	43.9956180	31.8519791
H	37.8460783	44.6859137	31.1276141
C	37.2438268	43.1600448	32.4755800
H	36.1751324	43.1143426	32.2746843
N	37.8941970	42.3997634	33.3521540
C	39.2200575	42.7667553	33.2816493
H	39.9763382	42.2774291	33.8923865
C	37.9596171	39.3892488	30.0358071
N	39.1982593	39.0613319	30.5417590
H	40.0210547	38.7313398	30.0167085
C	39.1745411	39.2817918	31.8691434
H	40.0147272	39.0730714	32.5278482
N	37.9810614	39.7393354	32.2449082
C	37.2091778	39.8086792	31.1030956
H	36.1731854	40.1406875	31.1204713
Fe	37.2283001	40.4751029	34.0970417
O	38.2122744	40.4959463	35.6876508
O	34.2129730	39.0614126	33.9923894
C	34.2431260	40.2953960	34.1330368
C	32.0171431	40.3781584	35.3979000
C	30.5318870	40.8297320	35.2528930
O	35.3525227	40.9783219	34.0156097
O	29.8154911	40.6112290	36.2595876
C	32.9801267	41.0770452	34.4316941
O	30.1720263	41.2996965	34.1557579
H	32.0102974	39.2966728	35.1851611
H	32.3201792	40.4871113	36.4497012
H	33.2430465	42.0902753	34.7655542
H	32.4234026	41.1928775	33.4854506
O	36.6897806	38.5407223	34.5890888
H	35.8308599	38.3450962	34.1429046
H	37.4760081	37.9017046	34.3670286
N	41.4533216	41.0382060	40.4911894
H	40.9486739	41.8804377	40.7792167
C	41.1134167	40.6643952	39.0905780
H	41.6265452	39.7230162	38.8381826
C	39.6365235	40.4463583	39.0463124
H	39.0003790	41.3268907	39.1699982
H	37.8171376	39.9106412	36.3629952

C	38.9376971	39.1440956	38.8707208
O	37.7020197	39.2439774	38.6311150
O	39.5865621	38.0653313	38.9685404
C	41.4687422	41.8210612	38.0964742
O	41.4454853	42.9528998	38.5435601
H	42.4221392	41.2225083	40.6567087
H	41.7310697	41.5890614	37.0642792
H	40.2430074	44.2892978	31.9903517
H	37.6735058	39.3325145	28.9855749

TS_{REB}

C	39.5876839	43.9000300	32.5274317
N	38.2743970	44.1063327	32.1686677
H	37.9477543	44.7318710	31.4158264
C	37.5039166	43.3378148	32.9624628
H	36.4198941	43.2699556	32.8928633
N	38.2551539	42.6489823	33.8248976
C	39.5607903	42.9862892	33.5492429
H	40.3802592	42.5186253	34.0836795
C	38.0990879	39.5307037	30.3878060
N	39.3489548	39.1342966	30.8145454
H	40.1090738	38.7395276	30.2438956
C	39.4429498	39.4031304	32.1304185
H	40.3183479	39.1575049	32.7276892
N	38.3187477	39.9546184	32.5837182
C	37.4677789	40.0360337	31.4974993
H	36.4605654	40.4371269	31.5814751
Fe	37.7199611	40.6918892	34.5402416
O	38.7912769	40.6470088	36.6174210
O	34.8087736	39.2004424	34.3990785
C	34.7127091	40.4502300	34.4456877
C	32.3176788	40.3773477	35.3686612
C	30.8376215	40.8341435	35.2346373
O	35.7483268	41.2217301	34.4538224
O	30.1239067	40.5847789	36.2429452
C	33.3326280	41.1020899	34.4743520
O	30.4486243	41.3356996	34.1640637
H	32.3178075	39.3058574	35.1106301
H	32.5936587	40.4334170	36.4319488
H	33.4383969	42.1591274	34.7548309
H	32.9325330	41.0924783	33.4462355
O	37.2464280	38.8255045	35.1444649
H	36.3197837	38.7179079	34.7585327
H	37.9118138	38.1095279	34.7943496
N	41.4062201	41.1633781	40.2035766
H	40.9212021	42.0186252	40.4827711
C	41.1191879	40.8097134	38.7701947
H	41.6526004	39.8753817	38.5323603
C	39.6301647	40.5404501	38.6379302
H	38.9809518	41.3745943	38.9099318
H	38.1005690	40.0651400	36.9919161
C	39.0338866	39.1650846	38.8554389
O	37.7774661	39.1410627	38.8905258
O	39.7984027	38.1729193	38.9397025
C	41.5288343	41.9730736	37.8267939
O	41.5113471	43.0985273	38.2874974
H	42.3660438	41.2804462	40.4585376
H	41.8337018	41.7413834	36.8062834
H	40.4400737	44.4008636	32.0684506
H	37.7374115	39.4201850	29.3655330

