Supporting Information

Mechanism of Uncoupled Carbocyclization and Epimerization Catalyzed by Two Non-heme Iron/α-ketoglutarate Dependent Enzymes

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Table S1. Coordination bond lengths (r1-r6) during the SnoK-catalyzed reaction. All distances are given in angstroms.

	$^{(3)[5]}$R	$^{(3)[5]}$IM1	$^{(3)[5]}$IM2	$^{(3)[5]}$IM3
r1	(1.62)[1.62]	(1.78)[1.78]	(1.80)[1.79]	(2.02)[2.12]
r2	(2.06)[2.15]	(2.05)[2.13]	(2.03)[2.10]	(2.31)[2.19]
r3	(1.99)[2.10]	(2.00)[2.15]	(1.98)[2.13]	(2.00)[2.18]
r4	(2.12)[2.10]	(2.06)[2.04]	(2.04)[2.04]	(2.05)[2.16]
r5	(1.95)[2.04]	(1.99)[2.05]	(1.99)[2.05]	(2.25)[2.17]
r6	(1.98)[2.09]	(1.97)[2.12]	(1.97)[2.15]	(2.04)[2.21]

Table S2. Coordination bond lengths (r1-r5) at quintet spin state during the SnoN-catalyzed reaction. All distances are given in angstroms.

	R*	IM1*	IM2*	IM3*
r1	1.63	1.79	1.79	1.78
r2	1.99	1.99	1.99	1.99
r3	2.07	2.13	2.09	2.11
r4	2.09	2.03	2.03	2.04
r5	1.90	1.91	1.93	1.92

Table S3. Calculated spin density of reactant at triplet and quintet spin states for SnoK.

	Fe	O_{Fe}
^{3}R	1.20	0.81
^{5}R	3.13	0.60

Table S4. Calculated spin density of reactant at triplet and quintet spin states for SnoN.

	Fe	O_{Fe}
$^3R^*$	1.24	0.76
$^5R^*$	3.04	0.65

Table S5. Calculated spin density of involved species in path-I at quintet spin state for SnoK.

	Fe	O_{Fe}	substrate
^5R	3.13	0.60	0
$^5TS1$	3.95	0.07	-0.38
$^5IM1$	2.75	0.05	0.98
$^5TS2$	2.75	0.05	0.99
$^5IM2$	2.76	0.06	0.97
$^5TS3$	3.19	-0.08	0.69
$^5IM3$	3.68	0.05	0.01

Table S6. Calculated spin density of involved species in path-II at quintet spin state for SnoK.

	Fe	O_{Fe}	substrate		
			C2	C5″	sum
$^5IM2$-II	2.80	0.02	0	0.70	0.98
$^5TS3$-II	3.65	0.13	0.80	-0.79	-0.04
$^5IM3$-II	3.67	0.04	0.88	-0.80	0.02

Table S7. Calculated spin density of involved species in path-I at quintet spin state for penta-coordinate model of SnoK.

	Fe	O_{Fe}	substrate
$^5R_{penta}$	3.06	0.69	0
$^5TS1_{penta}$	3.85	0.15	-0.36
$^5IM1_{penta}$	2.80	0.15	0.96
$^5TS2_{penta}$	2.77	0.04	0.99
$^5IM2_{penta}$	2.79	0.04	0.96
$^5TS3_{penta}$	2.78	0.04	0.98
$^5IM3_{penta}$	3.68	0.06	0.01

Table S8. Calculated spin density of involved species at quintet spin state for SnoN.

	Fe	O_{Fe}	substrate	K110
$^5R^*$	3.04	0.65	0	0
$^5TS1^*$	3.91	0.14	-0.44	0
$^5IM1^*$	2.72	0.07	0.97	0
$^5TS2^*$	2.71	0.06	0.99	0
$^5IM2^*$	2.73	0.05	0.98	0
$^5TS3^*$	2.71	0.07	0.52	0.41
$^5IM3^*$	2.71	0.06	0.01	0.87

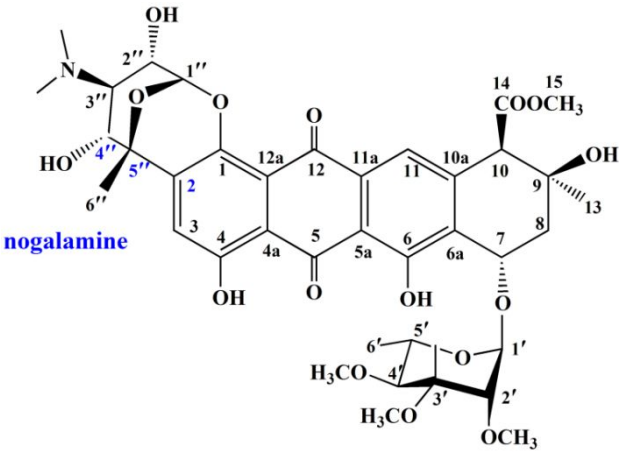

Figure S1. Definition of the numbering system for nogalamycin.

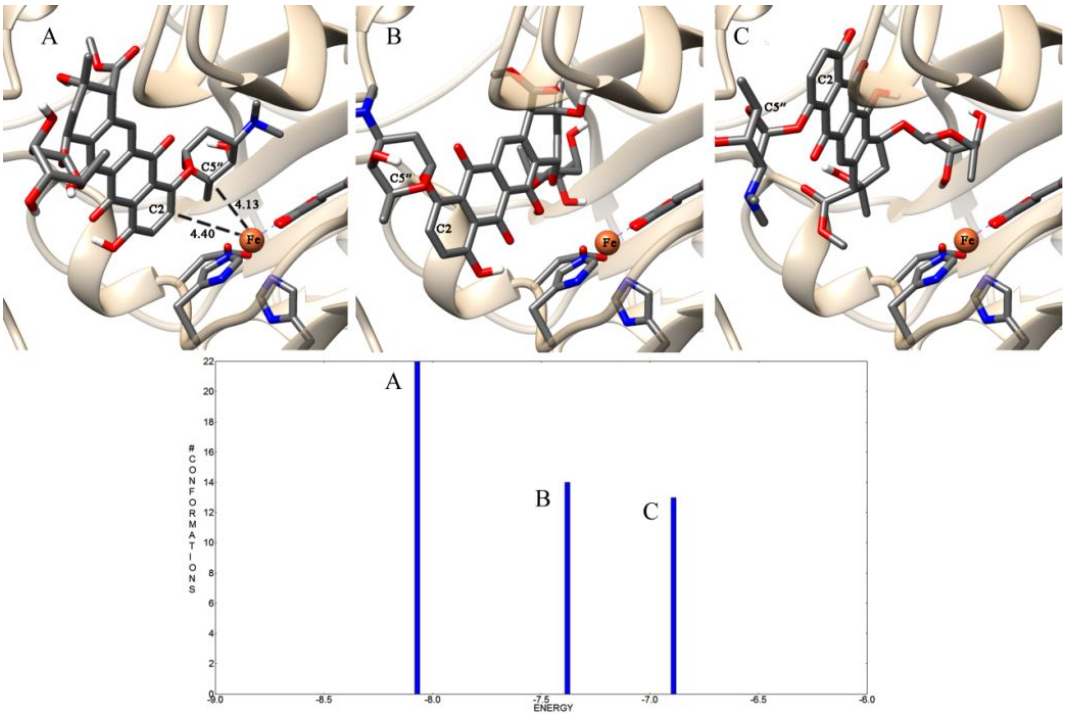

Figure S2. Substrate nogalamycin KO was docked into the active site of SnoK enzyme. During the docking, the crystal structure of SnoK (PDB ID: 5EPA, resolution of 2.24 Å) was used. Three representative conformations and docking results at the criterion of a RMSD of 2.0 Å are presented in column diagram. Energies are given in kcal/mol, and distances are given in Å. Docking scheme: during the docking process, three-dimensional grid map was generated in the active site, which was set to 32 Å × 30 Å × 50 Å with a grid spacing of 0.375 Å. The protein was kept rigid. Then fifty independent docking runs were carried out.

