Electronic Supporting Information

Computational studies of DNA base repair mechanisms by nonheme iron dioxygenases: Selective epoxidation and hydroxylation pathways

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QM/MM calculations

Table S1. Absolute energies (Hartree) for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{300}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown alongside the single stable dioxygen species (**Reoo***). The energies are broken down into separate MM and QM contributions as well as the combined total energies.

	$QM_{Turbomole}$	MM_{DL_poly}	$QMMM_{Total}$
$^3R_{OO}$*	-3306.886852	-103.979836	-3410.866688
$^3R_{OO}$	-3306.89148	−103.986474	-3410.877954
$^5R_{OO}$	-3306.912856	−103.980312	-3410.893168
$^7R_{OO}$	-3306.913601	−103.980158	-3410.893759
$^3Re_{Cyc}$	-3306.94486	−103.993571	-3410.938431
$^5Re_{Cyc}$	-3306.965479	−104.001547	-3410.967026
$^7Re_{Cyc}$	-3306.896847	−103.983259	-3410.880106
^3I_P	-3306.963497	−103.995344	-3410.95884
^5I_P	-3306.976063	−103.999213	-3410.975276
^7I_P	-3306.98011	−103.978433	-3410.958543

Table S2. Absolute energies (Hartree) for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{400}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown. The energies are broken down into separate MM and QM contributions as well as the combined total energies.

	$QM_{Turbomole}$	MM_{DL_poly}	$QMMM_{Total}$
$^3R_{OO}$	-3306.953522	−103.765796	-3410.719318
$^5R_{OO}$	-3306.972756	−103.761067	-3410.733823
$^7R_{OO}$	-3306.973599	−103.761283	-3410.734882
$^3Re_{Cyc}$	-3307.002789	−103.777868	-3410.780657
$^5Re_{Cyc}$	-3307.021458	−103.77596	-3410.797417
$^7Re_{Cyc}$	-3306.964413	−103.760432	-3410.724846
^3I_P	-3307.050834	−103.754474	-3410.805308
^5I_P	-3307.062671	−103.752004	-3410.814675
^7I_P	-3306.985073	−103.722586	-3410.707659

Table S3. Absolute energies (Hartree) for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{500}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown. The energies are broken down into separate MM and QM contributions as well as the combined total energies.

	$QM_{Turbomole}$	MM_{DL_poly}	$QMMM_{Total}$
$^3R_{OO}$	-3306.936762	−103.894914	-3410.831676
$^5R_{OO}$	-3306.973147	−103.870705	-3410.843852
$^7R_{OO}$	-3306.962929	−103.880245	-3410.843175
$^3Re_{Cyc}$	-3306.940199	−103.874952	-3410.815151
$^5Re_{Cyc}$	-3307.039706	−103.878672	-3410.918378
$^7Re_{Cyc}$	-3306.896832	−103.983277	-3410.880109
^3I_P	-3307.041241	−103.870006	-3410.911247
^5I_P	-3307.048999	−103.869045	-3410.918044
^7I_P	-3307.047534	−103.868693	-3410.916227

Table S4. Grouped spin populations for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{300}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown alongside the single stable dioxygen species (**Reoo***). The coordinating amino acids, iron co-factor as well as the distal (**O_1**) and proximal (**O_2**) oxygens of the bound dioxygen are all considered. The spin densities on the αKG co-enzyme is split into two groups for both the succinate (**suc**) and CO_2 components.

	Fe	**O_1**	**O_2**	**CO_2**	**suc**	**HIS_{131}**	**His_{187}**	**ARG**	**ASP**
$^3R_{OO}$*	3.67	-0.92	-0.93	0.06	0.01	0.04	0.05	-0.01	0.02
$^3R_{OO}$	2.98	-0.54	-0.62	0.07	0.04	-0.01	0.05	-0.01	0.05
$^5R_{OO}$	4.19	-0.30	-0.53	0.16	0.10	0.14	0.10	-0.01	0.16
$^7R_{OO}$	4.18	0.56	0.61	0.17	0.07	0.13	0.11	0.01	0.18
$^3Re_{Cyc}$	2.04	0.02	-0.02	0.01	-0.05	0.01	0.04	0.01	-0.06
$^5Re_{Cyc}$	3.75	0.06	0.01	0.00	0.03	0.07	0.03	0.00	0.04
$^7Re_{Cyc}$	4.29	0.20	0.12	0.52	0.49	0.12	0.10	0.00	0.15
^3I_P	2.84	-0.59	-0.24	0.01	-0.05	0.02	0.09	0.02	-0.10
^5I_P	4.21	-0.55	0.06	0.00	0.09	0.11	0.11	0.05	-0.08
^7I_P	4.20	1.01	0.32	0.01	0.12	0.08	0.12	0.00	0.15

Table S5. Grouped spin populations for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{400}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates. The coordinating amino acids, iron co-factor as well as the distal (**O_1**) and proximal (**O_2**) oxygens of the bound dioxygen are all considered. The spin densities on the αKG co-enzyme is split into two groups for both the succinate (**suc**) and CO_2 components.

	Fe	O_1	O_2	CO_2	suc	HIS_{131}	His_{187}	ARG	ASP
$^3R_{OO}$	3.20	-0.66	-0.70	0.07	0.02	0.00	0.04	-0.01	0.03
$^5R_{OO}$	4.18	-0.30	-0.50	0.16	0.09	0.13	0.10	0.00	0.14
$^7R_{OO}$	4.17	0.61	0.61	0.14	0.06	0.12	0.11	0.01	0.17
$^3Re_{Cyc}$	1.99	0.05	-0.02	0.00	-0.05	0.03	0.04	0.00	-0.05
$^5Re_{Cyc}$	3.76	0.07	0.01	0.01	0.03	0.07	0.03	0.00	0.03
$^7Re_{Cyc}$	4.17	0.61	0.61	0.14	0.06	0.12	0.11	0.01	0.17
^3I_P	2.84	-0.59	-0.24	0.01	-0.05	0.02	0.09	0.02	-0.10
^5I_P	4.20	-0.54	0.02	0.00	0.10	0.13	0.12	0.05	-0.08
^7I_P	4.46	0.11	-0.01	0.93	0.25	0.10	0.04	0.04	0.06

Table S6. Grouped spin populations for the minima structures in the oxygen activation path catalyzed by snapshot Sn_{500}. The superoxo (**Reoo**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates. The coordinating amino acids, iron co-factor as well as the distal (**O_1**) and proximal (**O_2**) oxygens of the bound dioxygen are all considered. The spin densities on the αKG co-enzyme is split into two groups for both the succinate (**suc**) and CO_2 components.

	Fe	O_1	O_2	CO_2	suc	HIS_{131}	His_{187}	ARG	ASP
$^3R_{OO}$	3.32	-0.76	-0.71	0.07	0.01	0.01	0.05	0.00	0.00
$^5R_{OO}$	4.19	-0.31	-0.52	0.18	0.07	0.13	0.09	-0.01	0.19
$^7R_{OO}$	4.18	0.52	0.64	0.15	0.07	0.12	0.10	0.01	0.20
$^3Re_{Cyc}$	1.12	0.05	0.09	0.44	0.35	0.00	-0.03	0.00	-0.02
$^5Re_{Cyc}$	3.76	0.06	0.01	0.01	0.02	0.07	0.03	0.00	0.04
$^7Re_{Cyc}$	4.32	0.16	0.09	0.55	0.49	0.12	0.09	0.00	0.16
^3I_P	1.37	0.63	0.04	0.00	-0.03	0.04	-0.03	0.00	-0.02
^5I_P	4.14	-0.29	-0.29	0.02	0.08	0.09	0.11	0.01	0.14
^7I_P	4.18	1.06	0.25	0.00	0.12	0.09	0.09	0.00	0.21

Table S7. Relative energies (kcal mol^{-1}) for the reaction landscape in the oxygen activation path catalyzed by snapshot Sn_{300}. The superoxo (**Re$_{OO}$**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown alongside the transition state for the initial attack of the superoxo on the beta carbon of the co-enzyme (**TS$_{O,C}$**) and the barrier for the OO cleavage of the peracid (**TS$_{C,C}$**). The energies are given for all possible spin states.

	S = 1	S = 2	S = 3
R_{OO}	9.92	0.37	0.00
$TS_{O,C}$	21.15	9.31	10.77
Re_{Cyc}	-28.03	-45.98	8.57
$TS_{O,O}$	-26.80	-41.26	24.25
I_P	-40.84	-51.15	-40.65

Table S8. Relative energies (kcal mol^{-1}) for the reaction landscape in the oxygen activation path catalyzed by snapshot Sn_{400}. The superoxo (**Re$_{OO}$**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown alongside the transition state for the initial attack of the superoxo on the beta carbon of the co-enzyme (**TS$_{O,C}$**) and the barrier for the OO cleavage of the peracid (**TS$_{C,C}$**). The energies are given for all possible spin states.

Sn400	S = 1	S = 2	S = 3
R_{OO}	9.77	0.66	0.00
$TS_{O,C}$	19.68	13.53	13.14
Re_{Cyc}	-28.72	-39.24	6.30
$TS_{O,O}$	-19.98	-32.73	28.97
I_P	-44.19	-50.07	17.08

Table S9. Relative energies (kcal mol^{-1}) for the reaction landscape in the oxygen activation path catalyzed by snapshot Sn_{500}. The superoxo (**Re$_{OO}$**), peracid (**Re$_{Cyc}$**) and ferryl oxo (**I$_P$**) intermediates are all shown alongside the transition state for the initial attack of the superoxo on the beta carbon of the co-enzyme (**TS$_{O,C}$**) and the barrier for the OO cleavage of the peracid (**TS$_{C,C}$**). The energies are given for all possible spin states.

Sn500	S = 1	S = 2	S = 3
R_{OO}	7.22	-0.42	0.00
$TS_{O,C}$	21.23	9.33	7.02
Re_{Cyc}	17.59	-47.19	-23.18
$TS_{O,O}$	24.22	-38.75	-7.49
I_P	-42.72	-46.98	-45.84

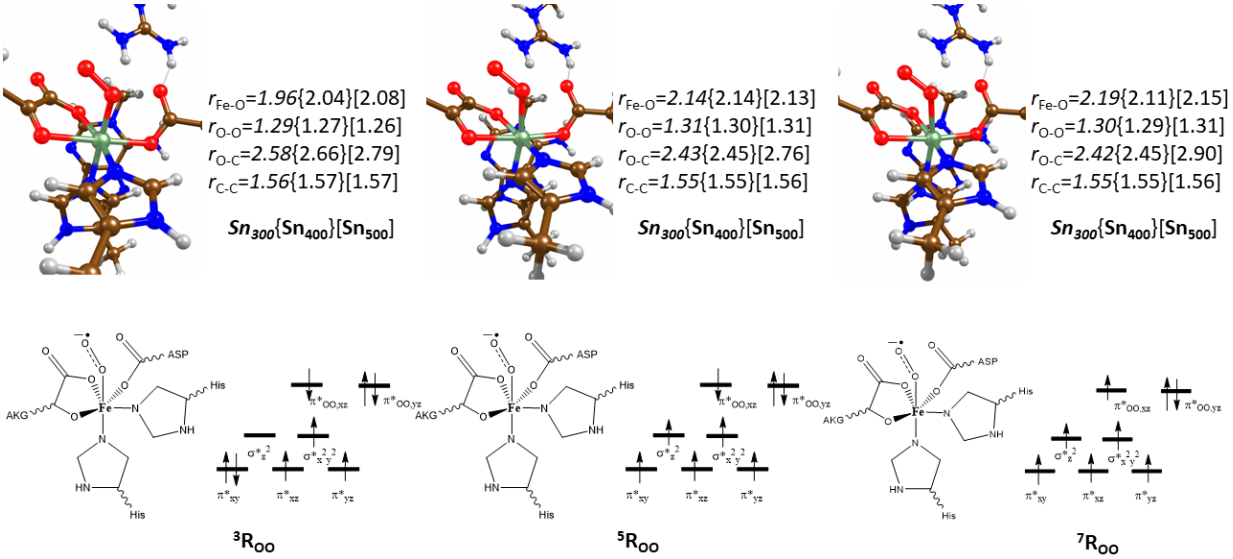

Fig. S1. Comparative orbital occupations and important bond lengths for the triplet (^{3}**Roo**), quintet (^{5}**Roo**) and septet (^{7}**Roo**) superoxo QM species.

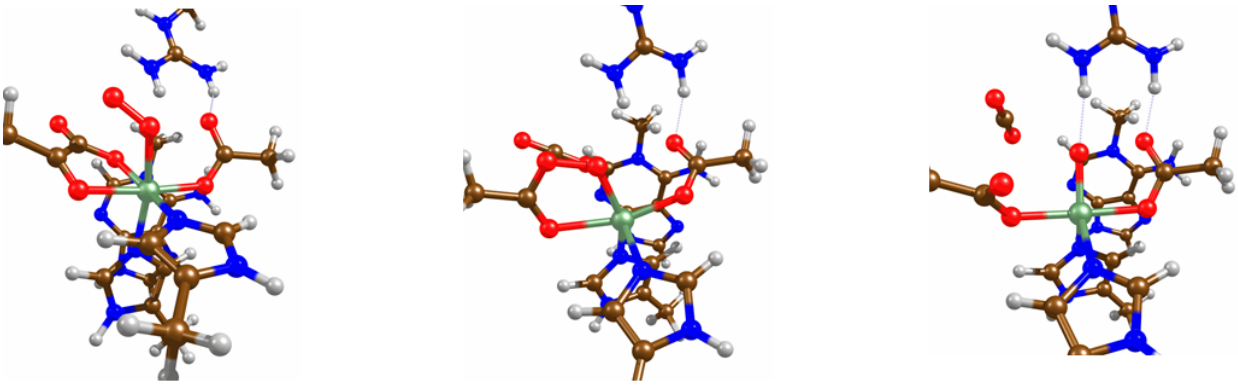

Fig. S2. Graphical representation of changes in the QM region at different minima point across the low energy quintet reaction pathways for oxygen activation. Important bond lengths for the superoxo ($^5R_{OO}$), peracid ($^5R_{Cyc}$) and ferryl oxo (^5I_P) species are all shown.

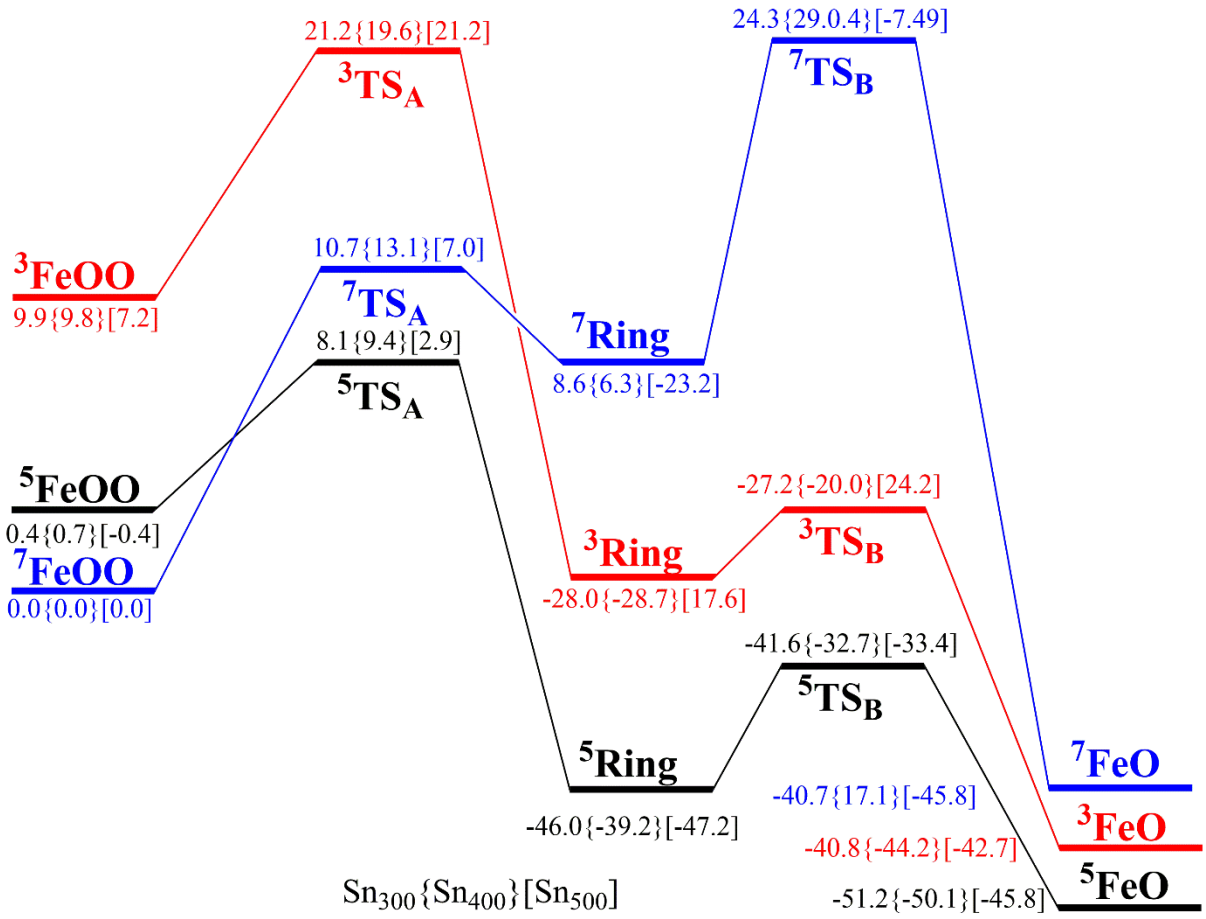

Fig. S3. QM/MM(Turbomole:Charmm) calculated potential energy landscapes for the conversion of the iron(II)-superoxo into and iron(IV)-oxo species, when S=1,2,3. All QM/MM energies were obtained BS3 are given in kcal mol^{-1} relative to the low-energy septet superoxo species. Data presented were derived from snapshots Sn_{300}, Sn_{400} and Sn_{500}.