PD

C	39.5885016	43.8842380	32.2362364
N	38.2990524	44.1838135	31.8637173
H	38.0147760	44.9131579	31.1930595
C	37.4783674	43.3239072	32.4893068

H	36.3952785	43.3229107	32.3799642
N	38.1779108	42.4796125	33.2461536
C	39.5041445	42.8161185	33.0932412
H	40.2919899	42.2529057	33.5892683
C	38.0049440	39.3257026	29.8072187
N	39.2547224	39.0470350	30.3126825
H	40.0918595	38.7449705	29.7927810
C	39.2219640	39.2647275	31.6379727
H	40.0744810	39.1080582	32.2949884
N	38.0080892	39.6689963	32.0133406
C	37.2357716	39.7094852	30.8719830
H	36.1878130	40.0024761	30.8836106
Fe	37.4101494	40.6144718	33.7493730
O	39.2830053	40.3873410	37.3876451
O	34.8889330	39.1350226	34.7053301
C	34.6590760	40.3584748	34.5910380
C	32.2386659	40.2644449	35.5430052
C	30.7545172	40.6919488	35.2636205
O	35.6380573	41.2035570	34.4112918
O	29.9736145	40.6207334	36.2369754
C	33.2571991	40.9295277	34.6156319
O	30.4853427	41.0098561	34.0832451
H	32.2683504	39.1721098	35.3916597
H	32.4572041	40.4367323	36.6087016
H	33.3260082	42.0119457	34.7976083
H	32.8452877	40.8326955	33.5928803
O	37.5411788	39.0548414	35.0981118
H	36.5946198	38.7505216	35.0205742
H	38.1934777	38.3226259	34.8035661
N	41.5900990	41.0761464	40.1608195
H	40.9818534	41.7778843	40.5775005
C	41.3123912	40.7750195	38.7562659
H	41.9800795	39.9567254	38.4355884
C	39.8486658	40.2549232	38.6855524
H	39.2607112	40.8533873	39.4120015
H	38.7670558	39.5381823	37.3406980
C	39.6806743	38.7514981	39.0730102
O	38.7827421	38.1849359	38.4044029
O	40.4021112	38.2162591	39.9416156
C	41.5400778	42.0120943	37.8392352
O	41.4892083	43.1124222	38.3564176
H	42.5368167	41.2615071	40.4241419
H	41.7904628	41.8636527	36.7888359
H	40.4604853	44.4035293	31.8386849
H	37.7222623	39.2996513	28.7548506

Snapshot 4

RC2

C	39.8386928	34.1284118	34.5423127
N	38.7149822	33.3986528	34.2250253
H	38.1561727	33.4939198	33.3648487
C	38.4962992	32.5128315	35.2062726
H	37.6813755	31.7934013	35.2249834
N	39.4346834	32.6376487	36.1445487
C	40.2836559	33.6447426	35.7429145
H	41.1507196	33.9201115	36.3369598
C	41.1312127	29.1624341	33.8679674
N	42.3354877	29.7298254	34.2137918
H	43.2132002	29.7028529	33.6690098
C	42.1800055	30.3366334	35.4002865
H	42.9753154	30.8552863	35.9297371
N	40.9297296	30.1816824	35.8331043
C	40.2584988	29.4459575	34.8847199
H	39.2125857	29.1695861	34.9953915
Fe	40.0339015	31.1889947	37.4258499
O	41.3138137	32.0931218	37.8371985
O	38.3896917	28.4978256	38.3588919
C	37.7123369	29.5171764	38.1363705
C	35.5963935	28.3356264	39.0230461
C	34.3050960	28.4990106	39.8907316
O	38.1997164	30.5459815	37.4970844
O	34.4634893	29.0059375	41.0368147
C	36.3003801	29.6496406	38.6787324
O	33.2547683	28.0874896	39.3754070
H	35.3313506	27.7776223	38.1127922
H	36.2918707	27.7148201	39.6107714
H	36.4151758	30.2304387	39.6120025
H	35.7064048	30.2862361	38.0042665
O	40.5650158	29.7909391	38.7031560
H	39.9446808	29.0251817	38.5285088
H	41.5798396	29.5387031	38.5573279
N	42.7255838	35.5409669	42.9944312
H	41.9743481	35.4718901	43.6846574
C	42.6642096	34.7957259	41.7421961
H	43.6486086	34.3286120	41.5493735
C	41.6421176	33.6680871	41.8947352
H	40.6906510	34.0917831	42.2516567
H	41.4234537	33.2361190	40.9022698
C	42.0459601	32.4746647	42.7686495
O	41.0872381	31.7350865	43.1312308
O	43.2524892	32.2476664	43.0057714
C	42.2333619	35.6266483	40.5101350
O	41.4491974	36.5518417	40.6629624
H	43.1714985	36.4359932	42.9867157
H	42.6802118	35.3506855	39.5550245
H	40.2675982	34.9025944	33.9061149
H	40.9298075	28.6471197	32.9288438