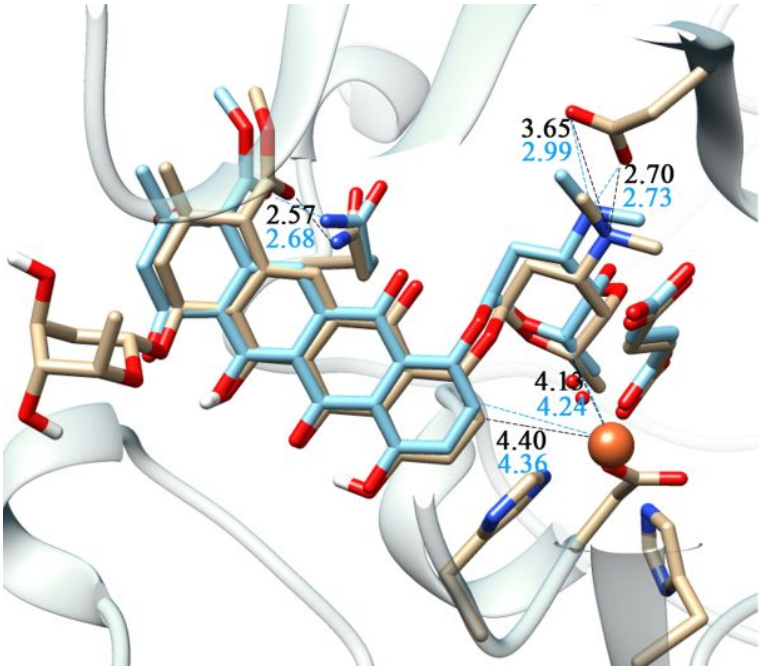

Figure S3. Overlap of the conformation A (in wheat color, chosen from Figure S2, substrate nogalamycin KO was docked into the active site of SnoK enzyme with 5EPA pdb file) and the docking model from Mikko Metsä-Ketelä group (in blue color, substrate nogalamycin K was docked into the active site of SnoK enzyme with 5EPA pdb file). All distances are given in Å. Note that we got the pdb file of SnoK-substrate complex model (in blue color) from Prof Mikko Metsä-Ketelä.

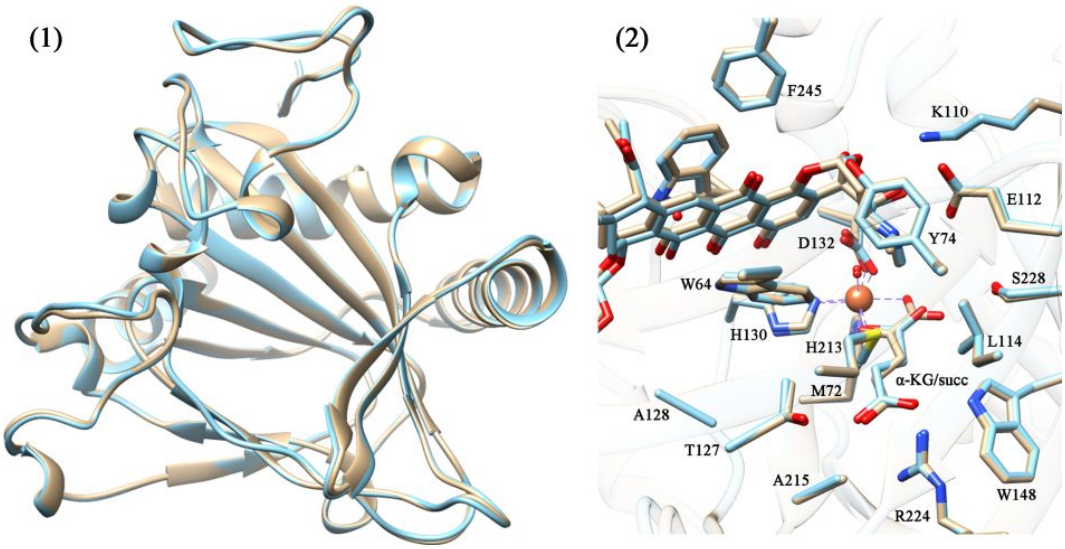

Figure S4. Overlap of two crystal structures (5EQU is with wheat color, 5ERL is with blue color). (1) enzyme peptide backbones; (2) active sites containing substrate nogalamycin RO.

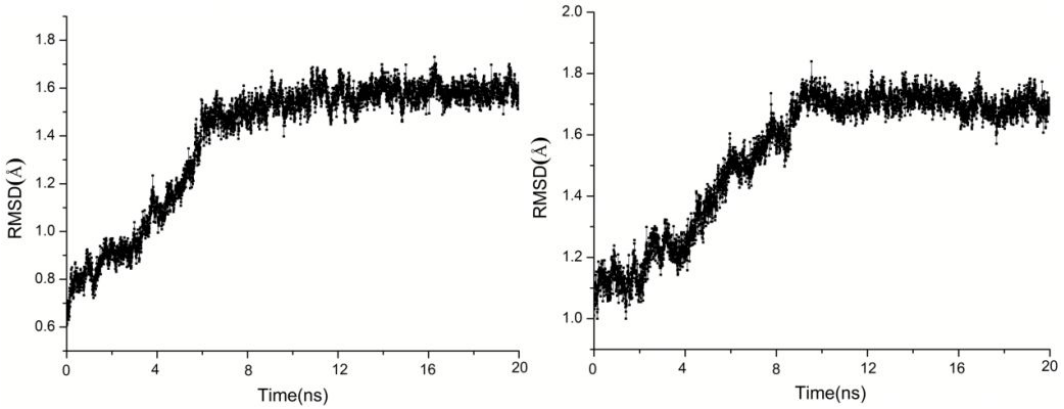

Figure S5. RMSDs for the backbone atoms of the enzyme-substrate complex in 20-ns MD simulations for SnoK (left) and SnoN (right).

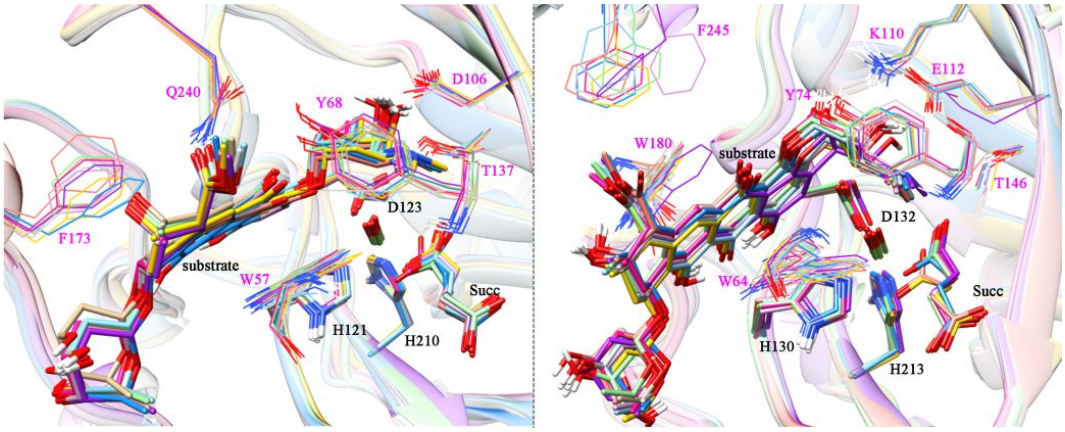

Figure S6. Left: overlap of ten QM/MM-optimized active site pockets from 11 to 20 ns MD simulation of SnoK. The calculated RMSD values of these optimized structures range from 0.33 to 0.50 Å. Right: overlap result for SnoN. The calculated RMSD values of these optimized structures range from 0.37 to 0.57 Å. The RMSD value of 20 ns corresponds to the lowest one.