DFT calculations: *Only the cluster model of Fe(IV)=O species was used to investigate epoxidation and hydroxylation reactions by nonheme iron dioxygenases.*

All calculations use methods as previously described but will be briefly summarized here.[1] We employ density functional theory with the unrestricted B3LYP method[2] throughout as implemented in *Gaussian*-09 program packages.[3] All geometries were fully optimized in *Gaussian*-09 using the Los Alamos type double-ζ quality LACVP basis set on iron in combination with 6–31G on the rest of the atoms; basis set B1.[4] Energies were improved by single point calculations using a triple-ζ type LACV3P+ basis set on iron and 6–311+G* on the rest of the atom; basis set B2. Frequency calculations were done in *Gaussian*-09 with basis set B1.

Local minima were found through a full geometry optimization without constraints and confirmed as local minima with an analytical frequency calculation. Subsequently, geometry scans were run whereby one degree of freedom (the reaction coordinate) was frozen but all other degrees of freedom varied. The maximum of these geometry scans were used as starting points of the transition state optimizations. Moreover, the geometry scans proved the connection between reactants and intermediates or between intermediates and products. Free energies reported in this work contain zero-point energies, thermal corrections and entropy. Vibrational frequencies and entropies were unscaled.

References:

1. de Visser, S. P. *J. Am. Chem. Soc*. **2006**, *128*, 9813–9824.
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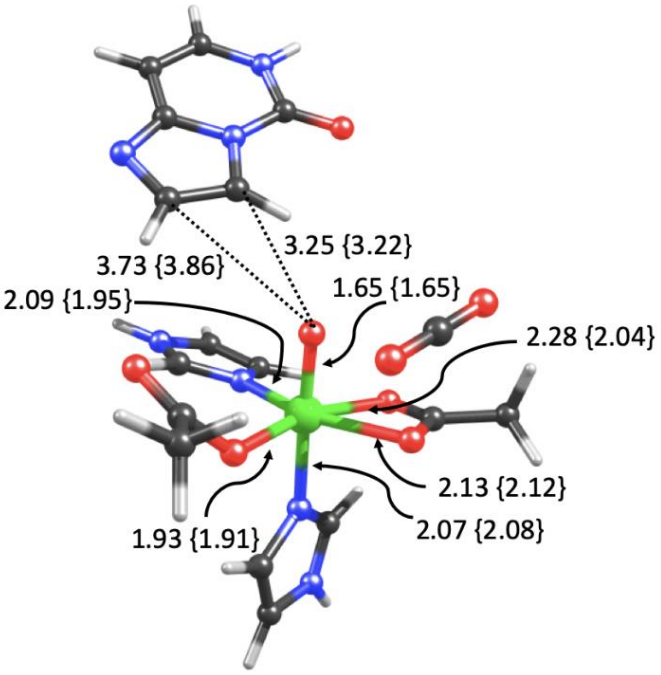

Fig. S4. DFT Optimized geometries for cluster model of ^{5}Re {^{3}R$_{e}$} in epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

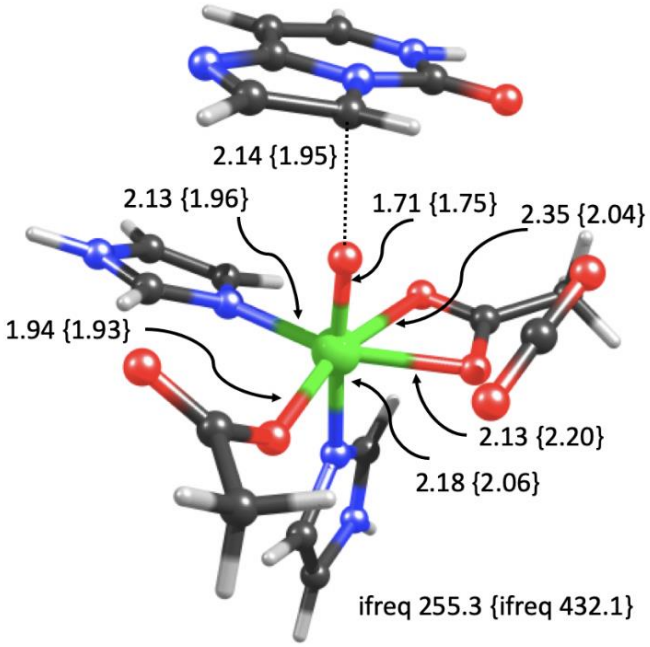

Fig. S5. DFT Optimized geometries for cluster model of ^{5}TS$_{E}$ {^{3}TS$_{E}$} in epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

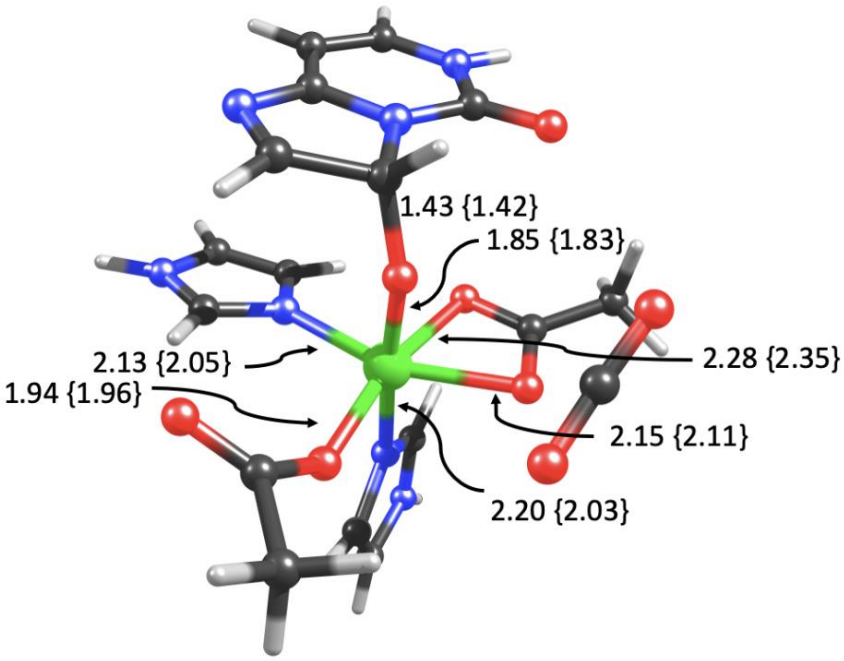

Fig. S6. DFT Optimized geometries for cluster model of $^{5}IM_{E}$ {$^{3}IM_{E}$} in epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

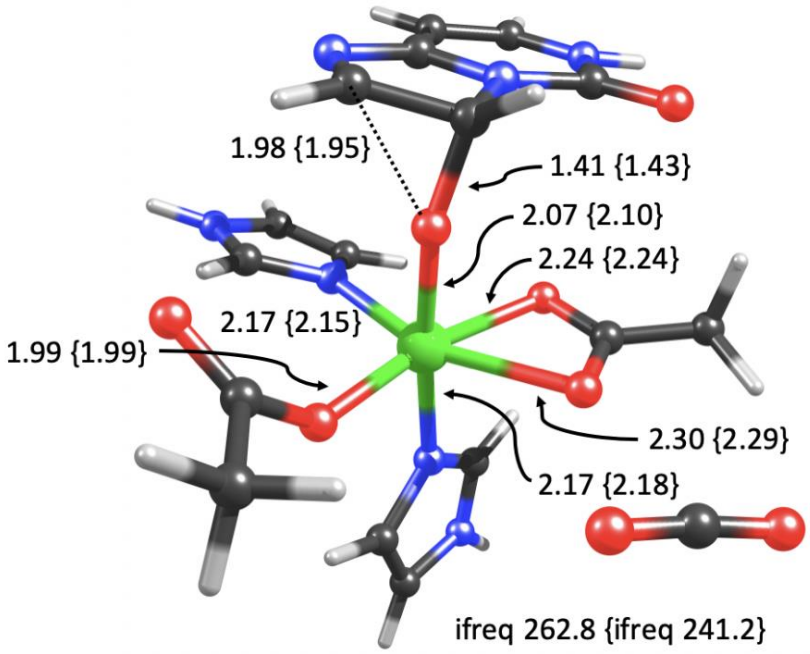

Fig. S7. DFT Optimized geometries for cluster model of $^{5}TS_{rc}$ {$^{3}TS_{rc}$} in epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

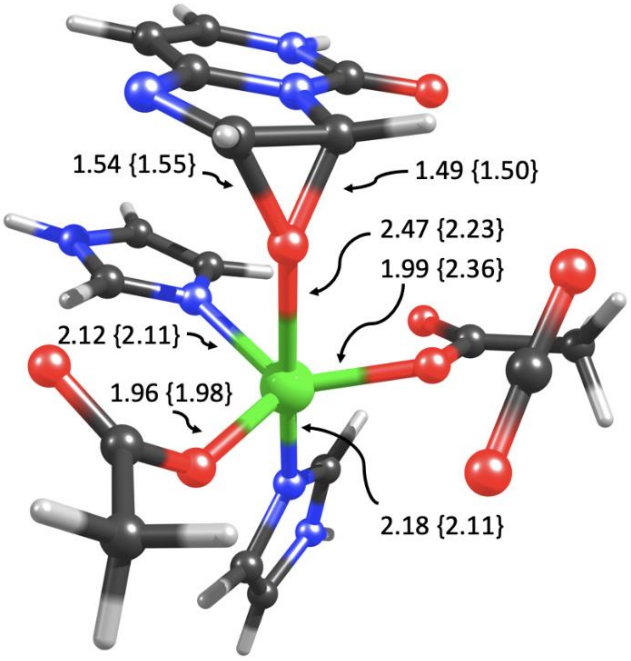

Fig. S8. DFT Optimized geometries for cluster model of $^{5}P_{E}$ {$^{3}P_{E}$} in epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

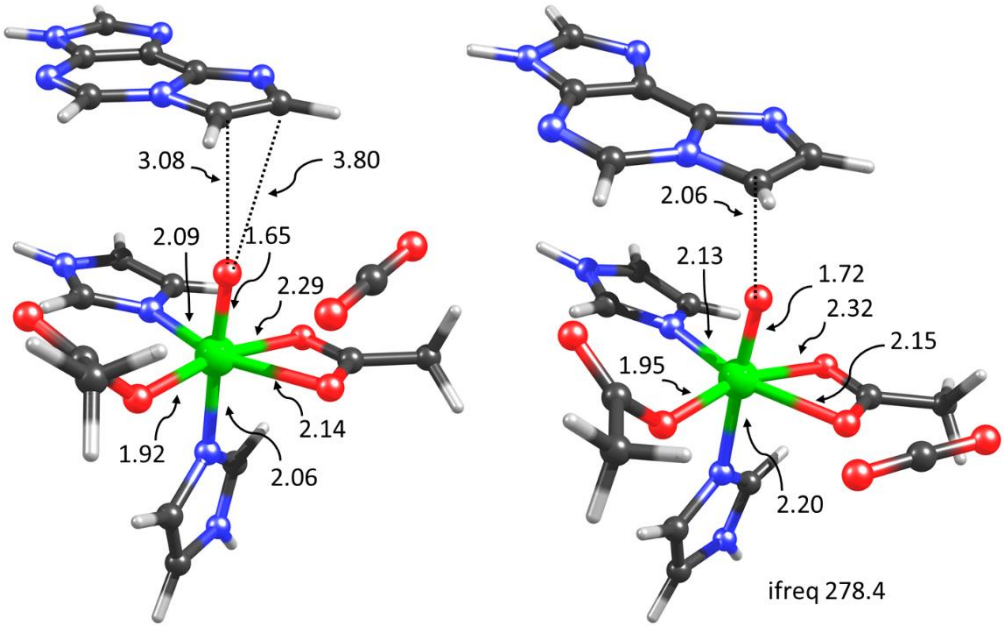

Fig. S9. DFT Optimized geometries for cluster model of ^{5}Re (left) and $^{5}TS_{E}$ (right) in epoxidation reaction by iron(IV)-oxo species with 1,N^{6}-etheno adenine (εA) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

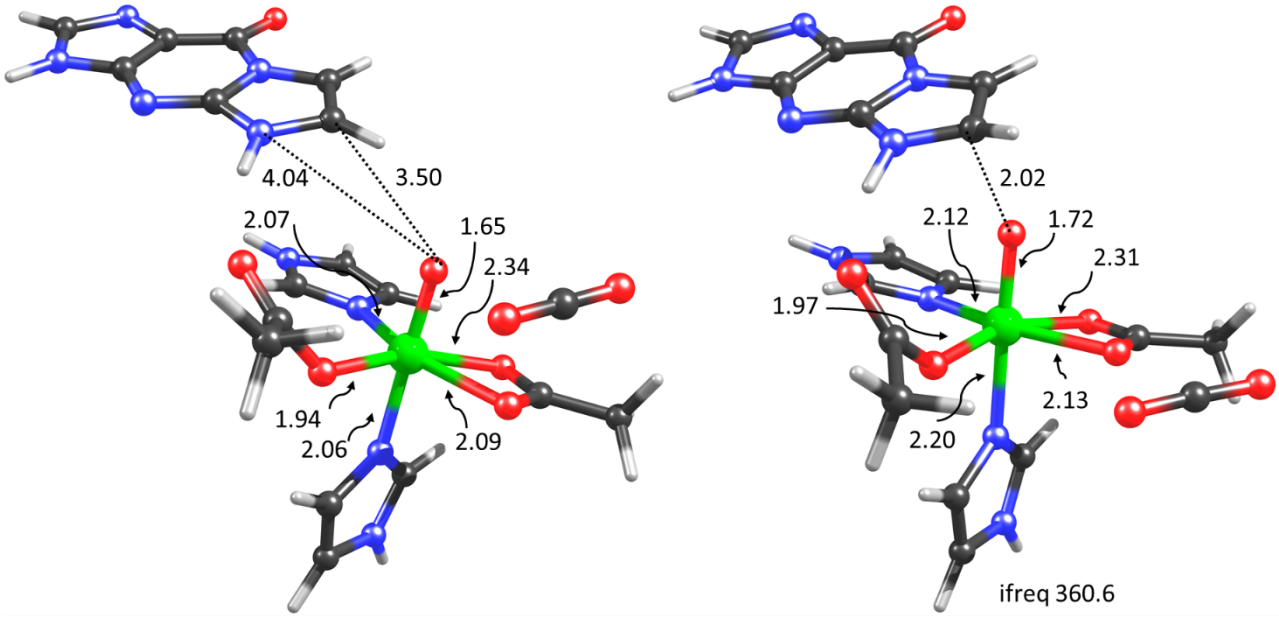

Fig. S10. DFT Optimized geometries for cluster model of ^{5}Re (left) and ^{5}TS$_{E}$ (right) in epoxidation reaction by iron(IV)-oxo species with 1,N^{2}-etheno guanine (εG) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

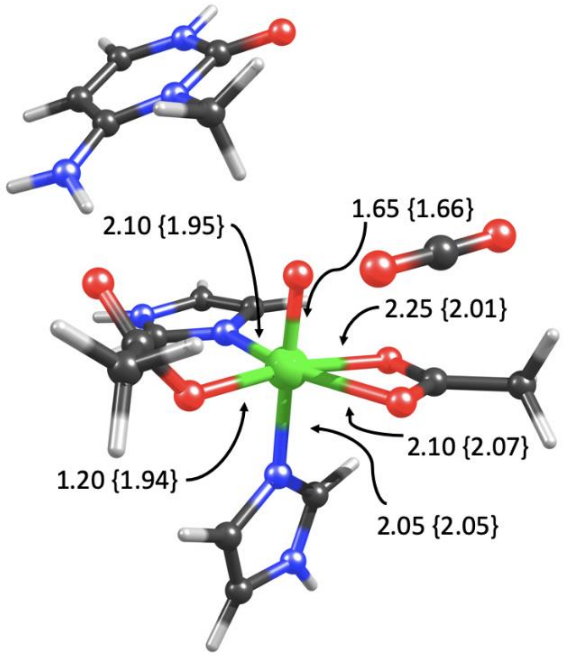

Fig. S11. DFT Optimized geometries for cluster model of ^{5}Re {^{3}Re} in hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