TS_{proR}

C	40.0103638	34.3080132	34.7178635
N	38.8699718	33.5776380	34.4757268
H	38.3063829	33.6039911	33.6129761
C	38.6360688	32.8110605	35.5572273
H	37.8050447	32.1156454	35.6457450
N	39.5693211	33.0122469	36.4837779
C	40.4366462	33.9469914	35.9722687
H	41.3004011	34.2812871	36.5387315
C	41.1839919	29.5481959	34.2770888

N	42.4345134	30.0675847	34.5209563
H	43.2821066	29.9435303	33.9444316
C	42.3777923	30.7580579	35.6762293
H	43.2451494	31.2421999	36.1191189
N	41.1528986	30.7152826	36.1948359
C	40.3952892	29.9532771	35.3267797
H	39.3486683	29.7276358	35.5182993
Fe	40.1460839	31.6024135	37.9879865
O	40.9586232	32.6221165	39.1625201
O	38.3522494	28.7798205	38.3250829
C	37.7373132	29.8595729	38.4048695
C	35.5865355	28.5815268	39.0537498
C	34.3565283	28.5950287	40.0053428
O	38.2671181	30.9975514	38.0721099
O	34.5345515	29.0091270	41.1795878
C	36.3330054	29.9128494	38.9796181
O	33.2949362	28.1564711	39.5206861
H	35.2574397	28.2427733	38.0622782
H	36.2731987	27.8136457	39.4482484
H	36.4725940	30.2844681	40.0079427
H	35.7571189	30.6942337	38.4598109
O	40.6878451	29.8042636	38.8202258
H	40.0281362	29.1467240	38.4775102
H	41.6692743	29.5245810	38.6002774
N	42.5633213	35.5637980	42.7030464
H	41.8120774	35.4805130	43.3866784
C	42.5312994	34.8217382	41.4301538
H	43.5191450	34.3528993	41.2699546
C	41.5083833	33.6945542	41.5158645
H	40.4956274	34.0764970	41.7145931
H	41.2522024	33.1333577	40.3286830
C	41.8827643	32.5096657	42.4113102
O	40.9136733	31.8357957	42.8594217
O	43.0905954	32.2797764	42.6486013
C	42.1645904	35.7017970	40.2051279
O	41.4048227	36.6423238	40.3649042
H	43.0653315	36.4263791	42.7655858
H	42.6428629	35.4403491	39.2612177
H	40.4239550	35.0364194	34.0204162
H	40.9351414	28.9371315	33.4094830

TS_{proS}

C	40.0132195	34.3049315	34.7034319
N	38.8599985	33.5931851	34.4652412
H	38.2923655	33.6302990	33.6056152
C	38.6216340	32.8234866	35.5425123
H	37.7821861	32.1385078	35.6338746
N	39.5647912	33.0075801	36.4623844
C	40.4449642	33.9300696	35.9513634
H	41.3251882	34.2350309	36.5090942
C	41.1486952	29.5076309	34.2573766
N	42.3872176	30.0659673	34.4717324
H	43.2293613	29.9556742	33.8847399
C	42.3319394	30.7689227	35.6180493
H	43.1917413	31.2960349	36.0226732
N	41.1192116	30.6935631	36.1647829
C	40.3681458	29.8999084	35.3185664
H	39.3317785	29.6466147	35.5313275
Fe	40.1025224	31.6186143	37.9651368
O	40.7794961	32.6947953	39.1831320
O	38.4053289	28.7803569	38.3762050
C	37.7497729	29.8380645	38.4184602
C	35.6241442	28.5186641	39.0799150
C	34.3668650	28.5360454	40.0014531
O	38.2501935	30.9834626	38.0563961
O	34.5271307	28.9985689	41.1653195
C	36.3394899	29.8641665	38.9744706