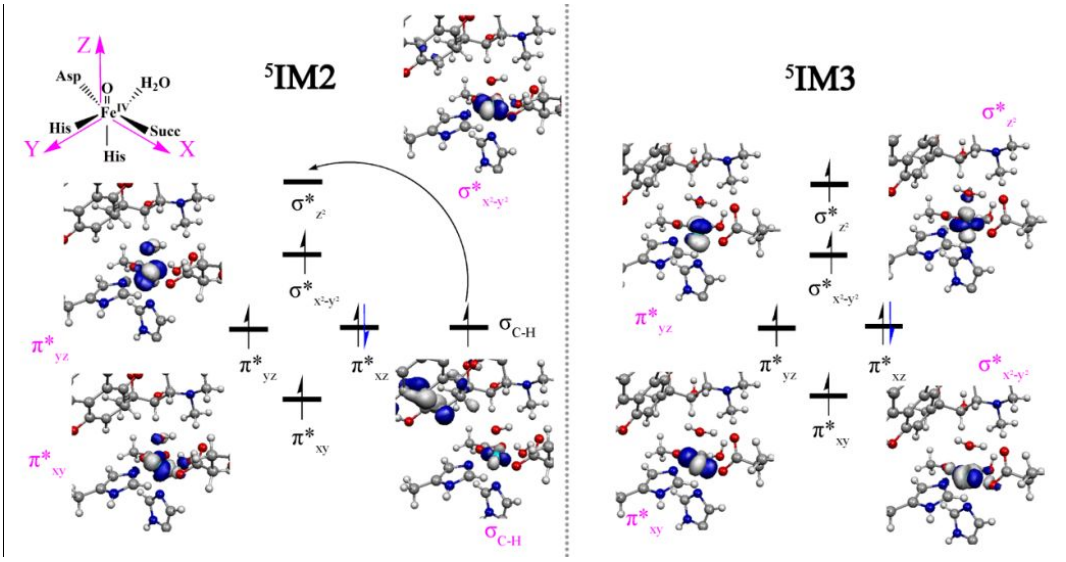

Figure S7. Molecular orbital occupations for iron-oxo of ^{5}IM2 and ^{5}IM3.

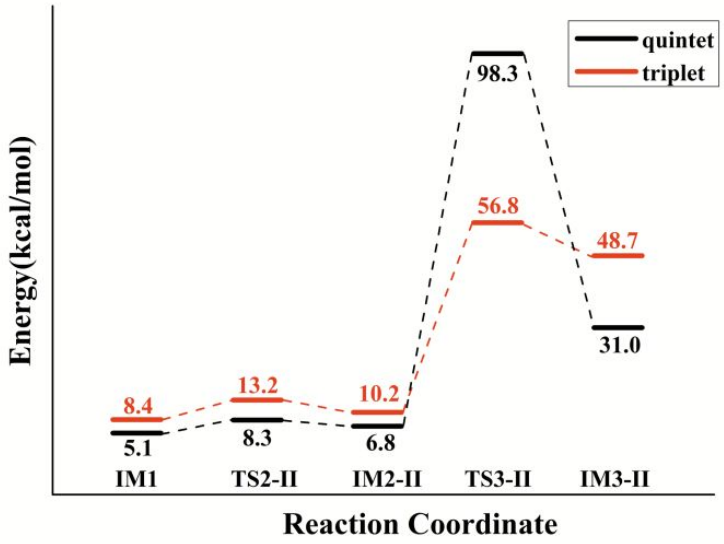

Figure S8. Calculated energy profiles in path-II for SnoK enzyme at triplet and quintet spin states. The energy of reactant at quintet state is set to zero.

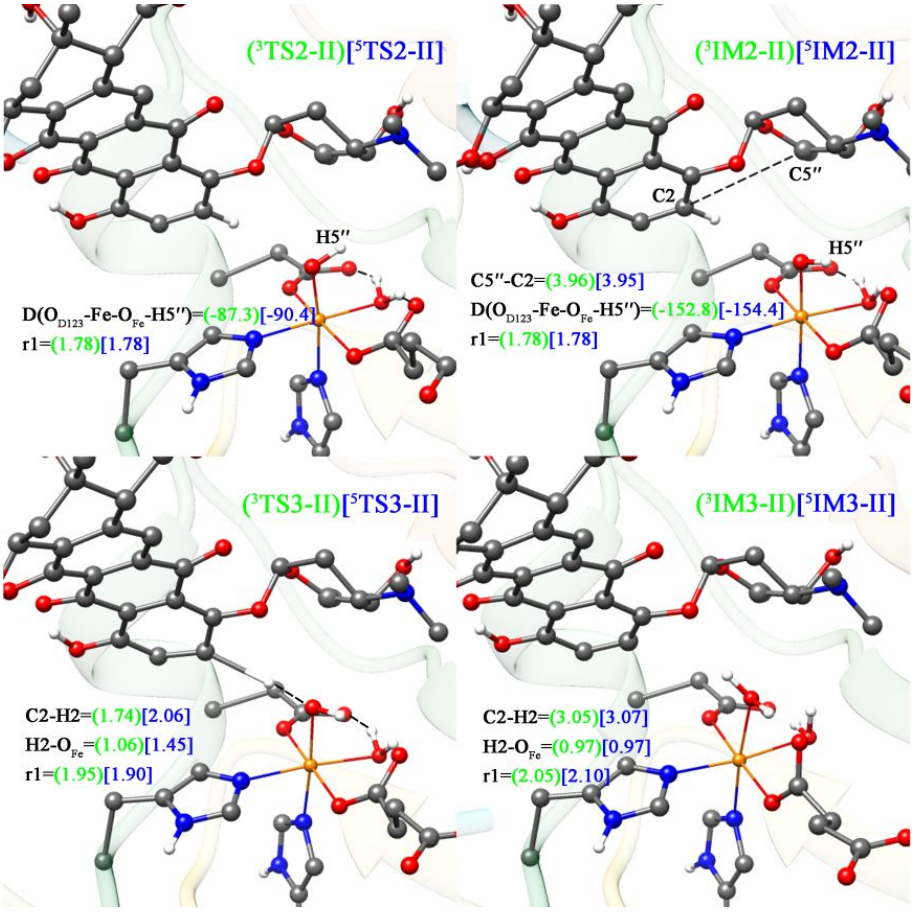

Figure S9. Optimized structures in path-II for SnoK enzyme. All distances are given in angstroms and angles in degrees.