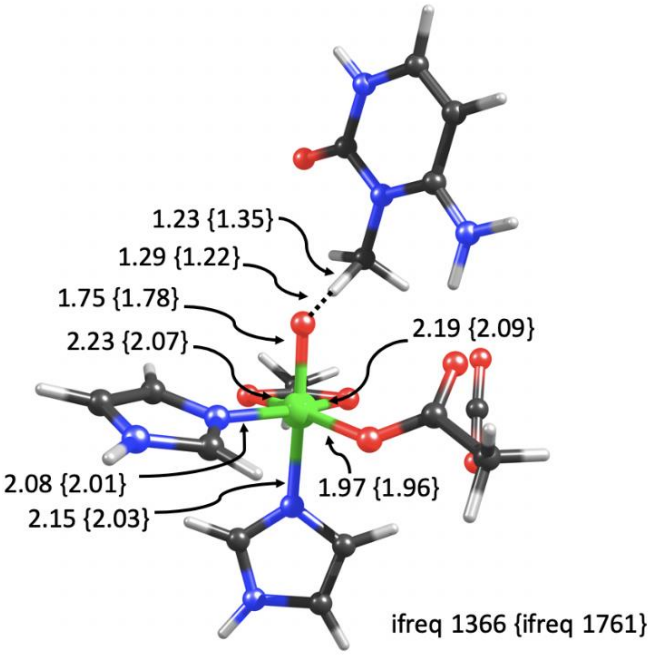

Fig. S12. DFT Optimized geometries for cluster model of $^{5}TS_{H}$ {$^{3}TS_{H}$} in hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

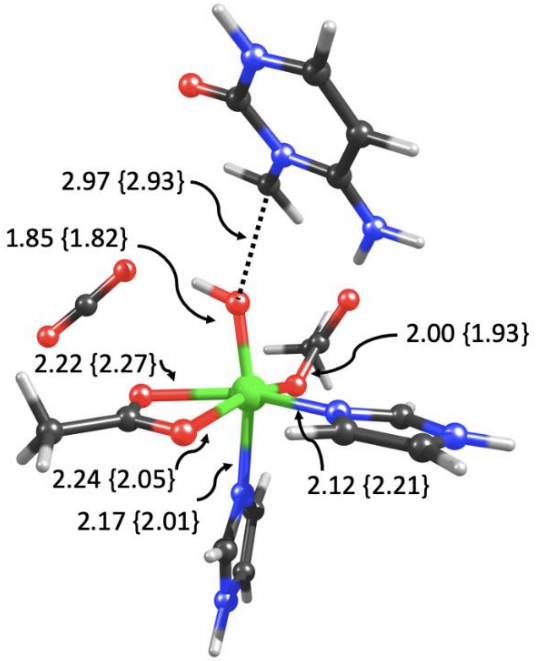

Fig. S13. DFT Optimized geometries for cluster model of $^{5}IM_{H}$ {$^{3}IM_{H}$} in hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

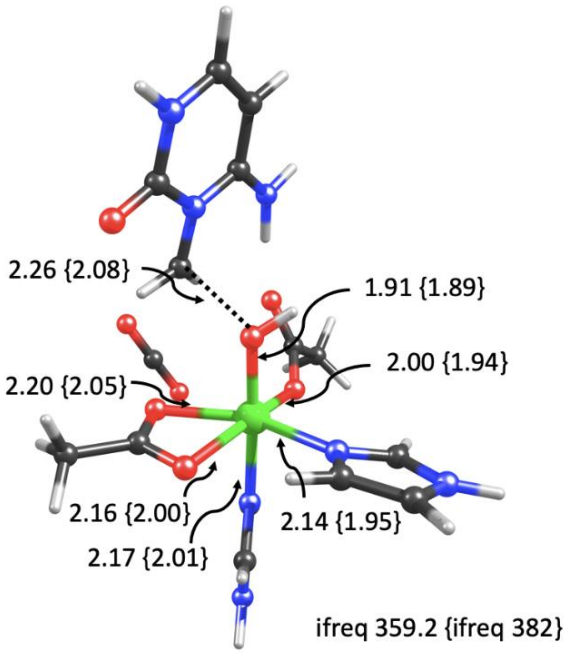

Fig. S14. DFT Optimized geometries for cluster model of $^{5}TS_{reb}$ {$^{3}TS_{reb}$} in hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

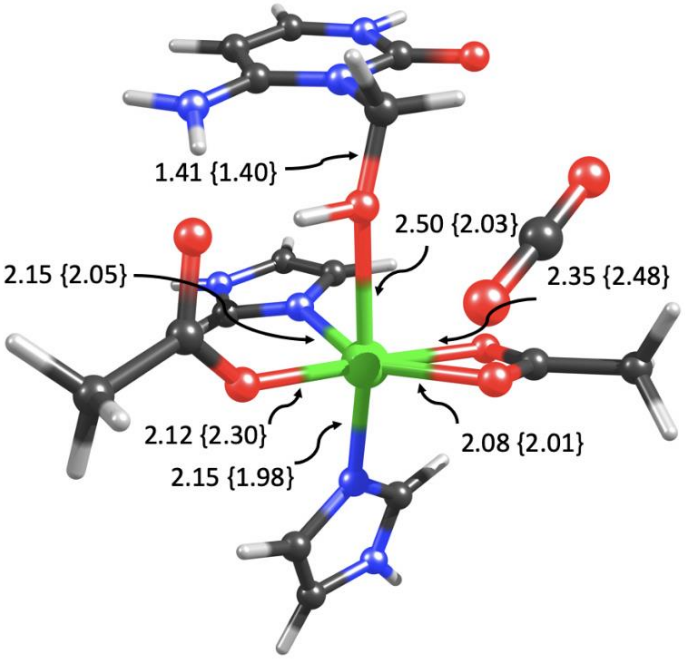

Fig. S15. DFT Optimized geometries for cluster model of $^{5}P_{H}$ {$^{3}P_{H}$} in hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

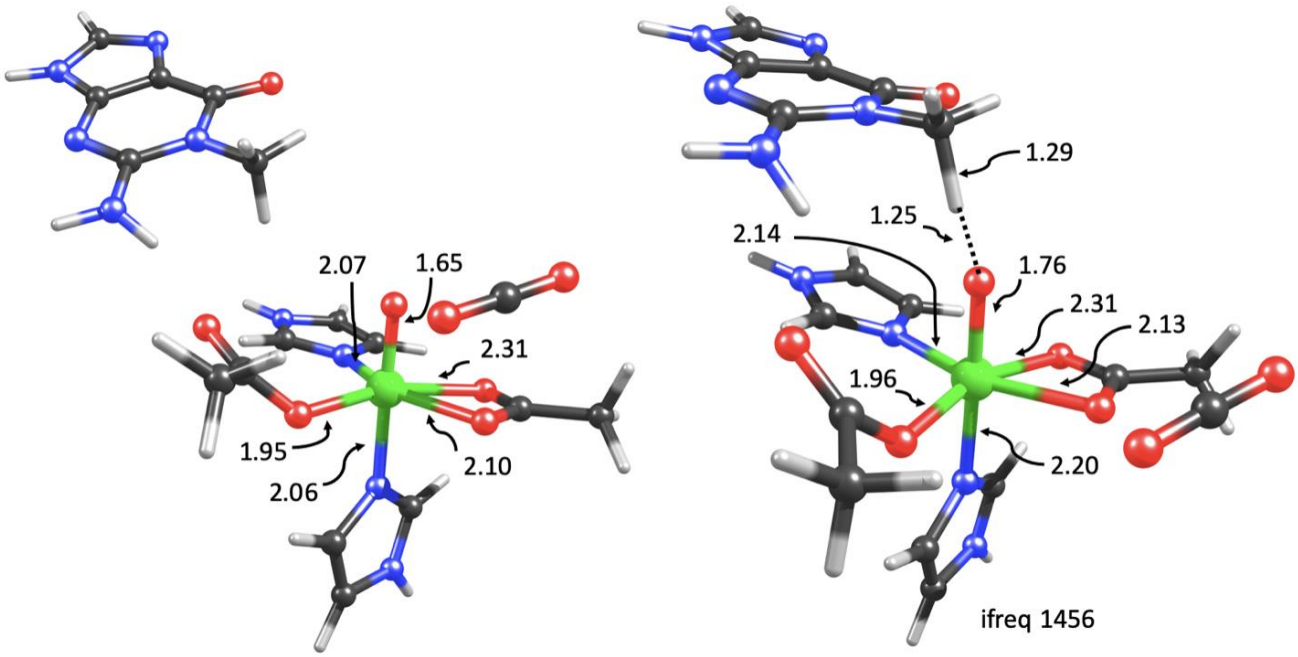

Fig. S16. DFT Optimized geometries for cluster model of ^{5}Re (left) and ^{5}TS$_{H}$ (right) in hydroxylation reaction by iron(IV)-oxo species with N^{1}-methyl guanine (1-meG) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

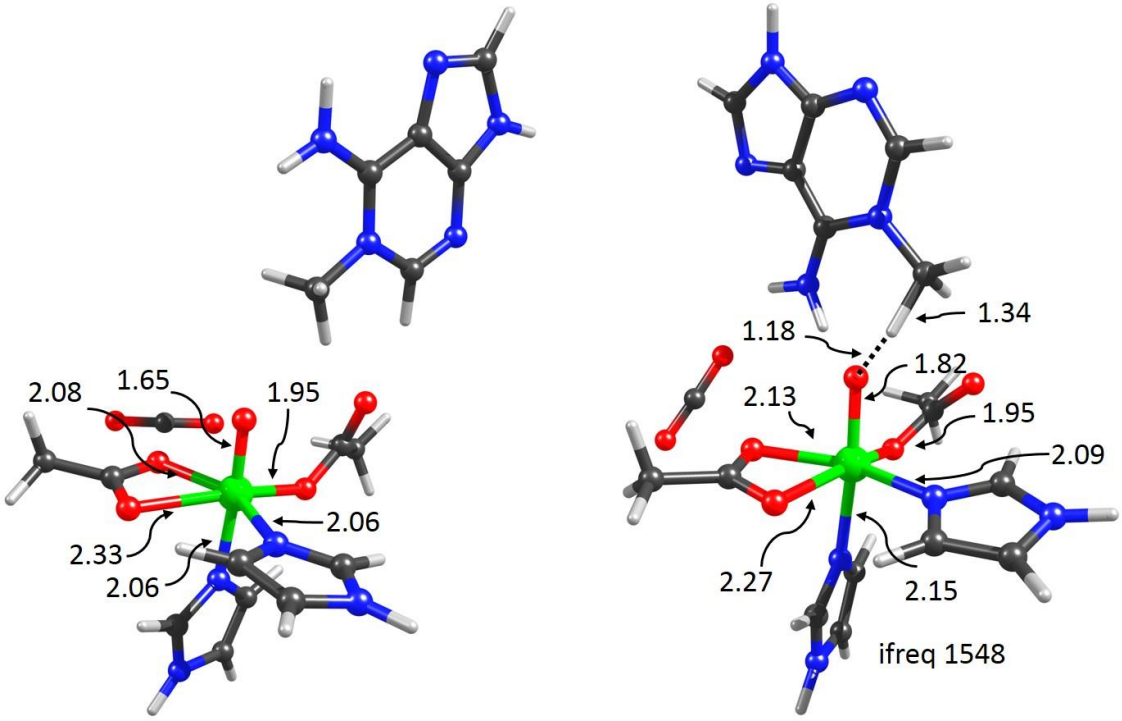

Fig. S17. DFT Optimized geometries for cluster model of ^{5}Re (left) and ^{5}TS$_{H}$ (right) in hydroxylation reaction by iron(IV)-oxo species with N^{1}-methyl adenine (1-meA) using UB3LYP/LACVP. All bond lengths are given in angstroms and the value of the imaginary frequency in the transition state in cm^{-1}.

Table S10. DFT absolute energies for cluster model using UB3LYP/LACVP for epoxidation reactions of 3,N^4-etheno cytosine (εC) by iron(IV)-oxo species.

	E (LACVP) (au)	**ZPE** (kcal/mol)	**G** (au)	**E (LACV3P+*)** (au)
^{1}**Re**	-1767.570763	0.378753	-1767.2541	-1768.273169
^{3}**Re**	-1767.619247	0.379556	-1767.3014	-1768.323704
^{5}**Re**	-1767.628520	0.378162	-1767.3157	-1768.338381
^{7}**Re**	-1767.610836	0.376252	-1767.2989	-1768.319167
^{1}**TS$_E$**	-1767.563873	0.378413	-1767.2471	-1768.262860
^{3}**TS$_E$**	-1767.593207	0.378456	-1767.2764	-1768.293683
^{5}**TS$_E$**	-1767.613687	0.376397	-1767.3026	-1768.325039
^{7}**TS$_E$**	-1767.600822	0.375990	-1767.2902	-1768.311652
^{1}**IM$_E$**	-1767.591178	0.378735	-1767.2725	-1768.297585
^{3}**IM$_E$**	-1767.603585	0.377239	-1767.2852	-1768.312414
^{5}**IM$_E$**	-1767.614469	0.374670	-1767.3026	-1768.325723
^{7}**IM$_E$**	-1767.641175	0.376734	-1767.3297	-1768.358120
^{1}**TS$_{rc}$**	-1767.597769	0.378468	-1767.2799	-1768.309723
^{3}**TS$_{rc}$**	-1767.578468	0.374595	-1767.2913	-1768.300033
^{5}**TS$_{rc}$**	-1767.629027	0.375842	-1767.3190	-1768.349898
^{7}**TS$_{rc}$**	-1767.571735	0.374394	-1767.2691	-1768.287445
^{1}**P$_E$**	-1767.614656	0.380195	-1767.2947	-1768.328372
^{3}**P$_E$**	-1767.612720	0.378152	-1767.2960	-1768.331372
^{5}**P$_E$**	-1767.636257	0.376903	-1767.3246	-1768.359487
^{7}**P$_E$**	-1767.635387	0.375709	-1767.3220	-1768.356517

Table S11. Group spin densities and charges of DFT optimized geometries using UB3LYP/LACVP for epoxidation reactions of 3,N^4-etheno cytosine (εC) by iron(IV)-oxo species.

	ρ_{Fe}	$\rho_{Ligands}$	ρ_{O}	$\rho_{Cytosine}$	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{O}	$Q_{Cytosine}$	Q_{Total}
^{1}**Re**	0.69	-0.06	-0.64	0.00	0.00	0.62	-0.27	-0.33	-0.02	0.00
^{3}**Re**	1.10	-0.05	0.96	0.00	2.00	0.60	-0.25	-0.33	-0.02	0.00
^{5}**Re**	2.95	0.33	0.72	0.00	4.00	0.74	-0.39	-0.34	-0.02	0.00
^{7}**Re**	3.98	0.63	1.39	0.00	6.00	0.90	-0.51	-0.36	-0.03	0.00
^{1}**TS$_E$**	0.81	-0.05	-0.34	-0.41	0.00	0.67	-0.40	-0.45	0.18	0.00
^{3}**TS$_E$**	2.74	0.23	-0.52	-0.45	2.00	0.78	-0.55	-0.44	0.22	0.00
^{5}**TS$_E$**	3.64	0.40	0.22	-0.25	4.00	0.82	-0.56	-0.46	0.20	0.00
^{7}**TS$_E$**	3.98	0.54	1.16	0.32	6.00	0.86	-0.61	-0.47	0.21	0.00
^{1}**IM$_E$**	0.99	-0.06	-0.01	-0.93	0.00	0.71	-0.31	-0.57	0.17	0.00
^{3}**IM$_E$**	2.83	0.22	-0.09	-0.96	2.00	0.81	-0.49	-0.52	0.20	0.00
^{5}**IM$_E$**	4.02	0.56	0.30	-0.89	4.00	0.93	-0.56	-0.61	0.24	0.00
^{7}**IM$_E$**	4.04	0.60	0.36	1.01	6.00	0.93	-0.54	-0.60	0.21	0.00
^{1}**TS$_{rc}$**	-0.06	-0.01	-0.06	0.13	0.00	0.60	-0.70	-0.48	0.57	0.00
^{3}**TS$_{rc}$**	1.98	0.11	0.06	-0.15	2.00	0.69	-0.80	-0.47	0.59	0.00
^{5}**TS$_{rc}$**	3.81	0.27	0.11	-0.19	4.00	0.79	-0.84	-0.50	0.55	0.00
^{7}**TS$_{rc}$**	4.06	0.66	0.24	1.04	6.00	0.99	-0.49	-0.58	0.08	0.00

	ρ_{Fe}	$\rho_{Ligands}$	$\rho_{Product}$	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	$Q_{Product}$	Q_{Total}
^{1}**P$_E$**	0.01	-0.01	0.00	0.00	0.58	-0.70	0.12	0.00
^{3}**P$_E$**	1.95	0.04	0.01	2.00	0.67	-0.76	0.09	0.00
^{5}**P$_E$**	3.74	0.25	0.01	4.00	0.83	-0.91	0.08	0.00
^{7}**P$_E$**	4.03	0.59	1.38	6.00	0.93	-0.53	-0.40	0.00

Table S12. Group spin densities and charges of DFT single point UB3LYP/LACV3P+ calculations on UB3LYP/LACVP optimized geometries in epoxidation reactions of 3,N^4-etheno cytosine (εC) by iron(IV)-oxo species.