O	33.3279276	28.0623961	39.5123793
H	35.3270549	28.1366907	38.0935590
H	36.3234025	27.7859386	39.5174170
H	36.4547255	30.2643885	39.9953434
H	35.7491423	30.6190207	38.4315100
O	40.7238450	29.8560313	38.8436012
H	40.0717836	29.1805108	38.5173221
H	41.6998251	29.6113466	38.5974320
N	42.5939106	35.5233330	42.5870691
H	41.7587534	35.4458509	43.1632407
C	42.7337542	34.8398720	41.2955612
H	43.8231156	34.7673086	41.1098925
C	42.2406797	33.3745153	41.2032138
H	41.2670338	33.1297911	40.3548213
H	42.9902439	32.8438587	40.6042294
C	42.1035666	32.5098457	42.4681139
O	41.0050605	32.0387766	42.8267984
O	43.2169966	32.2472210	42.9939182
C	42.1957677	35.6771652	40.0820620
O	41.4372255	36.5982435	40.3134965
H	43.0828773	36.3886398	42.6971929
H	42.5988045	35.4434529	39.0966656
H	40.4297237	35.0344764	34.0089144
H	40.9027547	28.9021834	33.3850161

IM4

C	39.8834129	34.1234588	34.5706088
N	38.7697277	33.4065422	34.2049446
H	38.2319517	33.5168292	33.3347005
C	38.5128605	32.5113704	35.1714406
H	37.6874864	31.8035100	35.1429466
N	39.4076849	32.6162883	36.1463961
C	40.2755978	33.6218250	35.7872988
H	41.1088331	33.9004043	36.4282512
C	41.1604329	29.2453064	33.9665336
N	42.3741673	29.8068265	34.2859343
H	43.2438439	29.7628932	33.7292039
C	42.2474906	30.4178666	35.4754975
H	43.0691692	30.9169482	35.9840209
N	41.0061522	30.2784054	35.9379062
C	40.3131739	29.5409614	35.0015788
H	39.2695727	29.2645981	35.1358276
Fe	39.9651698	31.1210616	37.5742087
O	40.8180986	32.3260568	38.6579968
O	38.1937819	28.3929259	38.2426020
C	37.5947451	29.4780433	38.2404521
C	35.4412381	28.3614102	39.1302459
C	34.2449004	28.5454123	40.1121139
O	38.1250138	30.5708047	37.7469824
O	34.5131815	29.0827824	41.2253899
C	36.2361529	29.6413338	38.8888461
O	33.1458477	28.1275075	39.7231170
H	35.0580475	27.9359297	38.1913648
H	36.1120112	27.6128936	39.5856707
H	36.4508048	30.0934068	39.8739920
H	35.6600970	30.4022822	38.3389020
O	40.5635831	29.4480479	38.6368925
H	39.9755761	28.7128783	38.3450872
H	41.5783401	29.2615554	38.4674417
N	42.7389146	35.5687686	43.0427095
H	42.0094725	35.4898675	43.7570985
C	42.6644590	34.7703039	41.8160530
H	43.6353565	34.2702916	41.6453000
C	41.6270490	33.7263951	42.0613596
H	40.5809855	34.0099137	41.9159742
H	40.3181113	32.8942794	39.2625756

C	41.9224433	32.4322796	42.7132665
O	40.9186687	31.7016352	42.9652807
O	43.1185692	32.1306444	42.9751647
C	42.2388770	35.5695467	40.5475587
O	41.4257052	36.4705882	40.6773132
H	43.1676001	36.4715129	43.0073103
H	42.7116108	35.2947109	39.6046620
H	40.3222517	34.9025521	33.9473108
H	40.9442071	28.7078775	33.0432336

TS_{REB}

C	40.0501344	34.3886947	34.6881877
N	38.8817772	33.6833755	34.5188806
H	38.2945586	33.6851333	33.6713278
C	38.6683808	32.9709170	35.6421712
H	37.8256689	32.3002841	35.7930693
N	39.6417963	33.1819356	36.5266539
C	40.5142333	34.0642388	35.9375041
H	41.4191917	34.3886158	36.4393672
C	41.1819945	29.6109766	34.3089033
N	42.4452721	30.1000992	34.5505713
H	43.2898385	29.9516848	33.9759299
C	42.4030554	30.8064082	35.6968181
H	43.2828479	31.2727144	36.1344701
N	41.1759891	30.8057182	36.2130533
C	40.4015651	30.0537175	35.3502706
H	39.3477347	29.8622855	35.5391847
Fe	40.1911602	31.7258719	37.9933480
O	40.9356413	32.6648507	39.7288649
O	38.4900231	28.9225131	38.5433060
C	37.8117465	29.9724301	38.5287884
C	35.6345487	28.6464110	39.0519257
C	34.3999562	28.6063205	40.0109853
O	38.3051218	31.1117403	38.1543549
O	34.5691907	29.0872964	41.1696463
C	36.3878549	29.9753261	39.0492641
O	33.3778497	28.0715412	39.5559931
H	35.2904896	28.3658360	38.0469088
H	36.3240105	27.8529638	39.3895846
H	36.4923545	30.2785308	40.1049869
H	35.8210861	30.7811747	38.5592893
O	40.7856637	30.0086023	38.9427933
H	40.0721882	29.3491857	38.6963457
H	41.7335320	29.6579126	38.6883217
N	42.5436734	35.5631523	42.6772444
H	41.7926287	35.4870334	43.3627066
C	42.4996265	34.8150226	41.4009805
H	43.4775757	34.3257570	41.2432988
C	41.4621453	33.7281480	41.5581151
H	40.4281713	34.0750471	41.6149985
H	40.5621433	32.0216559	40.3581570
C	41.8054795	32.4977418	42.3618781
O	40.8161321	31.7778656	42.6968376
O	43.0013179	32.2524454	42.6390129
C	42.1354862	35.6987299	40.1753489
O	41.3755230	36.6362807	40.3441938
H	43.0521166	36.4217830	42.7421325
H	42.6225711	35.4486789	39.2328581
H	40.4550462	35.0952445	33.9636878
H	40.9280903	28.9849768	33.4534952