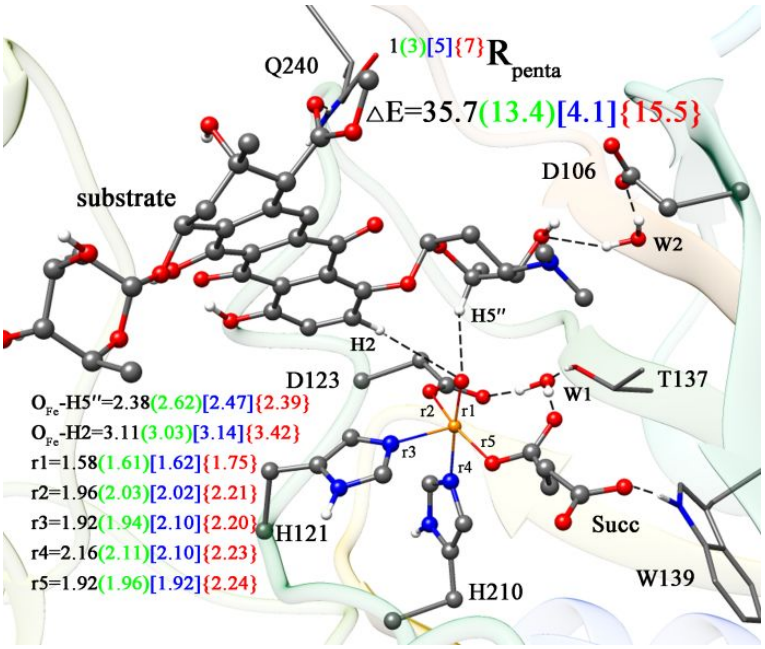

Figure S10. Optimized reactant structures at four possible spin states (singlet, triplet, quintet and septet) of penta-coordinate model for SnoK enzyme. All distances are given in angstroms and the relative energy (RE) data is in kcal/mol.

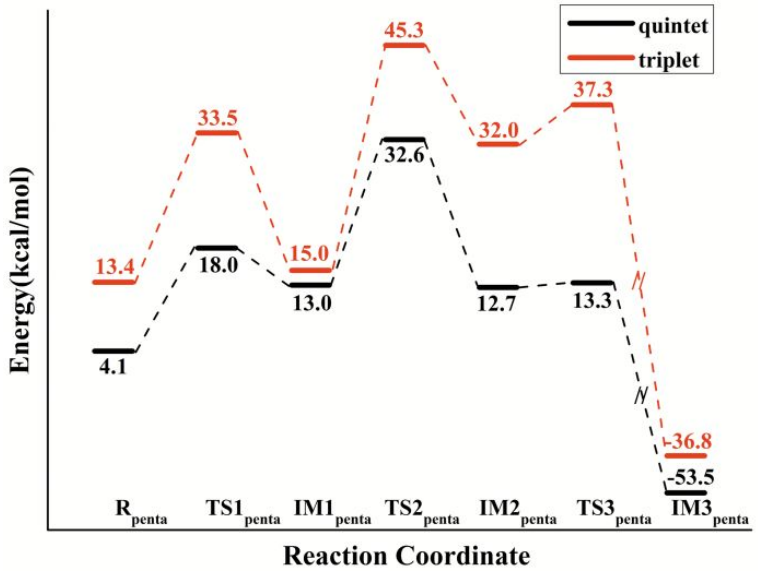

Figure S11. Energy profiles in path-I at both triplet and quintet spin states of penta-coordinate model for SnoK enzyme. The energy of ^{5}R is set to zero.

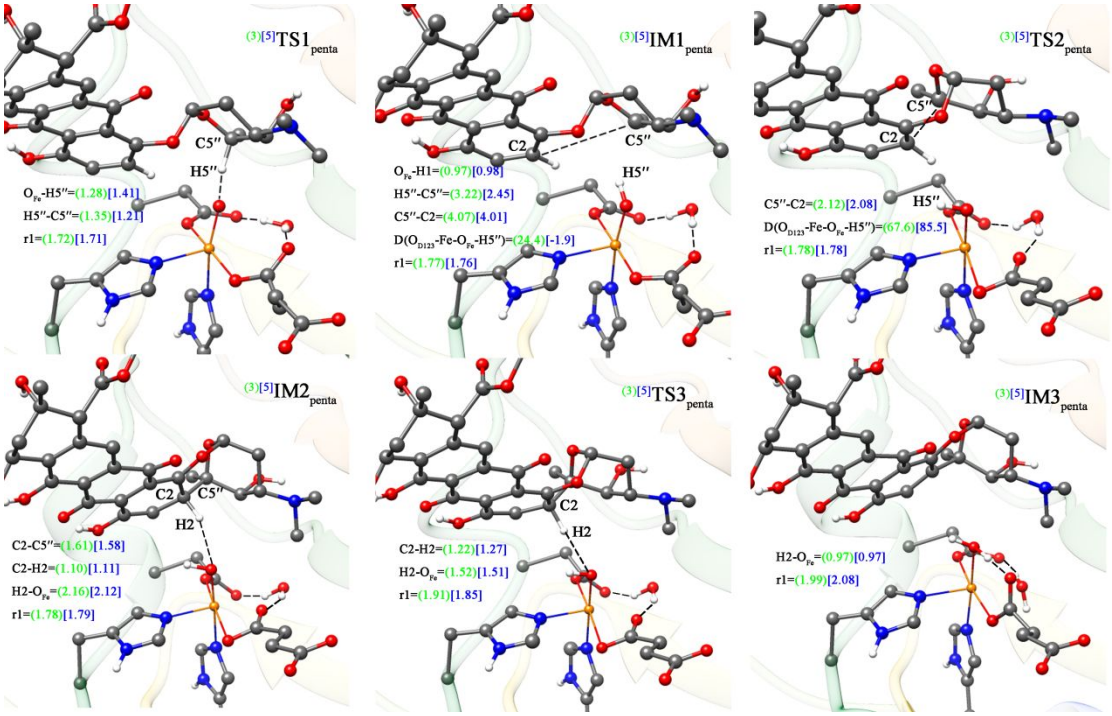

Figure S12. Optimized structures in path-I at both triplet and quintet spin states of penta-coordinate model for SnoK enzyme. All distances are given in angstroms and angles in degrees.

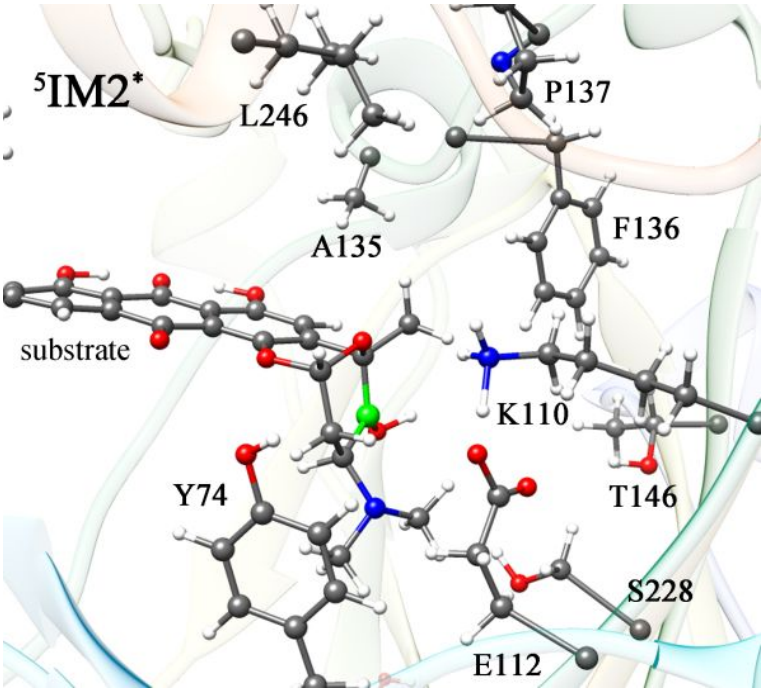

Figure S13. Relative positions of the surrounding residues for substrate in ^{5}IM2*. C4″ atom is marked green.