	ρ_{Fe}	$\rho_{Ligands}$	ρ_{O}	$\rho_{Cytosine}$	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{O}	$Q_{Cytosine}$	Q_{Total}
^{1}**Re**	0.70	-0.08	-0.61	0.00	0.00	0.62	-0.27	-0.33	-0.02	0.00
^{3}**Re**	1.16	-0.07	0.91	0.00	2.00	0.43	-0.21	-0.16	-0.06	0.00
^{5}**Re**	3.10	0.26	0.64	0.00	4.00	0.39	-0.21	-0.13	-0.05	0.00
^{7}**Re**	4.13	0.55	1.30	0.01	6.00	0.63	-0.42	-0.17	-0.04	0.00
^{1}**TS$_E$**	0.85	-0.07	-0.34	-0.44	0.00	0.62	-0.40	-0.21	-0.01	0.00
^{3}**TS$_E$**	2.81	0.18	-0.52	-0.47	2.00	0.70	-0.53	-0.19	0.02	0.00
^{5}**TS$_E$**	3.77	0.31	0.19	-0.27	4.00	0.59	-0.40	-0.21	0.01	0.00
^{7}**TS$_E$**	4.15	0.44	1.06	0.34	6.00	0.63	-0.44	-0.24	0.06	0.00
^{1}**IM$_E$**	1.03	-0.07	-0.01	-0.95	0.00	0.71	-0.34	-0.31	-0.05	0.00
^{3}**IM$_E$**	2.91	0.16	-0.10	-0.98	2.00	0.73	-0.44	-0.21	-0.07	0.00
^{5}**IM$_E$**	4.18	0.46	0.27	-0.91	4.00	0.77	-0.45	-0.34	0.01	0.00
^{7}**IM$_E$**	4.19	0.49	0.30	1.02	6.00	0.78	-0.42	-0.33	-0.03	0.00
^{1}**TS$_{rc}$**	-0.07	0.00	-0.06	0.13	0.00	0.67	-0.74	-0.22	0.29	0.00
^{3}**TS$_{rc}$**	2.01	0.09	0.05	-0.15	2.00	0.72	-0.83	-0.17	0.29	0.00
^{5}**TS$_{rc}$**	3.90	0.21	0.08	-0.19	4.00	0.75	-0.81	-0.21	0.27	0.00
^{7}**TS$_{rc}$**	4.22	0.55	0.18	1.05	6.00	0.76	-0.25	-0.19	-0.32	0.00

	ρ_{Fe}	$\rho_{Ligands}$	$\rho_{Product}$	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	$Q_{Product}$	Q_{Total}
^{1}**P$_E$**	0.02	-0.01	0.00	0.00	0.67	-0.96	0.29	0.00
^{3}**P$_E$**	1.97	0.02	0.01	2.00	0.77	-0.98	0.21	0.00
^{5}**P$_E$**	3.81	0.20	-0.01	4.00	0.71	-0.81	0.10	0.00
^{7}**P$_E$**	4.19	0.49	1.33	6.00	0.66	-0.35	-0.31	0.00

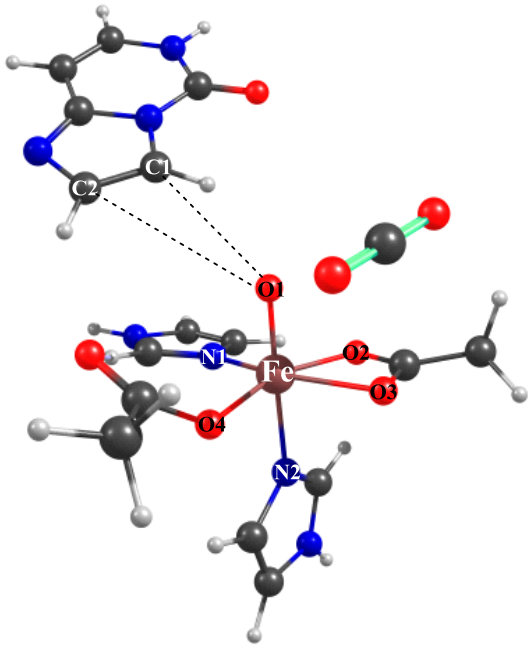

Table S13. Bond lengths (in angstroms) for DFT optimized geometries using UB3LYP/LACVP for epoxidation reactions of 3,N^4-etheno cytosine (εC) {above} by iron(IV)-oxo species .

	Fe-O1	Fe-O2	Fe-O3	Fe-O4	Fe-N1	Fe-N2	O1-C1	O1-C2
^{1}Re	1.70326	2.03158	2.11876	1.91060	1.95118	2.06322	3.20627	3.77641
^{3}Re	1.65250	2.04223	2.12473	1.91493	1.94702	2.07739	3.22303	3.85795
^{5}Re	1.64927	2.28205	2.13275	1.92770	2.08712	2.06879	3.25171	3.72760
^{7}Re	1.93592	2.36542	2.09256	1.93098	2.10234	2.17470	3.14594	3.85191
^{1}TS$_E$	1.75394	2.02674	2.20290	1.92225	1.94070	2.06782	1.92903	2.64566
^{3}TS$_E$	1.74732	2.03843	2.20072	1.93351	1.96169	2.06530	1.94638	2.67336
^{5}TS$_E$	1.71244	2.34825	2.13294	1.93837	2.12598	2.17696	2.13794	2.69638
^{7}TS$_E$	1.90480	2.31095	2.15125	1.94079	2.12895	2.22071	2.17446	2.64522
^{1}IM$_E$	1.85849	2.00346	2.12077	1.92395	1.96246	2.02423	1.40860	2.49953
^{3}IM$_E$	1.83218	2.36369	2.10034	1.96216	2.04779	2.02685	1.42300	2.50641
^{5}IM$_E$	1.84631	2.27555	2.15312	1.93699	2.12654	2.20339	1.42733	2.42206
^{7}IM$_E$	1.86934	2.28904	2.14956	1.92761	2.12566	2.19918	1.40732	2.42821
^{1}TS$_{rc}$	1.95220	2.10382	2.20286	2.00338	2.01417	1.98017	1.41033	2.00160
^{3}TS$_{rc}$	2.09999	2.24175	2.28532	1.98509	2.14590	2.16792	1.43155	1.94618
^{5}TS$_{rc}$	2.06541	2.24247	2.29726	1.98792	2.17221	2.17405	1.41456	1.98448
^{7}TS$_{rc}$	1.95048	2.27279	2.12851	1.91125	2.08059	2.15916	1.52640	1.65565
^{1}P$_E$	2.07269	2.09819	2.23115	2.00605	2.02209	2.00096	1.50436	1.56659
^{3}P$_E$	2.23910	2.03463	2.36329	1.98382	2.11388	2.10897	1.49577	1.55259
^{5}P$_E$	2.47254	3.17129	1.98886	1.95923	2.12496	2.17782	1.48550	1.54077
^{7}P$_E$	1.85611	2.28069	2.13706	1.92048	2.14957	2.21130	1.40689	2.43387

Table S14. DFT absolute energies for cluster model using UB3LYP/LACVP for hydroxylation reactions of N^3-methyl cytosine (3-meC) by iron(IV)-oxo species.

	E (LACVP) (au)	**ZPE** (kcal/mol)	**G** (au)	**E (LACV3P+*)** (au)
^{1}**Re**	-1731.101759	0.408898	-1730.7538	-1731.771229
^{3}**Re**	-1731.164160	0.410127	-1730.8191	-1731.833125
^{5}**Re**	-1731.172770	0.408783	-1730.8268	-1731.847229
^{7}**Re**	-1731.165185	0.407189	-1730.8238	-1731.837261
^{1}**TS$_H$**	-1731.112278	0.403607	-1730.7723	-1731.772673
^{3}**TS$_H$**	-1731.150624	0.403076	-1730.8109	-1731.813370
^{5}**TS$_H$**	-1731.157975	0.402022	-1730.8192	-1731.829716
^{7}**TS$_H$**	-1731.138744	0.400981	-1730.7990	-1731.808883
^{1}**IM$_H$**	-1731.101672	0.407345	-1730.7552	-1731.771548
^{3}**IM$_H$**	-1731.132768	0.405389	-1730.7929	-1731.810758
^{5}**IM$_H$**	-1731.151604	0.403100	-1730.8098	-1731.825897
^{7}**IM$_H$**	-1731.153942	0.403609	-1730.8150	-1731.838528
^{1}**TS$_{reb}$**	-1731.149271	0.408708	-1730.7989	-1731.814160
^{3}**TS$_{reb}$**	-1731.164602	0.407192	-1730.8266	-1731.827744
^{5}**TS$_{reb}$**	-1731.160190	0.403187	-1730.8197	-1731.832007
^{7}**TS$_{reb}$**	-1731.164979	0.405386	-1730.8240	-1731.846534
^{1}**P$_H$**	-1731.214112	0.411702	-1730.8631	-1731.884443
^{3}**P$_H$**	-1731.211195	0.409730	-1730.8606	-1731.880578
^{5}**P$_H$**	-1731.234052	0.408664	-1730.8951	-1731.915444
^{7}**P$_H$**	-1731.169729	0.406679	-1730.8229	-1731.851548

Table S15. Group spin densities and charges of DFT optimized geometries using UB3LYP/LACVP for hydroxylation reactions of N^3-methyl cytosine (3-meC) by iron(IV)-oxo species.

	ρ_{Fe}	$\rho_{Ligands}$	ρ_{O}	ρ_{ACH3}	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{O}	Q_{ACH3}	Q_{Total}
^{1}**Re**	0.80	-0.08	-0.72	0.00	0.00	0.61	-0.18	-0.38	0.94	1.00
^{3}**Re**	1.10	-0.06	0.95	0.00	2.00	0.59	-0.10	-0.34	0.85	1.00
^{5}**Re**	2.99	0.32	0.69	0.00	4.00	0.75	-0.25	-0.37	0.87	1.00
^{7}**Re**	3.99	0.64	1.37	0.00	6.00	0.90	-0.46	-0.37	0.93	1.00
	ρ_{Fe}	$\rho_{Ligands}$	ρ_{OH}	ρ_{ACH2}	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{OH}	Q_{ACH2}	Q_{Total}
^{1}**TS$_H$**	0.80	-0.04	-0.37	-0.39	0.00	0.57	-0.09	-0.11	0.63	1.00
^{3}**TS$_H$**	2.77	0.21	-0.51	-0.48	2.00	0.72	-0.28	-0.12	0.68	1.00
^{5}**TS$_H$**	3.70	0.41	0.15	-0.26	4.00	0.83	-0.33	-0.16	0.65	1.00
^{7}**TS$_H$**	4.05	0.56	0.84	0.55	6.00	0.87	-0.40	-0.19	0.72	1.00
^{1}**IM$_H$**	0.94	-0.06	0.10	-0.98	0.00	0.63	-0.14	-0.31	0.82	1.00
^{3}**IM$_H$**	2.02	0.16	0.03	-0.21	2.00	0.72	-0.26	-0.29	0.83	1.00
^{5}**IM$_H$**	4.05	0.53	0.40	-0.98	4.00	0.91	-0.44	-0.31	0.84	1.00
^{7}**IM$_H$**	4.06	0.58	0.37	0.99	6.00	0.90	-0.40	-0.36	0.86	1.00
^{1}**TS$_{reb}$**	0.85	-0.05	0.03	-0.84	0.00	0.60	-0.12	-0.23	0.75	1.00
^{3}**TS$_{reb}$**	2.55	0.18	0.00	-0.74	2.00	0.73	-0.32	-0.22	0.81	1.00
^{5}**TS$_{reb}$**	4.03	0.48	0.27	-0.78	4.00	0.87	-0.44	-0.30	0.87	1.00
^{7}**TS$_{reb}$**	4.11	0.69	0.23	0.96	6.00	0.95	-0.24	-0.25	0.53	1.00
	ρ_{Fe}	$\rho_{Ligands}$	ρ_{ACH2}	ρ_{Total}		Q_{Fe}	$Q_{Ligands}$	Q_{ACH2}	Q_{Total}	
^{1}**P$_H$**	0.00	0.00	0.00	0.00		0.54	-0.44	0.91	1.00	
^{3}**P$_H$**	1.98	0.03	-0.01	2.00		0.63	-0.54	0.92	1.00	
^{5}**P$_H$**	3.96	0.04	0.01	4.00		0.76	-0.63	0.87	1.00	
^{7}**P$_H$**	4.09	0.81	1.10	6.00		1.05	-0.24	0.19	1.00	

Table S16. Group spin densities and charges of DFT single point UB3LYP/LACV3P+ calculations on UB3LYP/LACVP optimized geometries in hydroxylation reactions of N^3-methyl cytosine (3-meC) by iron(IV)-oxo species.

	ρ_{Fe}	$\rho_{Ligands}$	ρ_{O}	ρ_{ACH3}	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{O}	Q_{ACH3}	Q_{Total}
^{1}**Re**	0.80	-0.10	-0.70	0.00	0.00	0.51	-0.21	-0.24	0.95	1.00
^{3}**Re**	1.17	-0.07	0.90	0.00	2.00	0.45	-0.14	-0.23	0.92	1.00
^{5}**Re**	3.13	0.24	0.63	0.00	4.00	0.48	-0.18	-0.22	0.92	1.00
^{7}**Re**	4.15	0.56	1.29	0.01	6.00	0.62	-0.37	-0.19	0.94	1.00
	ρ_{Fe}	$\rho_{Ligands}$	ρ_{OH}	ρ_{ACH2}	ρ_{Total}	Q_{Fe}	$Q_{Ligands}$	Q_{OH}	Q_{ACH2}	Q_{Total}
^{1}**TS$_H$**	0.83	-0.06	-0.38	-0.40	0.00	0.51	-0.20	0.18	0.52	1.00
^{3}**TS$_H$**	2.84	0.16	-0.51	-0.49	2.00	0.61	-0.37	0.19	0.58	1.00
^{5}**TS$_H$**	3.83	0.32	0.10	-0.25	4.00	0.62	-0.32	0.18	0.52	1.00
^{7}**TS$_H$**	4.21	0.48	0.77	0.55	6.00	0.70	-0.41	0.10	0.62	1.00
	4.21	0.47	0.75	0.57	6.00	0.69	-0.41	0.10	0.63	1.00
^{1}**IM$_H$**	0.97	-0.07	0.10	-0.99	0.00	0.56	-0.17	-0.24	0.85	1.00
^{3}**IM$_H$**	2.80	0.16	0.03	-0.99	2.00	0.72	-0.26	-0.29	0.83	1.00
^{5}**IM$_H$**	4.21	0.44	0.34	-0.99	4.00	0.86	-0.40	-0.29	0.83	1.00
^{7}**IM$_H$**	4.21	0.48	0.32	0.99	6.00	0.75	-0.39	-0.25	0.88	1.00
^{1}**TS$_{reb}$**	0.89	-0.06	0.04	-0.86	0.00	0.59	-0.27	-0.01	0.69	1.00
^{3}**TS$_{reb}$**	2.65	0.15	-0.01	-0.79	2.00	0.72	-0.44	0.01	0.70	1.00
^{5}**TS$_{reb}$**	4.17	0.40	0.24	-0.81	4.00	0.76	-0.44	-0.01	0.69	1.00
^{7}**TS$_{reb}$**	4.26	0.58	0.18	0.98	6.00	0.75	-0.19	0.01	0.43	1.00
	ρ_{Fe}	$\rho_{Ligands}$	ρ_{ACH2}	ρ_{Total}		Q_{Fe}	$Q_{Ligands}$	Q_{ACH2}	Q_{Total}	
^{1}**P$_H$**	0.00	0.00	0.00	0.00		0.54	-0.48	0.96	1.00	
^{3}**P$_H$**	2.03	-0.01	-0.02	2.00		0.53	-0.49	0.97	1.00	
^{5}**P$_H$**	3.84	0.17	-0.01	4.00		0.55	-0.50	0.95	1.00	
^{7}**P$_H$**	4.24	0.69	1.07	6.00		0.83	-0.24	0.41	1.00	

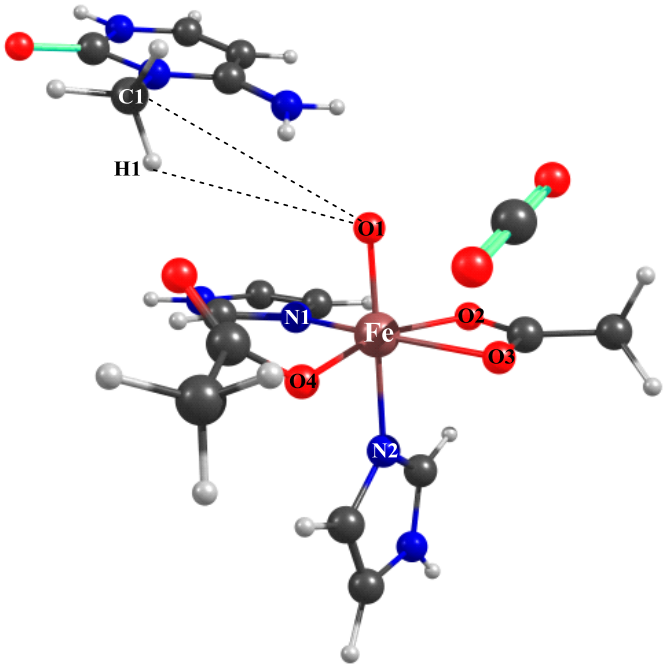

Table S17. Bond lengths (in angstroms) for DFT optimized geometries using UB3LYP/LACVP for hydroxylation reactions of N^3-methyl cytosine (3-meC) {above} by iron(IV)-oxo species .