PD

C	40.0610235	34.3898806	34.4718947
N	38.8802604	33.7099918	34.2918261
H	38.2660020	33.7697366	33.4671927
C	38.7080031	32.9019197	35.3522598

H	37.8618096	32.2312283	35.4861385
N	39.7246956	33.0256143	36.2027983
C	40.5840915	33.9514846	35.6605059
H	41.5213776	34.2146541	36.1433703
C	41.1639888	29.2318561	33.9019870
N	42.3923106	29.7959999	34.1511149
H	43.2409962	29.7280481	33.5682836
C	42.3131001	30.4559548	35.3154103
H	43.1495069	30.9955492	35.7498202
N	41.0955082	30.3408739	35.8386448
C	40.3617219	29.5744364	34.9599674
H	39.3181894	29.3259767	35.1416142
Fe	40.2594319	31.4163153	37.4157531
O	41.7938014	32.9091488	40.4280741
O	38.7400548	29.1440264	39.0551915
C	37.9264966	29.9948409	38.5936853
C	35.7919499	28.5798717	39.0834437
C	34.4878337	28.5506353	39.9499913
O	38.3059592	30.9443149	37.8278380
O	34.5608179	29.0938085	41.0908770
C	36.4803204	29.9476338	39.0474231
O	33.5149813	27.9687318	39.4457249
H	35.5415388	28.2183048	38.0754299
H	36.4894200	27.8524562	39.5336504
H	36.5136689	30.2823283	40.0976300
H	35.8954883	30.6881574	38.4834139
O	40.8799395	30.4612476	39.1494300
H	40.1223770	29.7639236	39.1643827
H	41.7679407	30.0201642	38.8828107
N	42.6554823	35.5370146	42.8486043
H	41.9050545	35.4425732	43.5345786
C	42.6650577	34.8045594	41.5889658
H	43.6821212	34.4040821	41.4082491
C	41.7420254	33.5789825	41.6928946
H	40.7172045	33.9357248	41.9006637
H	41.2383375	32.1070241	40.4500317
C	42.1419057	32.5086637	42.7366715
O	41.1919508	31.7610231	43.1111698
O	43.3441802	32.3526221	43.0235961
C	42.2175733	35.6620430	40.3625750
O	41.3957012	36.5442235	40.5439230
H	43.1243469	36.4195803	42.8834650
H	42.6996197	35.4647137	39.4050999
H	40.4615732	35.1139003	33.7623726
H	40.9174017	28.6942920	32.9864075