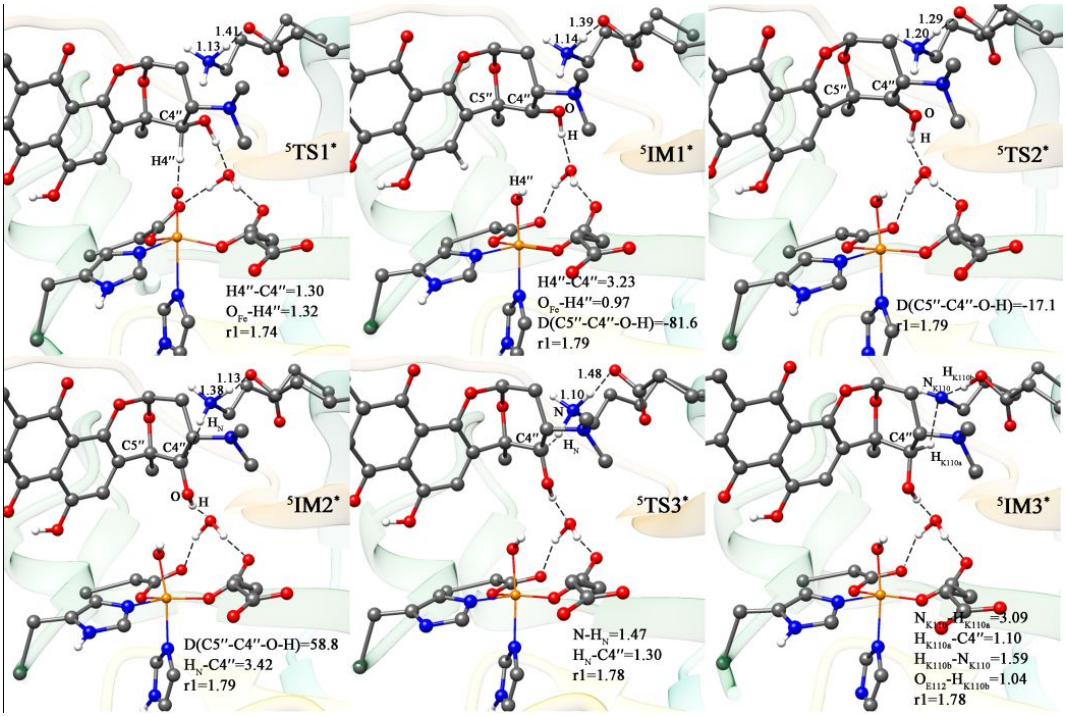

Figure S14. Optimized structures in hydroxyl epimerization reaction catalyzed by SnoN at quintet state. All distances are given in angstroms and angles in degrees.

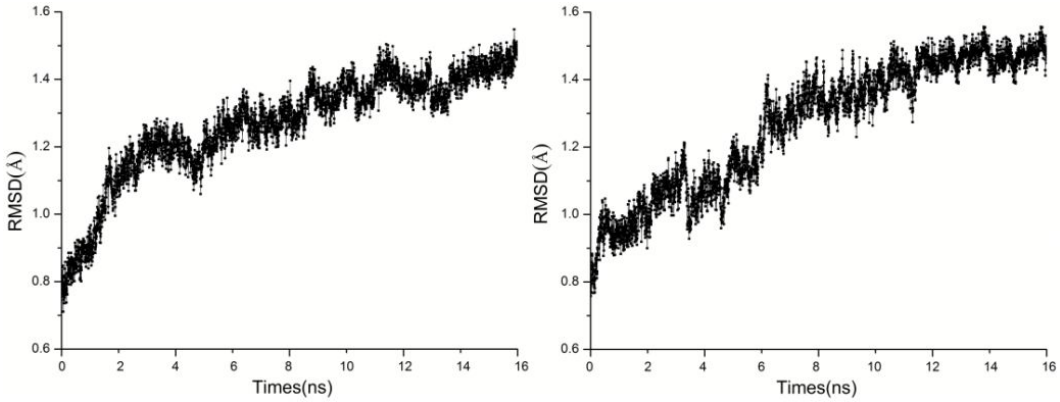

Figure S15. Left: RMSD for the backbone atoms of the mutant D106A enzyme-substrate complex in 16 ns MD simulation; Right: RMSD for the backbone atoms of the mutant D106N enzyme-substrate complex in 16 ns MD simulation.

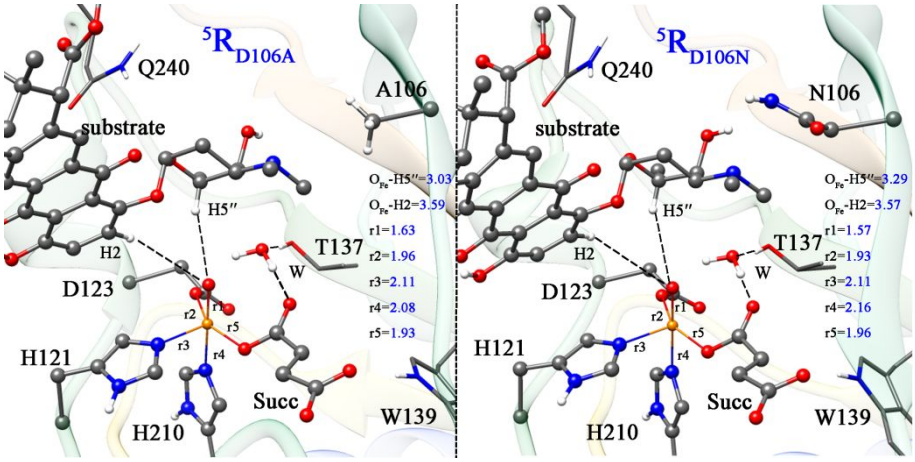

Figure S16. Optimized reactant structures at quintet state for mutant D106A (left) and mutant D106N (right). All distances are given in angstroms.

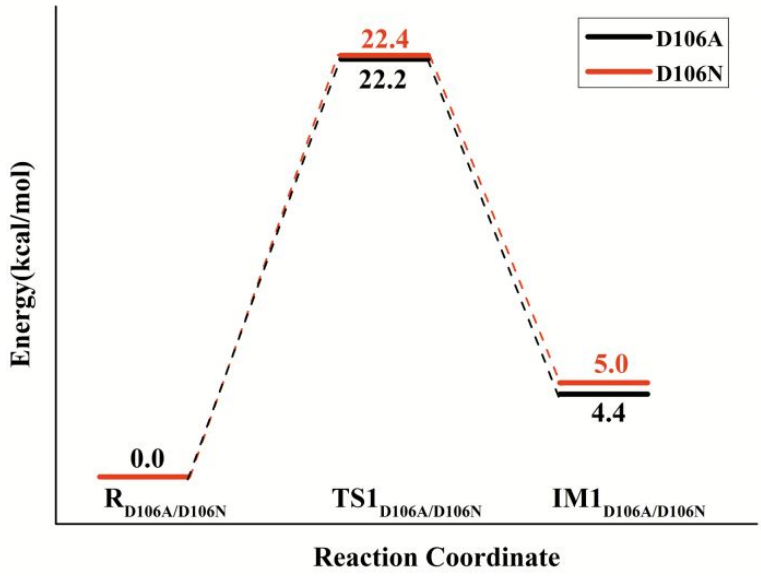

Figure S17. Energy profiles of H5″-abstraction at quintet state for mutant D106A and mutant D106N. The energy of $^5R_{D106A/D106N}$ is set to zero.