	Fe-O1	Fe-O2	Fe-O3	Fe-O4	Fe-N1	Fe-N2	O1-H1	H1-C1	O1-C1
^{1}Re	1.74346	2.04614	2.04915	1.89882	1.95509	2.04803	3.61496	1.09283	4.33017
^{3}Re	1.65568	2.01445	2.07153	1.93670	1.94867	2.05294	1.99734	1.09495	3.08993
^{5}Re	1.64995	2.24744	2.09589	1.95733	2.10113	2.04743	1.95870	1.09415	3.02665
^{7}Re	1.94090	2.33657	2.07411	1.94135	2.12006	2.16562	2.15901	1.09244	3.09906
^1TS_H	1.75326	2.01858	2.05638	1.91737	1.95000	2.02665	1.24603	1.34004	2.58562
^3TS_H	1.78251	2.07040	2.09459	1.95991	2.00576	2.02952	1.22450	1.35370	2.57795
^5TS_H	1.74556	2.23539	2.18663	1.97444	2.08353	2.14612	1.29417	1.22925	2.51828
^7TS_H	1.85239	2.08668	2.10592	1.95619	2.01861	2.08723	1.22147	1.34324	2.56216
^1IM_H	1.82031	2.03036	2.03170	1.93958	1.97078	2.02285	0.98036	3.15281	2.96202
^3IM_H	1.81880	2.05400	2.27944	1.92551	2.20514	2.01088	0.98228	3.13086	2.92549
^5IM_H	1.84838	2.24262	2.21821	2.00466	2.11811	2.17147	0.97954	2.82545	2.97008
^7IM_H	1.86324	2.33383	2.14215	1.94260	2.21081	2.15754	0.97596	3.02486	2.99143
$^1TS_{reb}$	1.85981	2.00575	2.04344	1.94203	1.95857	2.00445	0.98062	2.54284	2.12298
$^3TS_{reb}$	1.88607	1.99570	2.04713	1.93758	1.95466	2.01450	0.98210	2.50770	2.07661
$^5TS_{reb}$	1.90647	2.20376	2.16335	1.99757	2.14106	2.16942	0.97729	2.68542	2.26828
$^7TS_{reb}$	1.98228	2.16661	2.18238	1.96483	2.08898	2.14868	0.99887	2.24911	1.80415
^1P_H	2.03055	2.07331	2.09276	2.09422	1.99724	1.98202	1.06698	2.10221	1.39730
^3P_H	2.02596	2.47652	2.01485	2.29901	2.05438	1.98025	1.08950	2.13458	1.40241
^5P_H	2.50446	2.35400	2.07597	2.11548	2.14701	2.14738	1.02155	2.02381	1.41016
^7P_H	2.07470	2.24636	2.15561	1.89127	2.08590	2.11389	0.98337	2.04671	1.50046

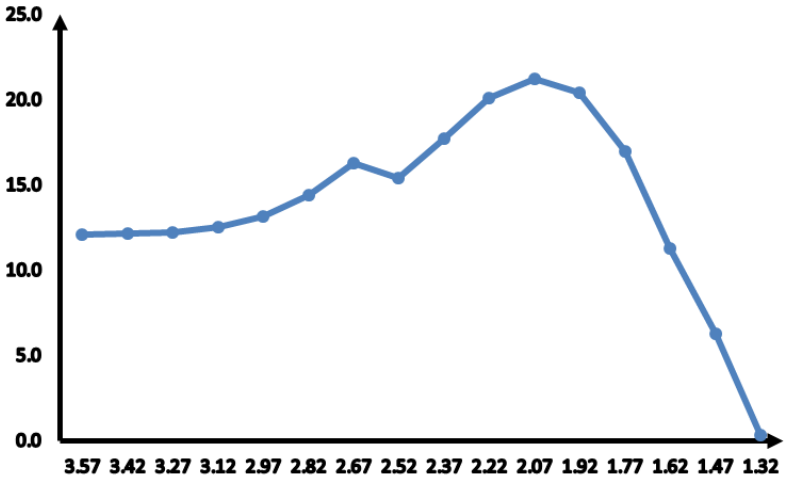

Fig. S18. Forward scan of C-O distance in ^{5}Re for epoxidation reaction by iron(IV)-oxo species with 1,N^{6}-etheno adenine (εA).

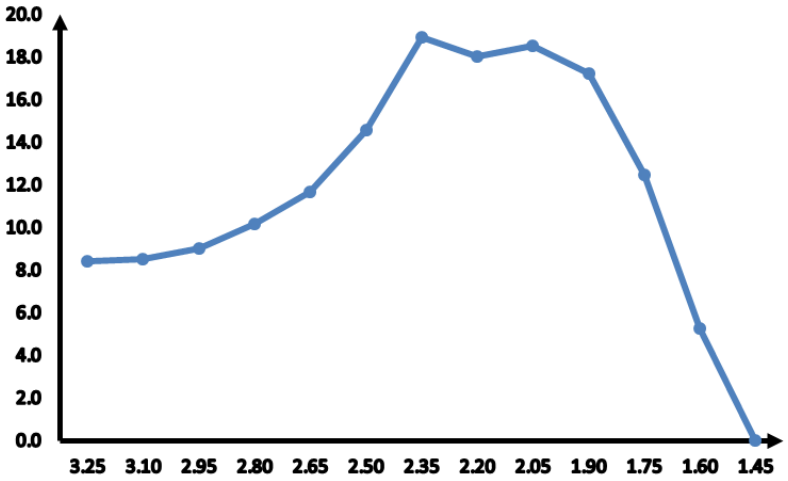

Fig. S19. Forward scan of C-O distance in ^{5}Re for epoxidation reaction by iron(IV)-oxo species with 1,N^{2}-etheno guanine (εG).

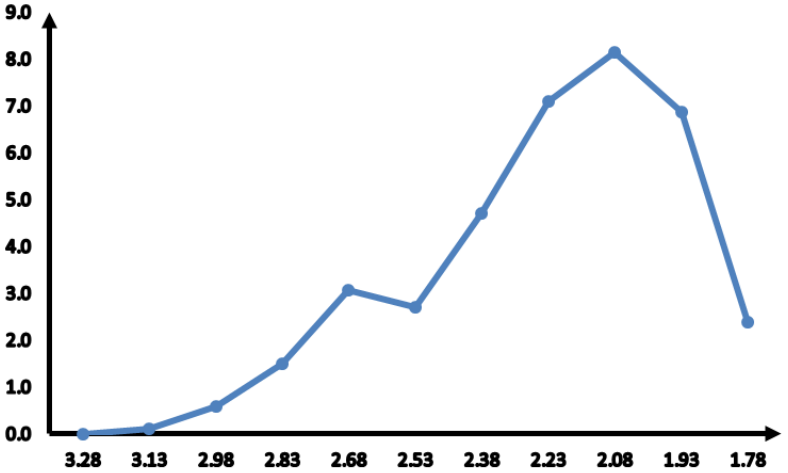

Fig. S20. Forward scan of C-O distance in ^{5}Re for epoxidation reaction by iron(IV)-oxo species with 3,N^{4}-etheno cytosine (εC).

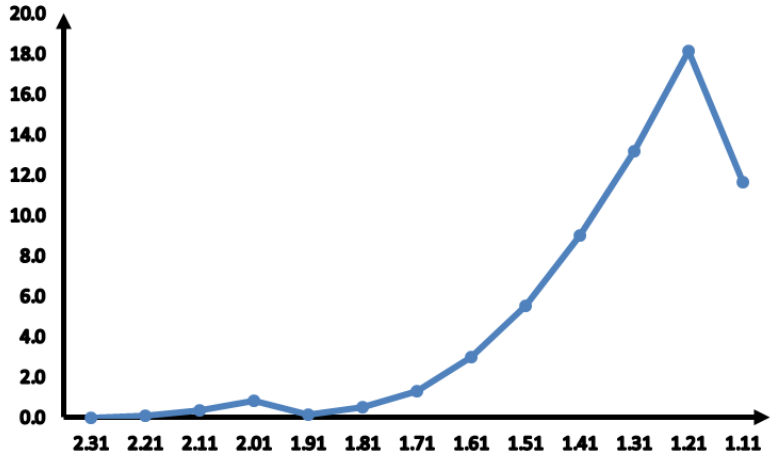

Fig. S21. Forward scan of H-O distance in ^{5}Re for hydroxylation reaction by iron(IV)-oxo species with N^{1}-methyl adenine (1-meA).

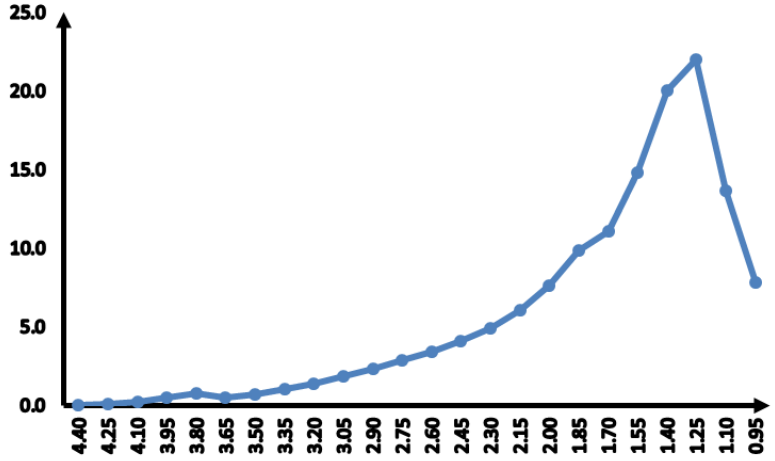

Fig. S22. Forward scan of H-O distance in ^{5}Re for hydroxylation reaction by iron(IV)-oxo species with N^{1}-methyl guanine (1-meG).

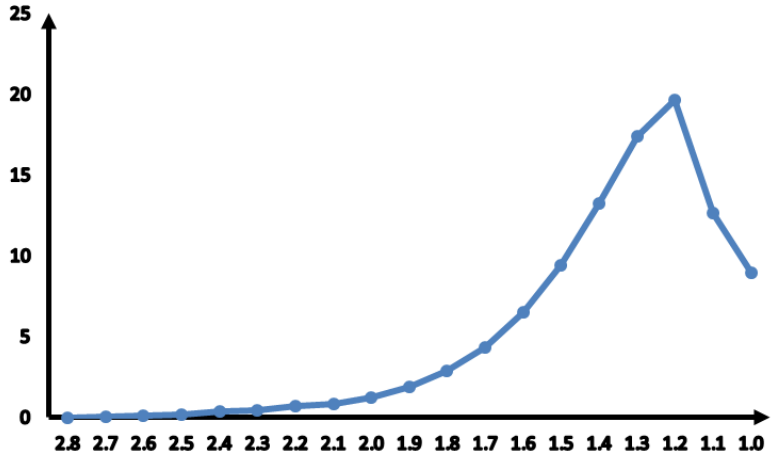

Fig. S23. Forward scan of H-O distance in ^{5}Re for hydroxylation reaction by iron(IV)-oxo species with N^{3}-methyl cytosine (3-meC).

Cytosine: ***Part 1: Epoxidation (DFT calculations in UB3LYP/LANL2DZ)***

$^{1}RE_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.951183393000
C	1.034372422000	0.000000000000	2.793392484400
N	0.557833516900	0.125298383900	4.064613635100
C	-0.832741410800	0.221322311500	4.021057681500
C	-1.171679091600	0.144493216300	2.695031253100
H	2.070269877100	-0.022975072900	2.477662396400
H	1.133972578800	0.200388967200	4.886977406900
H	-1.432862011200	0.341237119300	4.905787001200
H	-2.129487625500	0.220422799600	2.212999338000
N	-0.620746186600	-1.967590462700	0.011933128400
C	-1.853761052300	-2.428995575800	0.224771758300
N	-1.843621382300	-3.794485392500	0.179488930600
C	-0.539385576000	-4.214309230700	-0.078786800500
C	0.210912130700	-3.070563618400	-0.180732836100
H	-2.724019290700	-1.822094118400	0.395368920800
H	-2.644074248900	-4.392179857800	0.305121953100
H	-0.275814468700	-5.253418145000	-0.168275038900
H	1.255119958400	-2.924699915200	-0.382332482000
O	-0.676935833300	0.167453353500	-2.000716940700
C	-1.839750878500	0.479601917700	-1.533962913200
O	-1.970139566700	0.439833547200	-0.228905678700
C	-2.967676415300	0.908828206200	-2.412782399300
H	-3.920283941000	0.825243066000	-1.886740022600
H	-2.982143671900	0.315782803600	-3.330826523000
H	-2.809456341600	1.957114599100	-2.692942594500
C	0.875255882200	2.369583302700	-3.020761167700
O	1.895833360500	1.778896014500	-3.154054116500
O	-0.127808636600	3.002674943000	-2.943897960500
C	2.973019108700	-0.298442562800	-0.073682722800
O	1.739210736300	-0.714011833900	-0.340159372600
C	3.947815176100	-0.545094629900	-1.206107540000
H	3.817580047200	-1.552454174100	-1.613653480700
H	4.973593508800	-0.403624351200	-0.861913218400
H	3.725075086800	0.164374734500	-2.011821830800
O	0.487608811500	1.631046339500	-0.054844192700
O	3.334041114200	0.243697769500	1.001671976200
N	3.201119111500	3.552449381800	3.822766561800
C	2.327160527400	4.509764022800	4.120029818800
C	2.232402052000	5.385445384100	5.243212572700
N	1.349065298200	4.621500912000	3.095679849600
C	1.213420919700	6.280138687900	5.275881129100
H	2.969172270800	5.321076995100	6.030219746100
C	0.286090356900	5.532915711800	3.099973260900
N	0.282830873600	6.337439841100	4.236092230700
H	1.060577378700	6.986060651400	6.080066630800
O	-0.564884770100	5.624934155100	2.199567048700
H	-0.468435018700	7.010934987600	4.264532245300
C	1.661547330000	3.668179581100	2.125095594800
H	1.055538876200	3.510457037600	1.248346255700
C	2.794115101000	3.034189131800	2.585696651300
H	3.330851612100	2.232801585200	2.103730318200

$^{3}RE_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.947021406900
C	1.043463599000	0.000000000000	2.778492165600
N	0.577845052200	0.100238951500	4.055153195900
C	-0.814439479200	0.179101135300	4.026146525000
C	-1.166467421300	0.117040401800	2.702507054100
H	2.076203829200	0.004520867700	2.450916378300
H	1.160772776100	0.172010630200	4.873186451500

H	-1.407199220500	0.278805879400	4.918212045000
H	-2.129626062300	0.183480092600	2.229409411600
N	-0.547618084400	-2.002533736600	0.074348279900
C	-1.764403530500	-2.498425011200	0.305622277300
N	-1.700477938300	-3.862491315600	0.351616836600
C	-0.377437561300	-4.246383484700	0.134755807400
C	0.328134351300	-3.082154910800	-0.036752554700
H	-2.658794468900	-1.915819973300	0.431166332700
H	-2.478876151300	-4.482128440000	0.507048658700
H	-0.072052545600	-5.277880709700	0.117825047400
H	1.368731882500	-2.909334679000	-0.237928250300
O	-0.714063144900	0.040854399200	-2.000727650300
C	-1.881119903000	0.330084040300	-1.531761187000
O	-2.000951589200	0.341581399600	-0.224123972700
C	-3.033697832200	0.678296997800	-2.415454755200
H	-3.976950130400	0.588068965000	-1.873535184600
H	-3.038048555200	0.041153920500	-3.303616809400
H	-2.915235401500	1.716648592400	-2.747839849400
C	0.832333128300	2.524352001300	-2.980772144300
O	1.921236837900	2.055475821000	-3.012895013400
O	-0.241317593000	3.030482194300	-3.005154945100
C	2.975040563200	-0.178450277600	-0.081140565300
O	1.764051144300	-0.654809205800	-0.355416544900
C	3.964584088100	-0.356042728800	-1.212429011800
H	3.860763573300	-1.346566910900	-1.664493958900
H	4.983414456800	-0.204870672400	-0.851966026100
H	3.735080056700	0.385408126600	-1.986586205100
O	0.402440406600	1.600508018400	-0.084732733600
O	3.306646422900	0.368181075900	1.001679069500
N	3.051583318600	3.759515178000	3.837114452400
C	2.117923337700	4.673854968800	4.084112615400
C	1.991678095900	5.631961803300	5.134587765000
N	1.107795011300	4.632271625100	3.085545204300
C	0.914496559200	6.456193520100	5.126448029300
H	2.751623901100	5.683288936200	5.900111595100
C	-0.017488250300	5.465487692300	3.052353606100
N	-0.045654252500	6.361876943100	4.116779816500
H	0.734660116200	7.216138242200	5.873789373300
O	-0.902047585900	5.420025169400	2.181125898800
H	-0.841929247700	6.982405349800	4.114771739500
C	1.465965051500	3.628176956400	2.183618820200
H	0.863026940500	3.364568740900	1.330043061900
C	2.652790846000	3.115367880500	2.658418791300
H	3.238759118400	2.324144391200	2.218767225900

$^{5}RE_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.087124823900
C	1.117962950600	0.000000000000	2.816567054300
N	0.783497805600	0.126031844400	4.132749460000
C	-0.604295426800	0.221510532000	4.236392430600
C	-1.083151486200	0.142350042000	2.952127022800
H	2.119150821700	-0.031123680100	2.403963199700
H	1.443927895100	0.205505698400	4.889375052200
H	-1.105806083000	0.342611020100	5.180507927000
H	-2.087800310200	0.214411890300	2.574803146000
N	-0.678870586300	-1.953753494500	0.043500479900
C	-1.912265308300	-2.371712831300	0.337076226300
N	-1.947746187400	-3.735366140300	0.300425447700
C	-0.676314399500	-4.200851932800	-0.034609540700
C	0.104011563200	-3.083597875500	-0.191833296300
H	-2.745840985300	-1.729574131100	0.556425035900
H	-2.758728178700	-4.304840316500	0.479579480400
H	-0.452721649900	-5.248812447500	-0.129732143000
H	1.141357749200	-2.974460737500	-0.448697616800
O	-1.061071842100	0.247286626800	-1.833469751000