Snapshot 5

RC2

C	46.3250428	46.2317434	27.0677033
N	45.6999150	46.8497513	26.0092328
H	46.0903486	46.9827679	25.0664889
C	44.4789108	47.2380553	26.4236389
H	43.7616554	47.7475199	25.7842433
N	44.2832170	46.9019838	27.6919316
C	45.4301549	46.2720312	28.1124139
H	45.5190215	45.8933025	29.1283979
C	42.1500092	43.5780673	25.7301433
N	42.6694476	42.8223363	26.7583658
H	42.9800181	41.8418798	26.7175011
C	42.7246999	43.5998334	27.8565831
H	43.0641956	43.2476683	28.8281193
N	42.2696963	44.8195227	27.5894720
C	41.9005237	44.8185230	26.2596666
H	41.4544806	45.6921880	25.7875734
Fe	42.3790773	46.6548816	28.7285747
O	42.8656377	46.7259518	30.3568858
O	39.9709385	47.5993544	26.7899086
C	40.6463659	48.5370296	27.2263943
C	38.7881599	50.1546079	26.5328264
C	38.4104568	51.5809005	26.2694900
O	41.7072093	48.4115951	27.9574015
O	38.7443346	52.2072921	25.2326342
C	40.2658272	49.9878001	26.9126093
O	37.7351797	52.2604546	27.0912179
H	38.5722181	49.5620927	25.6294075
H	38.1472232	49.7913740	27.3493393
H	40.5167348	50.5975901	27.7910915
H	40.9192669	50.3430200	26.0965671
O	40.2643627	46.1709467	29.1299899
H	39.9365890	46.1030217	28.2114093
H	40.3566509	45.2003463	29.5222179
N	44.6604645	47.9662524	35.8884557
H	44.6083044	48.9786868	35.8032012
C	44.4325963	47.1893389	34.6633464
H	44.1932198	46.1533413	34.9627892
C	43.1940646	47.7489528	33.9496426
H	43.2509073	48.8477753	33.8941680
H	43.1693806	47.4075562	32.8894001
C	41.8396107	47.3582575	34.5499877
O	40.8450171	47.9292704	34.0365700
O	41.8036620	46.4791817	35.4478013
C	45.5955693	47.2064809	33.6496935
O	46.3558803	48.1616545	33.6276767
H	45.4238872	47.6990090	36.4764509
H	45.6547729	46.3397445	32.9914161
H	47.3128459	45.7777113	26.9891790
H	41.9971412	43.2270989	24.7095950

TS_{proR}

C	46.5789371	46.2174903	27.3388731
N	45.9268298	47.0014098	26.4143548
H	46.2389045	47.1829110	25.4489825
C	44.7924808	47.4514605	26.9885032
H	44.0706022	48.0905313	26.4867773
N	44.6774310	46.9949316	28.2335012
C	45.7892874	46.2200007	28.4623118
H	45.9337155	45.6998137	29.4030762

C	42.4232340	43.7822625	26.1656003
N	42.8724558	42.9203961	27.1422723
H	43.0566667	41.9119137	27.0445094
C	43.0732276	43.6323835	28.2681968
H	43.3886066	43.1843940	29.2077592
N	42.7780786	44.9152339	28.0754962
C	42.3643744	45.0196243	26.7591842
H	42.0198134	45.9587161	26.3322196
Fe	42.7966766	46.7554017	29.3354059
O	43.1286444	47.0042958	31.0682728
O	40.1898802	47.7263393	27.4790884
C	41.0114536	48.6163454	27.7412989
C	39.5722194	50.3592659	26.4725069
C	38.9256470	51.7439141	26.6648119
O	42.1510605	48.3822924	28.3333328
O	38.4850678	52.3137054	25.6313094
C	40.7175796	50.0795118	27.4436959
O	38.8206372	52.2301904	27.8116571
H	39.8834194	50.2555311	25.4225755
H	38.7736291	49.6170726	26.6388274
H	40.4383411	50.5281409	28.4128852
H	41.6516311	50.5746974	27.1371610
O	40.7992859	46.2145994	29.5575943
H	40.3936707	46.3668916	28.6729048
H	40.7235852	45.2064928	29.8378864
N	44.7186502	47.9741135	35.6880983
H	44.6893405	48.9852932	35.5854616
C	44.4733765	47.1660534	34.4694541
H	44.2259686	46.1435869	34.8034059
C	43.2648568	47.6782636	33.6973459
H	43.3546670	48.7445495	33.4403392
H	43.1944700	47.2313686	32.3025993
C	41.8980577	47.3571918	34.2946336
O	40.9186742	47.9870492	33.8205927
O	41.8511771	46.5110322	35.2270012
C	45.6596521	47.1495422	33.4762198
O	46.3919201	48.1212001	33.4068079
H	45.4330029	47.6904013	36.3277695
H	45.7460465	46.2376857	32.8853561
H	47.5322401	45.7208057	27.1583630
H	42.1415865	43.4760512	25.1581403

TS_{proS}

C	46.5950877	46.2184502	27.2938044
N	45.9577787	47.0174442	26.3714119
H	46.2795081	47.2063351	25.4106620
C	44.8181715	47.4648470	26.9351186
H	44.1032580	48.1118567	26.4333900
N	44.6882118	46.9923482	28.1720893
C	45.7909296	46.2075631	28.4064662
H	45.9058244	45.6670664	29.3393926
C	42.3909662	43.8000418	26.0867206
N	42.8835520	42.9497218	27.0514385
H	43.0904738	41.9459493	26.9518724
C	43.0948558	43.6637740	28.1719284
H	43.4603268	43.2215053	29.0950119
N	42.7596020	44.9396686	27.9895906
C	42.3135336	45.0357691	26.6826761
H	41.9391652	45.9675907	26.2647154
Fe	42.8336023	46.7737619	29.2725057
O	43.2205780	47.1163132	30.9866955
O	40.1568499	47.6815426	27.5453247
C	40.9780046	48.5849129	27.7484802
C	39.5321255	50.3408312	26.4828811
C	38.9086973	51.7487933	26.6948275
O	42.1490067	48.3654006	28.2966786
O	38.4411026	52.3029847	25.6722413