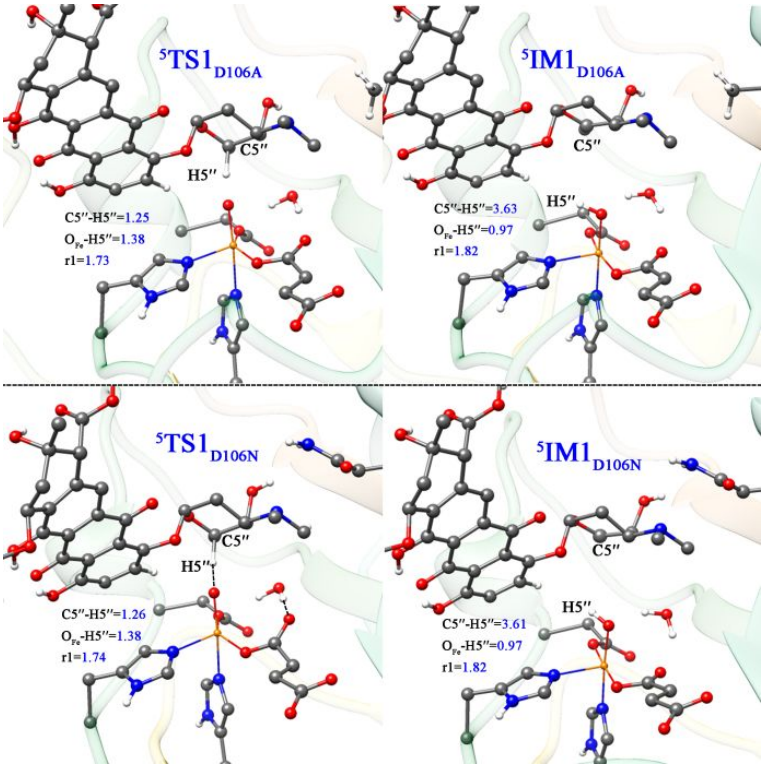

Figure S18. Optimized structures in hydrogen-abstraction catalyzed by mutant D106A and mutant D106N at quintet state. All distances are given in angstroms.

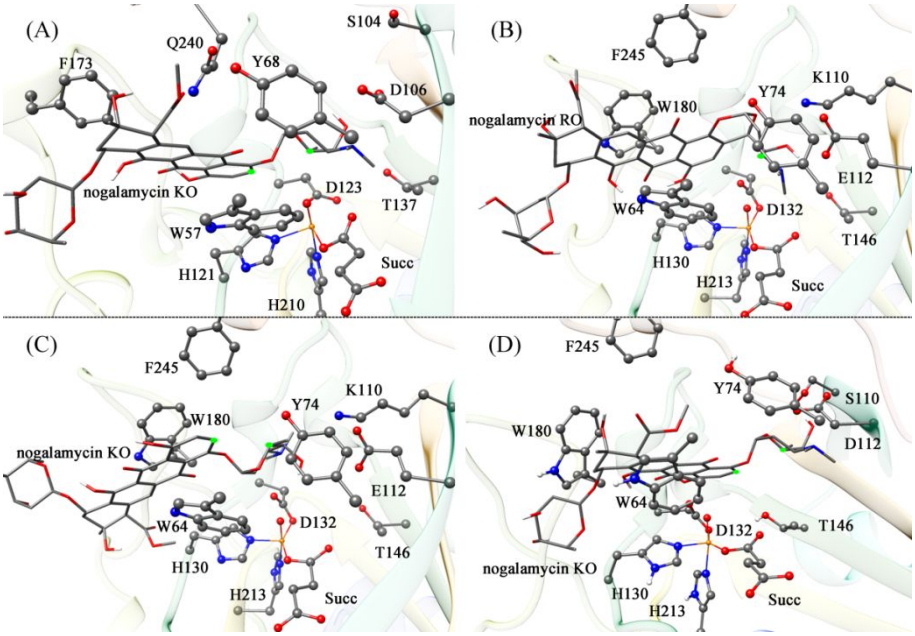

Figure S19. (A) Binding of nogalamycin KO in SnoK; (B) binding of nogalamycin RO in SnoN; (C) binding of nogalamycin KO in SnoN, and (D) binding of nogalamycin KO in the SnoN mutant (K110S/E112D). Substrates are shown in stick model and hydrogen atoms to be abstracted are marked with green.

Coordinates of QM regions for optimized species at the level of UB3LYP/B1 (LANL2DZ basis set chosen for iron ion and 6-31G(d,p) for other atoms) and absolute QM/MM single-point energies (E, a.u.) at the B2 level (Wachters+f basis set for iron and the 6-311++G(2d,2p) for others):

^{5}R

E=-4424.788474 (a.u.)

C	2.33200000	-2.46200000	5.97700000
H	2.19600000	-2.32100000	4.90200000
H	2.24000000	-3.52200000	6.23400000
C	1.26000000	-1.66700000	6.74200000
O	0.89500000	-0.55700000	6.24400000
O	0.83900000	-2.15300000	7.82100000
C	-9.85800000	-3.77100000	-1.03400000
H	-10.25000000	-2.95300000	-0.42200000
H	-10.27400000	-4.69900000	-0.63200000
N	-7.53700000	-4.83700000	-1.25200000
H	-7.79800000	-5.74500000	-1.65200000
C	-8.35600000	-3.76100000	-0.95000000
C	-6.25200000	-4.46900000	-1.08500000
H	-5.40000000	-5.10100000	-1.27700000
N	-6.19200000	-3.21400000	-0.67400000
C	-7.48900000	-2.76000000	-0.58000000
H	-7.70200000	-1.76000000	-0.24700000
C	-6.18900000	1.95400000	0.18600000
H	-6.08700000	2.78100000	-0.52200000
H	-5.89400000	2.33200000	1.17100000
C	-5.14900000	0.86500000	-0.16400000
O	-5.49500000	-0.35400000	-0.17900000
O	-3.97800000	1.28900000	-0.38100000
C	-5.17100000	-2.46800000	-6.26100000
H	-4.28000000	-3.06900000	-6.45700000
H	-5.16100000	-1.63000000	-6.97000000
N	-5.91100000	-0.89800000	-4.39200000
H	-6.54300000	-0.29800000	-4.92100000
C	-5.16400000	-1.97600000	-4.85000000
C	-5.71800000	-0.79100000	-3.06200000
H	-6.20800000	-0.05200000	-2.45400000
N	-4.87400000	-1.71900000	-2.63900000
C	-4.51800000	-2.46100000	-3.74300000
H	-3.81900000	-3.27700000	-3.66000000
O	-4.08700000	-2.44200000	0.92700000
C	-7.87100000	-5.18800000	6.55800000
C	-7.25100000	-6.05800000	7.44600000