C	-2.179640636500	0.553775624400	-1.244841221200
O	-2.232564740900	0.470430491200	0.045813827000
C	-3.351295082900	1.027357400400	-2.051648844000
H	-4.268948621800	0.980445733600	-1.462475084900
H	-3.449764103400	0.435226143000	-2.965196500300
H	-3.170742102300	2.067562847700	-2.347587971500
C	0.483276038000	2.460442171100	-2.946534822000
O	1.503263943500	1.870823906400	-3.079132337800
O	-0.514905314200	3.096364000300	-2.867057050800
C	2.964350851700	-0.236244291300	-0.243314374600
O	1.734412700600	-0.755424206600	-0.370395736900
C	3.801499186000	-0.297387019800	-1.497610951600
H	3.754852261300	-1.298369222200	-1.936936873200
H	4.835567153100	-0.028508747600	-1.277793873100
H	3.383847666600	0.400726743300	-2.231605788800
O	0.480684700500	1.576587926100	-0.058214678300
O	3.394383627100	0.242858878600	0.831885727600
N	3.039202282600	3.726129169500	3.792173719200
C	2.145826996400	4.649541622500	4.137736168500
C	2.108506660800	5.561128814400	5.235934987100
N	1.076484851500	4.677217895400	3.203038936400
C	1.053378149400	6.408439790700	5.331520668800
H	2.915767190900	5.561221429600	5.953350438200
C	-0.029539703900	5.533431023600	3.278224043200
N	0.030370707700	6.380515055200	4.381433823800
H	0.938908784600	7.137689252500	6.121428799600
O	-0.963982652400	5.547616046500	2.460138272100
H	-0.749062074800	7.017732737600	4.457126092700
C	1.353696073300	3.709766861500	2.235479708500
H	0.692653568200	3.503464034800	1.411241050000
C	2.553332071400	3.148545666200	2.611632379100
H	3.095398983400	2.367804552800	2.102398998400

$^{7}RE_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.102343141000
C	1.105865512300	0.000000000000	2.856283276600
N	0.742969796200	0.091047732600	4.165545008200
C	-0.649775495900	0.159022345200	4.244857542200
C	-1.101847842200	0.104139546400	2.952240947200
H	2.116216236400	-0.019477155900	2.463301606700
H	1.385056360700	0.149308435500	4.939161741100
H	-1.169532951700	0.246535765900	5.182507123100
H	-2.099876173900	0.156227631400	2.555094834300
N	-0.595259799600	-2.087941445400	-0.124366116400
C	-1.808581789900	-2.598364816200	0.095707809000
N	-1.762334582400	-3.957238547500	-0.035263607500
C	-0.454061613800	-4.324030482600	-0.355368395600
C	0.261254858000	-3.154320301700	-0.405931222700
H	-2.686439171300	-2.020826634900	0.326177080500
H	-2.542249188000	-4.585102250000	0.075059674600
H	-0.166007078400	-5.348510039300	-0.513932378900
H	1.299580672100	-2.972823743800	-0.617579688300
O	-1.007209993500	0.608311483800	-1.730397002600
C	-2.197946663200	0.710921857200	-1.181846312000
O	-2.347094176100	0.292770224900	0.025422239300
C	-3.316948076100	1.327775667500	-1.964411565300
H	-4.259403887100	1.235368941500	-1.423245764100
H	-3.397098491700	0.853823614900	-2.947553456200
H	-3.088669864500	2.385141128500	-2.133222817700
C	0.195413895300	2.822921000500	-2.902358387700
O	1.264432928400	2.309949218300	-2.924634019100
O	-0.846744534500	3.391631739400	-2.929054898500
C	3.015266610300	-0.043406314700	-0.197752304000
O	1.802329712300	-0.573766983400	-0.388682606200
C	3.828301294500	0.151785618200	-1.455036774200

H	3.866121516800	-0.780820255300	-2.028242053000
H	4.838721480400	0.481364856400	-1.207385601500
H	3.336968843500	0.902653198700	-2.083419243700
O	0.267721307800	1.909801758500	0.169622769500
O	3.448265892300	0.262279646300	0.939764066900
N	3.533613974900	3.746831605200	3.749122928700
C	2.614125059600	4.589305546500	4.209978438300
C	2.615676017800	5.457261674600	5.342773713100
N	1.460609016700	4.565352456700	3.381084682700
C	1.511323967600	6.209185431000	5.576261893000
H	3.487433345800	5.497973632700	5.978598125600
C	0.301130891500	5.318936005600	3.602562762500
N	0.403207842500	6.128357119200	4.730123347100
H	1.418298716100	6.897919679600	6.403860824700
O	-0.712302403000	5.277285595600	2.886503107200
H	-0.414527394600	6.691874476200	4.910458611800
C	1.711410076600	3.651924057200	2.355413685600
H	0.992283117600	3.431812147900	1.581125203700
C	2.977809762300	3.167751647000	2.600715912600
H	3.516336571500	2.427806529600	2.030274370400

$^{1}TS_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.940699060600
C	1.068587181600	0.000000000000	2.740873799800
N	0.643901631100	-0.045834270600	4.034856238900
C	-0.749864210400	-0.057868041600	4.054267738200
C	-1.141748403200	-0.030101192600	2.740195992700
H	2.089547944800	0.073529086600	2.381099633700
H	1.247388316300	0.007347559000	4.838514279400
H	-1.315574521000	-0.082673559400	4.968991141200
H	-2.124216281800	-0.003414782000	2.305560873000
N	-0.785804031200	-1.912469302600	-0.029340266500
C	-2.062358250900	-2.267206646400	0.112917467500
N	-2.182332362400	-3.619856050400	-0.048592396800
C	-0.915893106700	-4.141801203800	-0.309863864600
C	-0.057737817900	-3.071201008400	-0.296489553000
H	-2.877602066400	-1.591233013200	0.295665390900
H	-3.040911238600	-4.143735015200	-0.002904374200
H	-0.750012461200	-5.190722933900	-0.482698453300
H	1.000399354200	-3.006064987000	-0.467118386100
O	-0.793665198900	0.163064362500	-2.048477125500
C	-1.844325049300	0.662763626300	-1.505587161100
O	-1.916997330700	0.630916366000	-0.186378262300
C	-2.928942059700	1.321073890100	-2.295466952700
H	-3.907893952400	1.119191989600	-1.851610373600
H	-2.903180542900	0.987960591100	-3.333895562700
H	-2.756872892300	2.403913401200	-2.260207135100
C	1.286902617400	1.633663754400	-3.282961705500
O	2.084239126600	0.758556118000	-3.199385149000
O	0.540741075600	2.544037579000	-3.438598455300
C	2.942667964600	-0.503143572800	-0.051638056800
O	1.689403984200	-0.872469881900	-0.282390357800
C	3.934023629600	-1.107423172600	-1.027951331000
H	3.865718163000	-2.201376466500	-1.006423926900
H	4.949432032700	-0.798422969600	-0.774682368300
H	3.676329959800	-0.781363642400	-2.039965104000
O	0.651715199800	1.601657603400	-0.293730875900
O	3.321706351900	0.247411928200	0.886816710400
N	0.850579286100	3.201442686600	2.897103841200
C	-0.420669434000	3.521126360100	2.605138853300
C	-1.541900486400	3.751567356500	3.442273160600
N	-0.584238660500	3.645343264800	1.199583053700
C	-2.724706407900	4.085680774300	2.855513318800
H	-1.436123250100	3.665760565400	4.513749867200
C	-1.779209513200	3.992991437100	0.566251021600

N	-2.820954151400	4.200022791600	1.469369367100
H	-3.632675974500	4.282255143600	3.408377219400
O	-1.915785644400	4.132551404900	-0.660027985000
H	-3.700419393400	4.446775338800	1.039852948300
C	0.641805491300	3.315401549600	0.591781132300
H	0.862924628900	3.710296356600	-0.383819742800
C	1.514674140100	3.114869006800	1.697498706400
H	2.548521868800	2.819961670400	1.636354111000

$^{3}TS_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.942771432800
C	1.066687184700	0.000000000000	2.745381448300
N	0.639889020000	-0.045881351900	4.038587238500
C	-0.753830745900	-0.058432994200	4.055524894000
C	-1.143318704700	-0.030805322800	2.740671133400
H	2.088177425300	0.074229895900	2.387951306900
H	1.242036337500	0.008690503900	4.843164917600
H	-1.320977623300	-0.082659911800	4.969370982200
H	-2.125433528800	-0.004076984500	2.305160299800
N	-0.794700591500	-1.905386170000	-0.035794237800
C	-2.073730594400	-2.253663718200	0.102697511900
N	-2.199152053900	-3.606470530800	-0.052420394200
C	-0.933872855700	-4.135507795800	-0.304827327000
C	-0.070667066200	-3.068896491700	-0.292945174100
H	-2.886603117600	-1.573593315800	0.280746269800
H	-3.060178664800	-4.126378597000	-0.006353319900
H	-0.771876538500	-5.186098246900	-0.470782283200
H	0.988906506300	-3.009295965700	-0.456998335800
O	-0.779121642900	0.167562465100	-2.046263081600
C	-1.836996269200	0.662696609200	-1.512488742300
O	-1.916748703000	0.639253930600	-0.194104285600
C	-2.922560773000	1.303985031200	-2.315206772200
H	-3.902492476100	1.096597256700	-1.875612222500
H	-2.887019016100	0.960273257400	-3.350295270000
H	-2.760770615700	2.388939466500	-2.290070699500
C	1.319166755200	1.630567872800	-3.263900413600
O	2.109753363000	0.750834126300	-3.167385753800
O	0.579526715600	2.544292545800	-3.429351585300
C	2.941051934900	-0.515253158700	-0.030387604300
O	1.688918149300	-0.885568224600	-0.266090541300
C	3.937620422400	-1.128182105500	-0.996033625700
H	3.870962516000	-2.221985758100	-0.964735569500
H	4.951364087600	-0.815403795000	-0.740738676500
H	3.684695511600	-0.809707081700	-2.011607569500
O	0.663362472800	1.582963443500	-0.279803791100
O	3.315327701200	0.247110468900	0.900310917700
N	0.862873292400	3.193485052200	2.910467527700
C	-0.407403248500	3.500024355700	2.602441809200
C	-1.540337560000	3.725633854000	3.424787316000
N	-0.555394680500	3.615534837500	1.194111547200
C	-2.717763536300	4.050104461800	2.822756109300
H	-1.447100149700	3.644842274500	4.497574070100
C	-1.743064327600	3.958326780500	0.545675838400
N	-2.797283253500	4.159735932800	1.434993098500
H	-3.633762471900	4.242194397100	3.363609951900
O	-1.863552804600	4.098980057600	-0.682177011100
H	-3.671874587900	4.403335526800	0.994044507800
C	0.679318489300	3.291462181800	0.601929508400
H	0.915907686200	3.694052402400	-0.367297754700
C	1.540990392300	3.106014087200	1.718957852100
H	2.578544248500	2.822888068200	1.671875133000

$^{5}TS_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000

N	0.000000000000	0.000000000000	2.125982467200
C	1.141072885900	0.000000000000	2.819126686000
N	0.850582668800	0.099222992400	4.149252362700
C	-0.534334445100	0.175379053700	4.301844442800
C	-1.052164299900	0.112009152700	3.031799750400
H	2.127829138000	-0.063635814700	2.371916007700
H	1.533389659100	0.152722062900	4.887271614100
H	-1.004528226300	0.264393406400	5.265650062500
H	-2.072227199200	0.159244413900	2.694787478800
N	-1.121196611300	-1.864718869400	0.069974212000
C	-2.434263386300	-2.024880696800	0.230678856600
N	-2.744573222600	-3.356530573000	0.180927808900
C	-1.564701496500	-4.072085314000	-0.023966377000
C	-0.564633472200	-3.133989766800	-0.090396881400
H	-3.140406192600	-1.224456396000	0.363004305600
H	-3.667666103800	-3.749498780000	0.266848643400
H	-1.549180782900	-5.144941728300	-0.104519333300
H	0.493247983500	-3.239256021700	-0.247726183800
O	-1.008741539100	0.373531330200	-1.841837099000
C	-2.038380971100	0.954318846400	-1.297372310300
O	-2.161982493900	0.916524072800	-0.009048802800
C	-3.014020960400	1.702980735900	-2.156963133900
H	-3.995526685400	1.744900831900	-1.678888992600
H	-3.086592272400	1.248107370300	-3.147033015200
H	-2.638758915300	2.727505176300	-2.271499565200
C	0.926702288700	1.580001145400	-3.399594581600
O	1.687361904700	0.670611488800	-3.343300389300
O	0.225866691900	2.531548867400	-3.516421526300
C	2.863956262500	-0.889071274700	-0.206209929700
O	1.552016614700	-1.119565656900	-0.308397623900
C	3.668219819100	-1.357727205200	-1.399130489600
H	3.580175393800	-2.446083141900	-1.500426408900
H	4.718712463300	-1.087838316300	-1.279883940400
H	3.254568449900	-0.910190804600	-2.307839994400
O	0.771645087300	1.525256130400	-0.103003490200
O	3.400919959000	-0.362927069200	0.798340366000
N	1.698073558600	3.562393548200	2.529031384500
C	0.427576775400	3.954319591500	2.360850928900
C	-0.581613688100	4.286775196800	3.303564231600
N	0.111576920500	4.016357466900	0.981821933300
C	-1.809904896700	4.631104133000	2.831030639800
H	-0.358791930700	4.252838196400	4.359334669900
C	-1.140897387200	4.364462787600	0.462593130800
N	-2.061065604000	4.666722706400	1.462607500900
H	-2.643200852800	4.892017936000	3.468199200900
O	-1.407426933300	4.425301175000	-0.747671179400
H	-2.982239802100	4.900281720500	1.121746796200
C	1.231759076300	3.577946829900	0.278484328900
H	1.293203123800	3.672371767300	-0.788912171500
C	2.204051154700	3.358072697300	1.260618942500
H	3.204588893100	2.991242495800	1.108249571400

$^{7}TS_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.128945641300
C	1.135958787000	0.000000000000	2.834150336200
N	0.831655892800	0.037242374900	4.162659611500
C	-0.554571096400	0.076099088100	4.306544637400
C	-1.061120327800	0.050688287100	3.031290687400
H	2.127707427500	-0.063031450100	2.395269691100
H	1.505666313900	0.081882396400	4.909242663800
H	-1.033274330700	0.118181537700	5.269231562400
H	-2.079983999600	0.078025184300	2.688730176300
N	-1.064915948100	-1.945488717300	0.112247381100
C	-2.369707467400	-2.164728847400	0.266949669700
N	-2.615861546300	-3.511160153600	0.256741475800

C	-1.400880046100	-4.174871884100	0.086063777700
C	-0.446704591400	-3.191437161700	0.000136191300
H	-3.114970212300	-1.396328188900	0.371038720000
H	-3.519745338700	-3.945954863300	0.344904743000
H	-1.332554472900	-5.247688700400	0.040513303400
H	0.616704587000	-3.253453936200	-0.142785847000
O	-1.009113003300	0.301768385500	-1.875766162800
C	-2.072620561400	0.806389191400	-1.332884976100
O	-2.168463912400	0.798170484300	-0.034330544700
C	-3.132917622300	1.436650327100	-2.186316472300
H	-4.107458621900	1.379446616300	-1.694655076700
H	-3.168788752600	0.960864607800	-3.168398596800
H	-2.880927358300	2.496224235900	-2.314549140400
C	1.228873368500	2.172761228100	-2.882415413900
O	1.938691216500	1.227748230400	-2.984142337200
O	0.560898411800	3.155553942600	-2.868107746700
C	2.917800417500	-0.849693233500	-0.161453730300
O	1.606271891100	-1.037755256100	-0.331084520200
C	3.762872922200	-1.164538607700	-1.374872063700
H	3.650088610700	-2.221608445600	-1.643473038400
H	4.812916407200	-0.948136985800	-1.171896823100
H	3.405494198500	-0.571032629200	-2.221270966500
O	0.802765413800	1.709900997200	-0.245063147800
O	3.423883686500	-0.463226074200	0.920410694400
N	0.451296228800	3.360208303300	2.914220572000
C	-0.830568026800	3.568549108800	2.581708124000
C	-2.008383751400	3.608486721800	3.374006919100
N	-0.946740664000	3.774115457200	1.183993864600
C	-3.193899546700	3.841673514700	2.748037103600
H	-1.940079780900	3.455610052600	4.440323464000
C	-2.149465310400	4.029541015100	0.512779735300
N	-3.242844809500	4.049556217400	1.373489159600
H	-4.142947961200	3.885692530200	3.263746770400
O	-2.241143667700	4.246701211200	-0.704764788400
H	-4.128887459700	4.203209361800	0.914508849500
C	0.326883596100	3.642398553300	0.630868344000
H	0.523067772600	3.936884394800	-0.381907694100
C	1.164783440000	3.425590271000	1.735480552700
H	2.229280495700	3.271154689000	1.711319178500