C	40.6753620	50.0433822	27.4482070
O	38.8750763	52.2152975	27.8570639
H	39.8374288	50.2411990	25.4311305
H	38.7218273	49.6111644	26.6487012
H	40.3853576	50.4951377	28.4157459
H	41.6096780	50.5439747	27.1508725
O	40.8583309	46.1653865	29.6333352
H	40.4045497	46.2796846	28.7681796
H	40.8292041	45.1898512	29.9519032
N	44.7961664	47.8055748	35.5131639
H	44.8190374	48.7943413	35.2610423
C	44.6349322	46.8517031	34.3947116
H	44.7168995	45.8364532	34.8243959
C	43.2743973	46.8279354	33.6384606
H	43.2512090	47.1990214	32.2680369
H	43.1248037	45.7790744	33.3331028
C	41.9827426	47.1979972	34.3782510
O	41.1234660	47.9303158	33.8542670
O	41.8707438	46.5737949	35.4696379
C	45.7669590	46.9748028	33.3290194
O	46.4455157	47.9818589	33.3068296
H	45.4622553	47.5770708	36.2231520
H	45.8991166	46.1181812	32.6681110
H	47.5488644	45.7208558	27.1183737
H	42.1206549	43.4820886	25.0797927

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C	46.4332178	46.1873906	27.1151387
N	45.8301442	46.9057743	26.1089372
H	46.2219220	47.0870350	25.1732125
C	44.6231193	47.2996918	26.5489869
H	43.9199667	47.8826449	25.9583427
N	44.4116890	46.8656351	27.7889413
C	45.5383520	46.1649297	28.1574952
H	45.6256889	45.6905319	29.1327325
C	42.1856090	43.5744029	25.6983937
N	42.6584733	42.8108571	26.7423713
H	42.9307949	41.8172017	26.7183056
C	42.7552299	43.5994015	27.8259955
H	43.0645001	43.2405864	28.8053029
N	42.3728172	44.8406919	27.5301598
C	42.0084245	44.8373074	26.1989408
H	41.6294413	45.7248383	25.6958425
Fe	42.4509305	46.6387019	28.6333448
O	42.7908481	46.7896403	30.4610972
O	39.7432139	47.8474849	27.2156604
C	40.6649787	48.6579942	27.3655411
C	39.3368880	50.6034365	26.2738419
C	38.7652437	51.9877490	26.7063966
O	41.8525935	48.2986302	27.7986953
O	38.1762649	52.6312400	25.8141379
C	40.4924056	50.1462362	27.1552966
O	38.9014394	52.3245000	27.9077164
H	39.6097781	50.6520318	25.2096485
H	38.5054576	49.8841221	26.3542033
H	40.2737450	50.5638236	28.1593524
H	41.4557295	50.5818627	26.8493217
O	40.4699925	46.1932431	29.2122202
H	39.9061391	46.3312096	28.4233315
H	40.4641520	45.2045459	29.5514961
N	44.6538058	48.0203142	35.9783531
H	44.5586328	49.0315158	35.9304983
C	44.3778600	47.2539980	34.7535414
H	44.1024145	46.2297961	35.0621782
C	43.1647968	47.8604023	34.1225811
H	43.2759995	48.6972356	33.4289704

H	41.9335975	46.8348968	30.9191933
C	41.8004478	47.4101227	34.4782386
O	40.8440388	47.9668223	33.8695652
O	41.7003877	46.5018090	35.3517989
C	45.5293487	47.2321107	33.7112069
O	46.2719701	48.1955517	33.6321448
H	45.4353108	47.7456081	36.5384942
H	45.5971982	46.3322879	33.0998303
H	47.4111529	45.7172824	27.0116616
H	42.0261589	43.2160606	24.6814214