H	-6.20300000	-5.89200000	7.66000000
C	-7.97600000	-7.10100000	8.03200000
C	-9.29200000	-7.37200000	7.62100000
C	-9.93400000	-6.46600000	6.71800000
O	-11.18900000	-6.63200000	6.26700000
H	-11.44000000	-7.57300000	6.36600000
C	-9.22800000	-5.33900000	6.22700000
O	-5.90200000	-3.90100000	6.40600000
C	-7.02800000	-4.10600000	5.95600000
C	-9.86500000	-4.34100000	5.33700000
O	-11.10300000	-4.27500000	5.20300000
C	-7.60000000	-3.33400000	4.83000000
C	-8.99500000	-3.42900000	4.57600000
C	-9.57900000	-2.65600000	3.54300000
O	-10.89700000	-2.64400000	3.30500000
H	-11.28900000	-3.24200000	4.00800000
C	-8.75400000	-1.88200000	2.70800000
H	-9.22000000	-1.33600000	1.89400000
C	-7.39300000	-1.82600000	2.93400000
H	-6.74100000	-1.25600000	2.28100000
C	-6.80300000	-2.52400000	4.00400000
O	-5.44700000	-2.46800000	4.11600000
C	-4.87300000	-1.57700000	5.08600000
H	-5.51300000	-1.53800000	5.96800000
O	-4.83000000	-0.25800000	4.59200000
C	-3.96200000	-0.03700000	3.46600000
H	-4.38200000	-0.56300000	2.59900000
C	-2.54400000	-0.60000000	3.65700000
H	-2.09200000	-0.59300000	2.65300000
C	-2.58000000	-2.05200000	4.18300000
H	-3.00300000	-2.68500000	3.38200000
C	-3.49800000	-2.12200000	5.40700000
H	-3.08200000	-1.52900000	6.22500000
H	-3.62500000	-3.14600000	5.75200000
C	-3.97200000	1.46600000	3.23900000
H	-3.48000000	1.96600000	4.07600000
H	-3.45200000	1.72300000	2.31000000
H	-5.00500000	1.82100000	3.18000000
O	-1.76900000	0.22100000	4.52700000
H	-1.23600000	-0.38700000	5.08100000
N	-1.21100000	-2.46600000	4.52100000
C	-0.33200000	-2.41500000	3.35200000
H	0.61200000	-2.90500000	3.60100000
H	-0.75300000	-2.91600000	2.46200000

H	-0.08800000	-1.38000000	3.09600000
C	-1.14500000	-3.75900000	5.20500000
H	-1.61300000	-3.70700000	6.18800000
H	-1.62100000	-4.58000000	4.63800000
H	-0.09600000	-4.02100000	5.36900000
O	-0.64200000	-8.54600000	-0.95500000
C	-0.25400000	-7.36900000	-0.69400000
O	0.95600000	-6.99800000	-0.69800000
C	-1.28800000	-6.28100000	-0.34200000
H	-0.91900000	-5.76300000	0.55000000
H	-2.25800000	-6.72400000	-0.11000000
C	-1.43900000	-5.24100000	-1.47700000
H	-0.44200000	-5.00600000	-1.85700000
H	-2.03800000	-5.65400000	-2.29500000
C	-2.04900000	-3.91800000	-1.01000000
O	-3.29200000	-3.71300000	-1.32100000
O	-1.32300000	-3.11100000	-0.39200000
O	-2.65900000	-0.99000000	-0.87800000
H	-2.00900000	-1.64300000	-0.46800000
H	-2.85400000	-0.18800000	-0.35200000
O	1.03800000	0.92300000	4.01100000
H	1.18900000	0.30000000	4.76000000
H	0.07400000	0.84500000	3.90300000
Fe	-4.39000000	-2.14100000	-0.63600000

$^{5}R^{*}$

E=-4458.04899 (a.u.)

C	5.55500000	-3.65700000	-1.74600000
H	5.95800000	-3.69800000	-0.73100000
H	4.79200000	-2.88300000	-1.83800000
N	4.86600000	-4.92200000	-2.10000000
H	3.96700000	-5.01100000	-1.60200000
H	4.56900000	-4.83300000	-3.18000000
H	5.42600000	-5.77200000	-1.95300000
C	2.46000000	-3.70000000	-5.85300000
H	1.78400000	-4.54300000	-5.65900000
H	3.05700000	-3.99000000	-6.72500000
C	3.36100000	-3.63000000	-4.62400000
O	3.35000000	-2.71000000	-3.80500000
O	4.11500000	-4.70200000	-4.51900000
C	-3.20900000	-8.56100000	5.74900000
H	-2.15800000	-8.85400000	5.82100000
H	-3.77500000	-9.45800000	5.47500000
N	-4.54500000	-7.10600000	4.12400000

H	-5.44600000	-7.56800000	4.27100000
C	-3.35600000	-7.47500000	4.73100000
C	-4.32100000	-6.04400000	3.32300000
H	-5.09100000	-5.54200000	2.75300000
N	-3.03400000	-5.72000000	3.37600000
C	-2.42300000	-6.60500000	4.23800000
H	-1.36400000	-6.57200000	4.43100000
C	1.64500000	-4.03500000	5.29500000
H	1.26800000	-3.20400000	5.89700000
H	2.61800000	-3.77600000	4.87000000
C	0.74000000	-4.33300000	4.08500000
O	1.23900000	-4.92500000	3.12000000
O	-0.48100000	-3.91700000	4.18200000
C	-6.04800000	-2.25500000	6.50100000
H	-6.77800000	-1.89300000	5.77200000
H	-5.91700000	-1.46700000	7.24800000
N	-3.52900000	-2.54400000	6.51900000
H	-3.37500000	-2.41400000	7.52300000
C	-4.74400000	-2.57300000	5.84600000
C	-2.56200000	-2.91400000	5.66100000
H	-1.51300000	-2.94200000	5.89500000
N	-3.07100000	-3.16400000	4.46600000
C	-4.43300000	-2.95200000	4.56600000
H	-5.09800000	-3.11800000	3.73200000
O	-1.19900000	-4.75400000	1.68300000
N	0.29600000	-5.32300000	-3.11000000
C	-0.41700000	-5.74800000	-4.31000000
H	-0.59100000	-4.87300000	-4.94300000
H	-1.40200000	-6.20200000	-4.10100000
H	0.16800000	-6.45900000	-4.89500000
C	-0.47100000	-4.29700000	-2.42200000
H	-0.70000000	-3.50200000	-3.13900000
H	-1.43000000	-4.65900000	-2.00400000
H	0.10500000	-3.84600000	-1.62000000
C	3.05700000	-6.50000000	0.91800000
H	3.63500000	-7.31300000	1.36600000
H	2.48900000	-6.00500000	1.70400000
H	3.76200000	-5.78300000	0.49800000
O	2.22800000	-4.82800000	-1.14800000
H	1.96800000	-4.15700000	-0.47000000
C	2.50700000	-8.29100000	-2.19100000
H	3.29600000	-8.77600000	-2.77000000
C	1.73500000	-7.31000000	-3.05300000
H	1.23100000	-7.88600000	-3.83100000