$^{1}IM_{E,\varepsilon C}$

Fe	0.829610344200	-0.060283966500	-0.151488938900
N	-0.028539744300	-1.799991224400	0.145574353600
C	0.029595055200	-2.604760442600	1.209416339200
N	-0.637201950800	-3.757292772500	0.922077075600
C	-1.148489364200	-3.675862042900	-0.372579863000
C	-0.764958100100	-2.449567216600	-0.848265250800
H	0.469730092300	-2.318993183100	2.157579909100
H	-0.792878257000	-4.508980292900	1.574114314900
H	-1.727877991600	-4.466146838800	-0.817151072600
H	-0.973476117400	-1.968412042500	-1.787196603300
N	2.206338346000	-0.916378475900	-1.363604218000
C	2.051452449700	-1.206973510100	-2.656353760000
N	3.237062892000	-1.655361771800	-3.163559129000
C	4.184939050900	-1.640468003800	-2.140919469800
C	3.531222499200	-1.179959406800	-1.025064812700
H	1.144211229100	-1.082652297600	-3.217774814000
H	3.398794645500	-1.935778232800	-4.117176546400
H	5.205242228800	-1.941433982100	-2.298115674500
H	3.874965345700	-0.989615634900	-0.024790155900
O	1.388948870100	1.747563857600	-1.108831451900
C	0.413501967400	1.548975157300	-1.924849997300
O	-0.202969405500	0.385903081200	-1.809359097700
C	-0.043099791700	2.560325183100	-2.917444347200
H	-0.363149857400	2.075290795500	-3.843482425600
H	0.746660647800	3.285846328000	-3.116683540900

H	-0.911110240200	3.069686525800	-2.483513168900
C	1.119930559800	3.661495716900	1.061244155200
O	2.037301736000	3.211841949700	1.666030528300
O	0.225148665500	4.198857717200	0.495643650100
C	2.033496311700	-0.266560126100	2.581107094500
O	2.130363067800	-0.213083833500	1.257862098500
C	3.156060022300	0.445294131500	3.307276563600
H	4.127091811300	0.074849299900	2.961934049000
H	3.061377064600	0.291373550800	4.384338782500
H	3.109408944700	1.513310880500	3.070448964900
O	-0.292693728500	1.042110817800	0.838034124100
O	1.122938341700	-0.859385094800	3.220264321300
N	-2.776538772100	-1.009558553000	2.058481928200
C	-3.291297187400	-0.597242306500	0.861334806000
C	-4.277295949800	-1.189738158600	0.054105089600
N	-2.676032856800	0.606511491000	0.435916228400
C	-4.610078805600	-0.570419773000	-1.122436223400
H	-4.752117617300	-2.107737675100	0.372290295800
C	-3.018765298400	1.292132884700	-0.708502395300
N	-3.989488596800	0.630260862400	-1.478576217600
H	-5.352611331400	-0.947564601100	-1.811327358600
O	-2.563639687100	2.397792906200	-1.058453354900
H	-4.251211535500	1.113820912000	-2.324029122700
C	-1.581567169200	0.964626358900	1.401020408100
H	-1.784390566500	1.970145294900	1.796770571100
C	-1.828170679500	-0.141052609500	2.416034841700
H	-1.219446471000	-0.275108857500	3.296368981900

$^{3}IM_{E,\varepsilon C}$

Fe	0.835013687100	-0.066757717200	-0.116863037800
N	-0.055620751200	-1.794310662500	0.148102321400
C	-0.015386297800	-2.602785874800	1.210620779900
N	-0.669521508200	-3.758646753600	0.906367955800
C	-1.153870037600	-3.674843215200	-0.398327002400
C	-0.765508105500	-2.444753402300	-0.863296105200
H	0.421323666200	-2.325120580700	2.162345655200
H	-0.831854053700	-4.514387678400	1.552424494900
H	-1.720084220300	-4.464694086800	-0.857406871000
H	-0.955242418500	-1.961451718200	-1.804389561700
N	2.215702628800	-0.898968466200	-1.345789337400
C	2.064255274000	-1.188105729000	-2.638489263500
N	3.249843494900	-1.641007957300	-3.142614172600
C	4.194122659200	-1.633572210500	-2.117317627200
C	3.539104837200	-1.169675559200	-1.004279859700
H	1.159318191400	-1.058545936300	-3.202163027600
H	3.414180880700	-1.918121658600	-4.097121478400
H	5.213675727500	-1.941348924600	-2.270979928100
H	3.881852515800	-0.985365673200	-0.002659168500
O	1.380266795200	1.789827415500	-1.109757303900
C	0.416375286500	1.545255538100	-1.922541631500
O	-0.183786115900	0.369429278500	-1.793626411500
C	-0.061809676900	2.524104607100	-2.940640875000
H	-0.379251530700	2.010378884800	-3.852452650200
H	0.715804234000	3.256207011600	-3.162417237900
H	-0.934827688300	3.032885698300	-2.515485178300
C	1.141535455300	3.687618208200	1.063359940900
O	2.074040161200	3.233702870300	1.643344398300
O	0.229525966400	4.227840232600	0.528299641400
C	2.057832329900	-0.277092145300	2.602044369300
O	2.143862246800	-0.218697672500	1.272577721200
C	3.160825020300	0.475694683400	3.315642121400
H	4.139829794600	0.101484512900	2.997165410200
H	3.055473299100	0.359934520000	4.395937709600
H	3.107182955600	1.532255922300	3.035684179500
O	-0.270616157600	1.021455085900	0.876408235400
O	1.176810876700	-0.905069111400	3.242614920800

N	-2.787843135300	-1.033312815900	2.056636634100
C	-3.295233858200	-0.618167035700	0.861105167300
C	-4.308294523400	-1.180728192800	0.064946184000
N	-2.658067470100	0.576573434000	0.429970767300
C	-4.649863372300	-0.540076240400	-1.097656103800
H	-4.798580365700	-2.090247789500	0.382130054400
C	-3.014403961200	1.285259695700	-0.695180790600
N	-4.012797407200	0.653179411300	-1.452846205100
H	-5.413027169500	-0.893461897700	-1.776549071200
O	-2.546140741500	2.387767445700	-1.037478050000
H	-4.283018560400	1.152361288800	-2.286221981000
C	-1.581530289700	0.934653186700	1.404498587200
H	-1.787513235800	1.939788840200	1.799516287900
C	-1.835241793600	-0.169348942800	2.418951868800
H	-1.232886501300	-0.304041495200	3.303310288200

$^{5}IM_{E,\varepsilon C}$

Fe	0.879625303900	0.065495981500	0.004136539500
N	-0.012534385900	-1.864665262400	0.031007389600
C	-0.035126705200	-2.641787285100	1.119065463600
N	-0.671276079600	-3.806413274400	0.815775189500
C	-1.076635026200	-3.761294783200	-0.518346901200
C	-0.659984084400	-2.546520501500	-0.997570022100
H	0.378274192400	-2.364707858500	2.083628732700
H	-0.859154930200	-4.546743388300	1.469715469200
H	-1.609439749600	-4.566922912900	-0.984928044500
H	-0.791548176300	-2.093423405800	-1.964974325800
N	2.449940118600	-0.771962805500	-1.294974526300
C	2.386861319100	-0.982803656700	-2.609603768700
N	3.593599441100	-1.448331785300	-3.058745469600
C	4.461711267600	-1.533916360200	-1.971372668400
C	3.739606263500	-1.112580985200	-0.882135878700
H	1.522093136800	-0.799474999400	-3.222242666400
H	3.816776654700	-1.681921294400	-4.010185845000
H	5.480040633200	-1.868303943700	-2.069981342100
H	4.021659452000	-1.004771187900	0.146726108700
O	1.240034282800	1.897667084100	-1.067851901800
C	0.364197113300	1.620236530200	-1.985572238300
O	-0.153389870800	0.420526655700	-1.992105400200
C	-0.069814446000	2.668563365800	-2.962375539100
H	-0.387262589300	2.210046669300	-3.902381617500
H	0.728134397900	3.392324076700	-3.137448604300
H	-0.927318659500	3.187453435500	-2.523279005800
C	0.970334282600	3.709000712000	1.054618576200
O	1.897290852100	3.243149301300	1.640838090500
O	0.051006020800	4.245005102500	0.523334051500
C	2.112341494100	-0.287382161300	2.752782724100
O	2.177255837500	-0.176952494700	1.421641680600
C	3.061624812000	0.619823358100	3.505508946400
H	4.095459706000	0.317168390200	3.300630828400
H	2.876098019100	0.559974649800	4.577009682700
H	2.939056078300	1.644296876700	3.145024815500
O	-0.440348099600	0.874569456800	1.010077009900
O	1.354022499300	-1.105614369300	3.339185768200
N	-2.919693546600	-1.143739081100	1.980446002800
C	-3.357878661200	-0.745199778200	0.757041328700
C	-4.271135493700	-1.354527186200	-0.120146887800
N	-2.783282074900	0.499607394600	0.400464827100
C	-4.582257768000	-0.702458978000	-1.279387662500
H	-4.712879953500	-2.304738204000	0.136006221400
C	-3.114131159500	1.217869532000	-0.727674206500
N	-4.021495255500	0.540630143600	-1.556829302600
H	-5.270010372200	-1.092097688600	-2.016159140500
O	-2.695799408900	2.356218961800	-1.006723105800
H	-4.261957325600	1.033898761100	-2.398985295000
C	-1.801677866100	0.901568376200	1.438248954900

H	-2.026279403100	1.917514146000	1.780371383500
C	-2.075838780100	-0.207623767100	2.431485554000
H	-1.539731778400	-0.312319879200	3.361337152200

$^{7}IM_{E,\varepsilon C}$

Fe	0.884546955400	0.072756401500	0.006347522700
N	-0.001318184200	-1.859373038600	0.029453422100
C	-0.024029886900	-2.648911977200	1.116814274700
N	-0.663250476400	-3.814680651600	0.808067584100
C	-1.070023208100	-3.757791877700	-0.529103161900
C	-0.650689193700	-2.534866221600	-1.003657644100
H	0.390308516400	-2.375917014000	2.081504665300
H	-0.852579112700	-4.562768674700	1.459801373100
H	-1.605850553000	-4.557380520000	-0.999999425100
H	-0.780121499700	-2.074798484900	-1.968840117000
N	2.445860202400	-0.776498535300	-1.288824253600
C	2.383247381400	-0.994224133800	-2.603618152600
N	3.592233541000	-1.464664423600	-3.051041501600
C	4.463167736500	-1.546392804000	-1.961976090000
C	3.737844369600	-1.117659150800	-0.873509890500
H	1.517120949300	-0.811019770300	-3.217812078700
H	3.817668759500	-1.702301849000	-4.001281688300
H	5.481389871500	-1.883395939900	-2.061912634200
H	4.018332864500	-1.008682471500	0.154110649100
O	1.239399188400	1.904709535900	-1.060731107200
C	0.356459248300	1.628675152700	-1.985460484000
O	-0.160306077000	0.430842493100	-1.998581494300
C	-0.086153969900	2.675988932900	-2.959772725300
H	-0.407231963000	2.220880317000	-3.900565196200
H	0.710984610400	3.399293172200	-3.131953612300
H	-0.945535141400	3.193034190800	-2.519546414600
C	0.975333042000	3.717074903900	1.037258075000
O	1.894379553000	3.252339884200	1.620676077900
O	0.060193842500	4.256003946000	0.501928950400
C	2.110597480200	-0.289589811500	2.747412857400
O	2.177495150300	-0.181870569000	1.413167198400
C	3.058444352500	0.619715310800	3.500286698500
H	4.094728596200	0.319000559600	3.296094370500
H	2.871069113400	0.558089506200	4.575654126100
H	2.935621651500	1.643661726000	3.137715154500
O	-0.458103099400	0.888324684600	1.019553878100
O	1.351985175400	-1.099423394000	3.328639323000
N	-2.931902235600	-1.146459677000	1.992908624300
C	-3.363602905500	-0.751386530000	0.765606419700
C	-4.269688217300	-1.357604383500	-0.115093460500
N	-2.783591188500	0.495576212100	0.406886173500
C	-4.573659505200	-0.702517067900	-1.281030262200
H	-4.713471660400	-2.304320024400	0.144137035300
C	-3.104835739700	1.214888795100	-0.725405116700
N	-4.006922004500	0.545215418100	-1.558967050900
H	-5.252448241100	-1.084950180900	-2.023406751800
O	-2.685297393300	2.350830584900	-1.002341806100
H	-4.241708290700	1.045115535200	-2.406144798800
C	-1.799926381300	0.901715994000	1.443679645100
H	-2.037064810300	1.916557228300	1.797183837300
C	-2.085558044200	-0.215906621100	2.443732369700
H	-1.549641861900	-0.312762860100	3.371244161300

$^{1}TS_{rc,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.014173167300
C	1.109610209300	0.000000000000	2.758364638600
N	0.758316719200	-0.051194673300	4.079268498400
C	-0.632181299400	-0.080917136500	4.175466211600
C	-1.091327761300	-0.049110933500	2.881262356600

H	2.116288239400	0.077792686800	2.349433508200
H	1.407216058800	-0.041913428500	4.848558180600
H	-1.146533514200	-0.130103334200	5.119642456100
H	-2.100021903800	-0.050569349900	2.507303118500
N	-0.756430403500	-1.829288776400	-0.050706815400
C	-2.035630680800	-2.182081576800	0.073320882900
N	-2.149019290500	-3.540230816800	-0.060137699000
C	-0.875247280900	-4.063459004300	-0.283952591500
C	-0.018491263000	-2.991118397700	-0.276324835800
H	-2.853940484800	-1.501587348500	0.224339279000
H	-3.006320644300	-4.065617132600	-0.019318660800
H	-0.703269066100	-5.115705120100	-0.427868675200
H	1.045125293200	-2.918051301700	-0.414586181500
O	-0.669305624300	0.193523963700	-2.089776404900
C	-1.778296152200	0.670904858300	-1.643843051800
O	-1.920676879100	0.786198145700	-0.344864042100
C	-2.871536730500	1.119151849500	-2.571276282900
H	-3.852506450000	0.887676120700	-2.145633027300
H	-2.757362660900	0.646929807000	-3.548319178200
H	-2.804700716200	2.207194897800	-2.687772723600
C	0.360899954300	-0.381463163900	-4.500812321200
O	1.476681423400	-0.311745864700	-4.105832127500
O	-0.713508253100	-0.480330380700	-5.001582716200
C	3.017634137800	-0.320193540200	-0.062510179100
O	1.813695985400	-0.831394181000	-0.181133449000
C	3.954256082200	-0.609230227500	-1.224319740800
H	4.098350581500	-1.691701083800	-1.326050483800
H	4.921905538000	-0.128935417900	-1.066162006700
H	3.497674587100	-0.255199935300	-2.154374056200
O	0.903218250800	1.716021256600	-0.224855978500
O	3.433570330200	0.342342519300	0.940168109000
N	0.987270427100	3.219039872000	2.256886653000
C	-0.292449071700	3.531897257400	1.958032805000
C	-1.360093991800	3.826078343800	2.840298233100
N	-0.527698239100	3.556390167400	0.582453963100
C	-2.572727300200	4.122373308500	2.285351684800
H	-1.199918373100	3.801008520500	3.906723947700
C	-1.726966812100	3.894486114600	-0.019567672000
N	-2.741212352600	4.162617473000	0.919126860800
H	-3.449157353600	4.347334038600	2.878470212200
O	-1.913793408100	3.997379682600	-1.239656301000
H	-3.644996254100	4.362819089000	0.514648888700
C	0.713243834100	3.108615726000	-0.108186127800
H	0.888614496800	3.675853757500	-1.018866793100
C	1.637035620900	3.045962671000	1.078672682500
H	2.662270804200	2.717847742300	1.018431871000

$^{3}TS_{rc,\varepsilon C}$

Fe	-0.003093176000	-0.000885004000	-0.002138719000
N	-0.003730234000	-0.000992733000	2.143757304000
C	1.140380111000	0.000225533000	2.843000942000
N	0.856672924000	-0.048168350000	4.186450439000
C	-0.534057943000	-0.073157052000	4.346548253000
C	-1.054127559000	-0.044442223000	3.063651572000
H	2.130595856000	0.055523311000	2.396825310000
H	1.545824777000	-0.036590374000	4.925414613000
H	-1.010357520000	-0.117147676000	5.312495546000
H	-2.082901395000	-0.043063283000	2.740946179000
N	-0.874807900000	-1.977852521000	-0.179837185000
C	-2.162065103000	-2.334155508000	-0.135009109000
N	-2.281290208000	-3.692541381000	-0.332888347000
C	-0.995279001000	-4.216394736000	-0.512992383000
C	-0.132797033000	-3.138612432000	-0.414527511000
H	-2.987134219000	-1.658773530000	0.021531390000
H	-3.146202106000	-4.214638386000	-0.354244360000
H	-0.813418947000	-5.263206441000	-0.693049447000