TS_{REB}

C	46.6941274	46.1837631	27.3425789
N	46.0524906	47.0444496	26.4815362
H	46.3456243	47.2584644	25.5168698
C	44.9472931	47.4984704	27.1072670
H	44.2336352	48.1894008	26.6650274
N	44.8404179	46.9710165	28.3270755
C	45.9264966	46.1413402	28.4784438
H	46.0683139	45.5362874	29.3664584
C	42.4236569	43.8044565	26.1190037
N	42.8669412	42.9462710	27.1023197
H	43.0490360	41.9370278	27.0123057
C	43.0708206	43.6667285	28.2217339
H	43.3845217	43.2228117	29.1639860
N	42.7855803	44.9506434	28.0191789
C	42.3743014	45.0474947	26.7026913
H	42.0418027	45.9882598	26.2695665
Fe	42.9203350	46.7368154	29.2996454
O	43.0325225	47.1806948	31.5539435
O	40.2331074	47.7331769	27.7484468
C	41.0851430	48.6377755	27.8485763
C	39.5963484	50.3433755	26.5321056
C	38.9458564	51.7480314	26.7546831
O	42.2663381	48.4257010	28.3514079
O	38.4239743	52.2743975	25.7482486
C	40.7690750	50.0749060	27.4709833
O	38.9592606	52.2131847	27.9216973
H	39.8759252	50.2467706	25.4729048
H	38.8058995	49.5970216	26.7207139
H	40.4931713	50.5713389	28.4209688
H	41.6941610	50.5629168	27.1292019
O	40.9845472	46.2965327	29.8250494
H	40.4993955	46.5647278	28.9971463
H	40.8407465	45.2826452	30.0331562
N	44.7832917	48.0584279	35.5817061
H	44.8668004	49.0609484	35.4301372
C	44.5073883	47.2361349	34.3788757
H	44.2479430	46.2217947	34.7255330
C	43.2694122	47.8058708	33.7213575
H	43.3520348	48.8129940	33.3122935
H	42.0703975	47.2454043	31.7091034
C	41.9040279	47.4097646	34.2435286
O	40.9184385	47.9695133	33.6962397
O	41.8732280	46.5778394	35.1848038
C	45.6835239	47.2079593	33.3676025
O	46.4141921	48.1780312	33.3000242
H	45.4375047	47.7388666	36.2671676
H	45.7763622	46.2856371	32.7942187
H	47.6335288	45.6757956	27.1244953
H	42.1430467	43.4877011	25.1145186

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C	46.7388266	46.0681922	27.1640047
N	46.1002798	46.9025395	26.2760659
H	46.4312168	47.1462160	25.3309946

C	44.9328394	47.2749694	26.8334096
H	44.2120815	47.9381933	26.3597855
N	44.7831791	46.7128812	28.0316659
C	45.9070425	45.9506293	28.2490921
H	46.0266646	45.3501560	29.1474056
C	42.2452249	43.5317319	25.7195266
N	42.7420376	42.7143488	26.7107679
H	43.0025953	41.7212468	26.6402617
C	42.8931893	43.4522449	27.8212036
H	43.2555066	43.0506372	28.7635913
N	42.5155116	44.7086780	27.6036900
C	42.1052498	44.7720745	26.2874580
H	41.7340371	45.6910510	25.8385789
Fe	42.8526044	46.3622330	28.8297804
O	43.0991410	47.2563498	32.5358719
O	40.0631275	47.7236101	28.3328191
C	40.9959881	48.5241471	28.0843311
C	39.5786918	50.1332622	26.5852337
C	38.7668954	51.4580855	26.8271883
O	42.2370452	48.2187630	28.2918717
O	38.4306113	52.1042249	25.8223239
C	40.6875606	49.9314251	27.6279058
O	38.5153604	51.7111593	28.0416626
H	39.9737437	50.1318980	25.5589514
H	38.8588590	49.2984669	26.6602412
H	40.3016661	50.4373607	28.5355577
H	41.6204505	50.4308577	27.3336006
O	41.2171354	46.3023790	30.1478838
H	40.5464659	46.6919578	29.5046836
H	41.0442093	45.3185754	30.3252316
N	44.7167942	48.0190617	35.7655767
H	44.7239511	49.0296191	35.6494938
C	44.4889238	47.2198322	34.5590435
H	44.2415172	46.1909513	34.8777800
C	43.2238800	47.7819994	33.8769611
H	43.3145253	48.8837091	33.8275501
H	42.1504919	47.3525586	32.3231091
C	41.8889877	47.4294817	34.5782294
O	40.8971530	47.9745966	34.0366903
O	41.8891063	46.5857342	35.5039202
C	45.6757986	47.2238288	33.5578022
O	46.3926466	48.2044796	33.4968587
H	45.4289989	47.7263852	36.4036022
H	45.7965112	46.3137112	32.9702815
H	47.6918956	45.5789105	26.9631836
H	42.0609788	43.2091775	24.6947934