H	2.46200000	-6.65400000	-3.54600000
C	0.74100000	-6.44000000	-2.26200000
H	-0.11600000	-7.07600000	-1.96000000
C	1.37600000	-5.93600000	-0.93200000
H	0.56800000	-5.63900000	-0.25300000
C	2.17000000	-7.05900000	-0.19500000
O	3.12500000	-7.67800000	-1.09600000
O	1.67200000	-9.38900000	-1.74500000
C	1.15500000	-9.34600000	-0.50300000
C	1.27600000	-8.17800000	0.30600000
C	0.65700000	-8.12200000	1.53800000
C	-0.03500000	-9.23300000	2.05500000
C	-0.10900000	-10.42200000	1.29400000
C	0.49800000	-10.47900000	0.00000000
H	0.70800000	-7.22600000	2.14900000
O	-0.56100000	-9.11200000	3.28200000
H	-1.01200000	-9.97500000	3.47800000
C	0.46600000	-11.73400000	-0.76400000
O	0.96200000	-11.88300000	-1.87700000
C	-0.80000000	-11.56700000	1.85700000
O	-1.32500000	-11.50200000	3.01000000
C	-0.22700000	-12.90500000	-0.13600000
C	-0.89300000	-12.81000000	1.09000000
C	-1.64900000	-13.90900000	1.59400000
C	-1.75900000	-15.07900000	0.78300000
C	-0.93100000	-15.18600000	-0.34400000
C	-0.19600000	-14.10500000	-0.82900000
H	0.40200000	-14.14500000	-1.73200000
O	-2.23200000	-13.82600000	2.78600000
H	-2.02800000	-12.91400000	3.14900000
C	-2.49300000	-2.43300000	0.49700000
O	-1.35500000	-2.22600000	0.04700000
O	-2.75200000	-2.68200000	1.76100000
C	-3.71900000	-2.35400000	-0.38600000
H	-4.40600000	-1.63100000	0.06900000
H	-3.42500000	-1.97200000	-1.36400000
C	-4.45800000	-3.69000000	-0.54500000
H	-4.59400000	-4.17200000	0.42600000
H	-3.85400000	-4.37000000	-1.15900000
C	-5.82900000	-3.52900000	-1.23500000
O	-5.90400000	-2.66700000	-2.16000000
O	-6.76500000	-4.27300000	-0.84000000
O	1.15400000	-3.38600000	0.82300000
H	1.13700000	-3.96800000	1.61300000

H	0.20900000	-3.24000000	0.61500000
Fe	-1.98800000	-4.00300000	2.88900000

$^{5}R_{penta}$

E=-4424.781796 (a.u.)

C	2.32700000	-2.44600000	5.97000000
H	2.18800000	-2.28900000	4.89800000
H	2.23200000	-3.50900000	6.21300000
C	1.26300000	-1.65600000	6.75100000
O	0.90600000	-0.53500000	6.27300000
O	0.84100000	-2.15800000	7.82200000
C	-10.04800000	-3.81500000	-1.07500000
H	-10.44100000	-2.98500000	-0.48100000
H	-10.50200000	-4.73100000	-0.68700000
N	-7.73700000	-4.92100000	-1.23600000
H	-7.98600000	-5.81300000	-1.67500000
C	-8.55200000	-3.84000000	-0.93500000
C	-6.45400000	-4.57900000	-1.01400000
H	-5.61200000	-5.22800000	-1.19400000
N	-6.39000000	-3.33700000	-0.56400000
C	-7.68400000	-2.86600000	-0.50500000
H	-7.89600000	-1.87400000	-0.14900000
C	-6.25100000	1.81300000	0.14100000
H	-6.12000000	2.68100000	-0.50800000
H	-5.92400000	2.09400000	1.14800000
C	-5.29500000	0.69900000	-0.32400000
O	-5.59200000	-0.51800000	-0.03800000
O	-4.24900000	1.04200000	-0.90800000
C	-5.22000000	-2.46800000	-6.18200000
H	-4.31900000	-3.06300000	-6.35500000
H	-5.19700000	-1.62600000	-6.88500000
N	-6.02700000	-0.91100000	-4.32900000
H	-6.63400000	-0.29900000	-4.87600000
C	-5.25900000	-1.98200000	-4.76900000
C	-5.87700000	-0.80900000	-2.99700000
H	-6.37900000	-0.05800000	-2.41600000
N	-5.03900000	-1.73200000	-2.54800000
C	-4.64500000	-2.46700000	-3.64700000
H	-3.94000000	-3.27600000	-3.54700000
O	-4.20600000	-2.49600000	0.99400000
C	-7.87600000	-5.17700000	6.55700000
C	-7.25300000	-6.04900000	7.44300000
H	-6.20600000	-5.88000000	7.65800000
C	-7.97600000	-7.09300000	8.02800000

C	-9.29200000	-7.36800000	7.61700000
C	-9.93500000	-6.46200000	6.71500000
O	-11.19000000	-6.63100000	6.26400000
H	-11.43900000	-7.57200000	6.36400000
C	-9.23200000	-5.33200000	6.22600000
O	-5.91300000	-3.87800000	6.40900000
C	-7.03700000	-4.08900000	5.95700000
C	-9.87400000	-4.33300000	5.34000000
O	-11.11200000	-4.27100000	5.20800000
C	-7.61300000	-3.31800000	4.83200000
C	-9.00900000	-3.41400000	4.58200000
C	-9.59800000	-2.63600000	3.55700000
O	-10.91700000	-2.62600000	3.32300000
H	-11.30400000	-3.23100000	4.02300000
C	-8.77800000	-1.85200000	2.72600000
H	-9.25100000	-1.30000000	1.92000000
C	-7.41600000	-1.79500000	2.94700000
H	-6.76800000	-1.21900000	2.29500000
C	-6.82000000	-2.50100000	4.00800000
O	-5.46400000	-2.44900000	4.11600000
C	-4.88600000	-1.53100000	5.06200000
H	-5.52600000	-1.47300000	5.94300000
O	-4.84000000	-0.22600000	4.53600000
C	-3.95900000	-0.03800000	3.40900000
H	-4.37600000	-0.58800000	2.55600000
C	-2.54300000	-0.59300000	3.62300000
H	-2.08700000	-0.59400000	2.62400000
C	-2.58600000	-2.03100000	4.18100000
H	-3.00400000	-2.68000000	3.39100000
C	-3.51300000	-2.07300000	5.40000000
H	-3.10100000	-1.46300000	6.20700000
H	-3.64500000	-3.08800000	5.76800000
C	-3.95700000	1.45500000	3.12700000
H	-3.45400000	1.98100000	3.94200000
H	-3.43000000	1.65800000	2.18900000
H	-4.98600000	1.82400000	3.06000000
O	-1.78000000	0.25000000	4.49100000
H	-1.26100000	-0.34600000	5.06700000
N	-1.22100000	-2.44200000	4.54000000
C	-0.33200000	-2.40000000	3.37900000
H	0.61300000	-2.88000000	3.64500000
H	-0.74200000	-2.91500000	2.49200000
H	-0.09500000	-1.36800000	3.10800000
C	-1.16600000	-3.73400000	5.22600000

H	-1.65200000	-3.68200000	6.20000000
H	-1.63300000	-4.55600000	4.65100000
H	-0.12100000	-3.99600000	5.40900000
O	-0.72400000	-8.37600000	-1.03300000
C	-0.35200000	-7.19900000	-0.75700000
O	0.85500000	-6.81600000	-0.74900000
C	-1.40400000	-6.13000000	-0.37600000
H	-1.07900000	-5.69000000	0.57300000
H	-2.38200000	-6.59300000	-0.22500000
C	-1.50900000	-4.99700000	-1.42400000
H	-0.49500000	-4.73000000	-1.73400000
H	-2.06400000	-5.34200000	-2.30200000
C	-2.13700000	-3.70600000	-0.88200000
O	-3.37600000	-3.47400000	-1.27200000
O	-1.47600000	-2.94700000	-0.17500000
O	-1.98200000	-0.18200000	-0.00900000
H	-1.83500000	-1.14900000	0.00600000
H	-2.88300000	-0.01100000	-0.33000000
O	1.06000000	0.92900000	4.02700000
H	1.19300000	0.31200000	4.78400000
H	0.10200000	0.83900000	3.88000000
Fe	-4.62200000	-2.21100000	-0.54600000