H	0.940103039000	-3.086634526000	-0.499997910000
O	-0.923689439000	0.455370505000	-2.043468310000
C	-2.012934138000	0.857293797000	-1.475343594000
O	-2.077727667000	0.833450392000	-0.160965795000
C	-3.178248623000	1.369861306000	-2.291165597000
H	-4.127672922000	1.087415966000	-1.823102677000
H	-3.122720235000	0.986557263000	-3.313326480000
H	-3.122962992000	2.465384001000	-2.322826792000
C	0.051540674000	0.257902404000	-4.466638288000
O	1.166357543000	0.198195211000	-4.049951065000
O	-1.022840839000	0.310660653000	-4.986993330000
C	3.023269334000	-0.299375166000	-0.185711297000
O	1.794976818000	-0.798406372000	-0.269540227000
C	3.861729133000	-0.440672994000	-1.450378498000
H	4.017267955000	-1.505020156000	-1.670168029000
H	4.829261709000	0.053859322000	-1.330538312000
H	3.310145033000	-0.011929402000	-2.295251400000
O	0.874207773000	1.900355074000	-0.162157086000
O	3.492350553000	0.244612875000	0.862309364000
N	1.074136714000	3.292854253000	2.301340089000
C	-0.213003940000	3.627759407000	2.068546197000
C	-1.262264803000	3.874164515000	3.000553913000
N	-0.502366099000	3.737108495000	0.690036428000
C	-2.498729869000	4.196204441000	2.496149127000
H	-1.074693190000	3.789030830000	4.060970267000
C	-1.730252832000	4.091261810000	0.145981753000
N	-2.716190956000	4.308398523000	1.132160380000
H	-3.355701377000	4.380904217000	3.133731032000
O	-1.963418074000	4.231758821000	-1.070114064000
H	-3.638321383000	4.517797496000	0.766189578000
C	0.701929560000	3.318054601000	-0.063262527000
H	0.857774411000	3.885923776000	-0.977630324000
C	1.681422291000	3.166049388000	1.076400242000
H	2.723466191000	2.910690809000	0.960980092000

$^{5}TS_{rc,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.172213839300
C	1.147996853900	0.000000000000	2.856797968700
N	0.873384991200	-0.041373782500	4.196233049400
C	-0.510274497600	-0.062442635200	4.368929991100
C	-1.039747000700	-0.038223537100	3.101387287900
H	2.135446866200	0.045980114200	2.402465497800
H	1.563786801300	-0.031981264000	4.928948783500
H	-0.970108424600	-0.101190918500	5.341371005900
H	-2.067936219600	-0.041262424000	2.783762653500
N	-0.863346335200	-1.989272387800	-0.154623038000
C	-2.147061487700	-2.336028091900	-0.103523321100
N	-2.267232481800	-3.689137775900	-0.287149492300
C	-0.988429957100	-4.217632564500	-0.464613761000
C	-0.126516530800	-3.151713834500	-0.380096724300
H	-2.965921062300	-1.653835789200	0.043379416900
H	-3.129237962500	-4.208797196600	-0.304800418900
H	-0.818268894800	-5.266628259900	-0.633491839500
H	0.944297166200	-3.096860621200	-0.464981309800
O	-0.897384527600	0.433411053800	-2.069842934100
C	-1.989676592900	0.823810346800	-1.513953137800
O	-2.085722916800	0.797058493000	-0.207730095700
C	-3.135483122900	1.340872573100	-2.341816086900
H	-4.091289525100	1.056034689700	-1.892199452600
H	-3.064765707600	0.967266361800	-3.364628079800
H	-3.081889271700	2.435629649200	-2.360663913300
C	0.145557151400	0.318592450100	-4.518805319600
O	1.253454835800	0.245845202900	-4.099899952900
O	-0.914409301100	0.383727105000	-5.054328321200
C	3.026341333200	-0.355337944600	-0.126759917900

O	1.794148318600	-0.826547859300	-0.222873160000
C	3.876909326700	-0.519816832100	-1.371744437400
H	4.008618844700	-1.585680763400	-1.592942189700
H	4.854425426000	-0.054277980500	-1.232543027700
H	3.359097728400	-0.074576240600	-2.227636582600
O	0.856354711600	1.872638917500	-0.160600991600
O	3.497142873100	0.177732318600	0.918102186900
N	1.048373860700	3.305827694500	2.313313019700
C	-0.244723063200	3.609272754300	2.074647187200
C	-1.287029522600	3.841512949200	3.003926656200
N	-0.529777773400	3.689490675600	0.707147016500
C	-2.526365467300	4.125375753100	2.504977773800
H	-1.089025584300	3.774235426300	4.062226602300
C	-1.762528656900	4.006514477900	0.163546987000
N	-2.745831892900	4.213849355500	1.147072720300
H	-3.386746454200	4.301018782900	3.136823690200
O	-1.998894365400	4.135118718700	-1.046348156100
H	-3.670331591400	4.398002611200	0.784112146100
C	0.685558880400	3.271704163200	-0.040484485700
H	0.824644759500	3.847970480800	-0.950800778400
C	1.652378152000	3.178882449200	1.103609971200
H	2.685234561000	2.893931417700	0.994765753100

$^{7}TS_{rc,\varepsilon C}$

Fe	-0.004323110000	0.000514315000	-0.002738895000
N	-0.003055537000	0.003531620000	2.077851969000
C	1.118804541000	0.005374696000	2.811353252000
N	0.792768277000	0.212400513000	4.120206735000
C	-0.593762731000	0.368974433000	4.220646854000
C	-1.078577063000	0.238607199000	2.938486231000
H	2.119647579000	-0.099533040000	2.408515554000
H	1.458780503000	0.320935379000	4.871167425000
H	-1.091497719000	0.573691341000	5.154524798000
H	-2.083260909000	0.341169985000	2.564588745000
N	-0.899786630000	-1.961861171000	-0.098750085000
C	-2.170765378000	-2.300520712000	0.138474293000
N	-2.317697660000	-3.654893587000	-0.003592172000
C	-1.076394132000	-4.199000333000	-0.348272472000
C	-0.203752248000	-3.134512069000	-0.402818126000
H	-2.957515904000	-1.610815356000	0.393566294000
H	-3.178132825000	-4.168626372000	0.117211303000
H	-0.929170860000	-5.251973777000	-0.519403006000
H	0.847342980000	-3.102666146000	-0.630465733000
O	-0.971252907000	0.448368118000	-1.845304037000
C	-2.105328161000	0.792717490000	-1.289248110000
O	-2.179276568000	0.660135204000	0.005185163000
C	-3.233214908000	1.347405761000	-2.104345197000
H	-4.196187069000	1.068525258000	-1.665925791000
H	-3.160088044000	1.006659684000	-3.139981328000
H	-3.149481586000	2.443057904000	-2.081656842000
C	0.102323514000	0.471168527000	-4.346887559000
O	1.200112299000	0.494124282000	-3.892297528000
O	-0.964500191000	0.446568576000	-4.871907108000
C	2.961604969000	-0.488763153000	-0.298239665000
O	1.665338896000	-0.853324620000	-0.371609413000
C	3.709312910000	-0.548483124000	-1.616556277000
H	3.794990348000	-1.593301069000	-1.941981365000
H	4.709160230000	-0.124512243000	-1.501778506000
H	3.146297354000	-0.014054750000	-2.388925592000
O	0.735624814000	1.805182289000	0.001008862000
O	3.501369057000	-0.156125134000	0.781777962000
N	1.149828060000	3.299379599000	2.099208840000
C	-0.149941060000	3.786091453000	2.001304079000
C	-1.062957753000	4.228428665000	2.943846056000
N	-0.547543323000	3.843165965000	0.588117457000
C	-2.321869653000	4.697178987000	2.530090697000

H	-0.796469199000	4.221073325000	3.992545782000
C	-1.804625456000	4.238040475000	0.136528792000
N	-2.640464328000	4.680597870000	1.141617886000
H	-3.084522490000	5.079641235000	3.193800213000
O	-2.143575551000	4.202894733000	-1.074569336000
H	-3.550855695000	4.989510781000	0.828252219000
C	0.495323779000	3.300501038000	-0.189175003000
H	0.611661033000	3.623655975000	-1.213339245000
C	1.546747710000	2.986361968000	0.830507915000
H	2.594098472000	2.831966633000	0.616904550000

$^{1}P_{E,\varepsilon C}$

Fe	-1.120973596400	0.011824758400	-0.199576768000
N	-1.743524130000	1.809381382700	-0.885187291600
C	-1.885985428300	2.965557686300	-0.233328503200
N	-2.182362381800	3.953074434000	-1.133308939900
C	-2.226674671900	3.394567290300	-2.410037030300
C	-1.951588552000	2.060922399300	-2.243526780000
H	-1.748725691800	3.081351412500	0.835681792900
H	-2.323728710700	4.923428786100	-0.904976177900
H	-2.433827945000	3.979820955800	-3.288753585600
H	-1.846389872200	1.272616463300	-2.967364855700
N	-2.941171418700	-0.819073978300	-0.217703318100
C	-3.583645403900	-1.280933212700	-1.290936423100
N	-4.784948231500	-1.814729252600	-0.909879938300
C	-4.903014573000	-1.684045116100	0.472998515200
C	-3.752058916100	-1.064498707100	0.890994016500
H	-3.199849121700	-1.256267836300	-2.295038843000
H	-5.459806767900	-2.238039934800	-1.524979079800
H	-5.764286331000	-2.036895068200	1.014328054200
H	-3.416615976000	-0.791204962600	1.874032384400
O	-0.078543045400	-1.951213671300	-0.394135135400
C	-0.206536754800	-1.820154633400	-1.673081688000
O	-0.842035374900	-0.775281694900	-2.124428701800
C	0.366004930500	-2.824700162800	-2.636138112300
H	-0.410015319400	-3.156642369100	-3.334097494000
H	0.783287318100	-3.678276997000	-2.101058333900
H	1.154092735100	-2.349087398100	-3.233355315700
C	1.501360093200	-3.595757959300	0.998438889400
O	1.364872938600	-2.897200009900	1.947809565600
O	1.666394338300	-4.371628970900	0.113326792000
C	-1.281373142000	1.065057399000	2.754030039900
O	-1.263374950300	0.176164859500	1.794651911800
C	-1.463976886600	0.498888729000	4.154648597400
H	-2.461863441800	0.054687009300	4.253138146700
H	-1.347792895200	1.287181590000	4.900431643200
H	-0.736492352200	-0.299802664500	4.332272602600
O	0.811854552400	0.758343977200	-0.253725945900
O	-1.150152838500	2.321948447200	2.593355731300
N	2.428070088200	2.570301668700	0.355088749700
C	3.413160657200	1.770138804000	0.023578390500
C	4.697672464500	2.090565970500	-0.523732043400
N	3.143213482400	0.387990797000	0.284605266300
C	5.571600346300	1.077583256000	-0.743864318500
H	4.936544468200	3.119967800100	-0.743059905500
C	4.020016558000	-0.664549019500	0.069406682700
N	5.249121220100	-0.240304172400	-0.453316041200
H	6.559223637800	1.236353188800	-1.155901443400
O	3.780696750400	-1.860125124600	0.306404699300
H	5.907787970500	-0.983666198800	-0.633996916700
C	1.801950970400	0.304934827100	0.784176175900
H	1.510026629800	-0.539817320800	1.388601407800
C	1.367129260700	1.735606768600	0.837522527900
H	0.592755668600	2.156491833300	1.464841428900

$^{3}\mathbf{P}_{E,\varepsilon C}$

Fe	-1.220295095800	0.045287797500	-0.187752814000
N	-1.722377151900	1.960999914700	-0.926987787700
C	-1.846974698400	3.113182131300	-0.264031837300
N	-2.105405565900	4.118083505600	-1.154230856500
C	-2.141168276200	3.576954541100	-2.440720878700
C	-1.898780333100	2.235656495900	-2.285667794800
H	-1.717689623000	3.212712015500	0.807848997100
H	-2.226278493600	5.089025019800	-0.916073584400
H	-2.322223417300	4.179183422100	-3.314660974300
H	-1.806912228200	1.452380897800	-3.017379745700
N	-3.040931536400	-1.019004386800	-0.169858073000
C	-3.650705847600	-1.518002541000	-1.244613988900
N	-4.818039651300	-2.125809578900	-0.868242945000
C	-4.944785147000	-2.007655476100	0.517080392300
C	-3.835051582300	-1.317914204700	0.936650898700
H	-3.271325369200	-1.459883949300	-2.249156307900
H	-5.468530818900	-2.584858142900	-1.484226695200
H	-5.782630243700	-2.416599903700	1.055191705900
H	-3.519941465100	-1.019595871900	1.918921536100
O	0.009534062600	-1.959593206300	-0.418166405900
C	-0.174215679500	-1.755139119500	-1.670442006100
O	-0.878902680500	-0.712311677200	-2.044960472800
C	0.410530848600	-2.663556808800	-2.717542686700
H	-0.359839566700	-2.955122639700	-3.439842010300
H	0.845763344400	-3.546703673700	-2.250713363400
H	1.188976859700	-2.127056692400	-3.272629360400
C	1.512009503500	-3.605180073700	1.041088418200
O	1.409174663300	-2.879006998900	1.975093912000
O	1.639642627100	-4.410152374500	0.178773384000
C	-1.382477832500	1.159456204500	2.718305382300
O	-1.426189327700	0.250709942500	1.774631770700
C	-1.617516632300	0.628023457700	4.124889106000
H	-2.625831910300	0.205359712000	4.204338535200
H	-1.503407908800	1.430003302700	4.856267382000
H	-0.910554020600	-0.180656714900	4.340414647800
O	0.891968625500	0.787785395800	-0.162933324400
O	-1.152265266000	2.395168483500	2.537930333300
N	2.577057345400	2.547235300200	0.394713976300
C	3.525826025200	1.725654574100	0.018301124000
C	4.794112540500	2.015371688500	-0.582891480200
N	3.230752034100	0.348247689800	0.279333941300
C	5.628846493700	0.980234860400	-0.851075202100
H	5.051309571600	3.039736155000	-0.803983442800
C	4.066286280800	-0.725406355100	0.014142260400
N	5.282599892100	-0.331180003200	-0.558787316700
H	6.601648555400	1.114677806400	-1.305069761300
O	3.804032858200	-1.916344834900	0.247536496400
H	5.911018522000	-1.090582994900	-0.775441170000
C	1.903429446200	0.292896373300	0.821625501400
H	1.616364979200	-0.553256005400	1.425957462200
C	1.506517699500	1.734954481400	0.902776191600
H	0.765299069900	2.172592571800	1.556659644400

$^{5}\mathbf{P}_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.124964544100
C	1.130667324300	0.000000000000	2.837856786300
N	0.822143928700	-0.170525836900	4.159873913900
C	-0.563580051500	-0.277949469400	4.286182873800
C	-1.064383743100	-0.169190129300	3.011751009100
H	2.122812821100	0.136085355400	2.412160896400
H	1.493303915400	-0.213551793000	4.909154172900
H	-1.045936472500	-0.422537681100	5.237176588900
H	-2.078998033000	-0.182413020400	2.649761824100

N	-0.856713896100	-1.994754102600	-0.172938736700
C	-2.121055002700	-2.355172988100	0.065414144600
N	-2.254423145800	-3.703773178500	-0.121781772000
C	-1.014438262000	-4.222192325500	-0.494176892000
C	-0.155436415500	-3.150588682900	-0.521947459400
H	-2.910515841200	-1.668140895300	0.327716931400
H	-3.108629410800	-4.226930993300	-0.019677541500
H	-0.865107775000	-5.267752026400	-0.700060581400
H	0.893041753200	-3.101013959900	-0.760046980500
O	-1.367728543600	0.919655094400	-1.113161187900
C	-2.664194664900	0.869337251300	-0.858142832700
O	-3.142258146600	0.375684018800	0.205329490800
C	-3.561953905400	1.413294668600	-1.949082057100
H	-4.604563596200	1.394012361600	-1.629714469100
H	-3.441940384900	0.810080614500	-2.857219461400
H	-3.267167218000	2.438470492100	-2.194156935400
C	0.224573338300	2.608351756600	-2.881594623400
O	0.862269294800	1.695863582200	-3.289197407000
O	-0.375198754200	3.573882109800	-2.532761721700
C	3.031534464300	0.089927385900	-0.231894950600
O	1.849612120600	-0.469590648500	-0.443835514600
C	3.910402732100	0.218869029800	-1.462051729800
H	4.121656094900	-0.774195139400	-1.873889232300
H	4.848154644700	0.716991190800	-1.210317897200
H	3.376652232300	0.780511523100	-2.235617931200
O	0.899742096900	2.291356542000	0.231567428600
O	3.431596331200	0.486096796700	0.896445501100
N	1.919114225900	3.270706894500	2.335089006800
C	0.732634252500	3.275548874700	2.896232242200
C	0.381151030600	3.138082922300	4.278312260700
N	-0.337891232600	3.468173691200	1.972912227700
C	-0.933270742100	3.173069850100	4.612158534700
H	1.161383743900	3.001651225300	5.010991420500
C	-1.688612036800	3.529443029200	2.289695482100
N	-1.923907651400	3.359062037200	3.661395667300
H	-1.280468973600	3.062396611500	5.631046573800
O	-2.599561962600	3.729185768500	1.474796647900
H	-2.898783046100	3.361455314900	3.923616510400
C	0.230698210700	3.547225621700	0.658052924000
H	-0.303465871100	4.091561267600	-0.103955936500
C	1.702010170200	3.409313517400	0.924764882400
H	2.511370180500	3.778541177100	0.317313569500

$^{7}P_{E,\varepsilon C}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.149570212100
C	1.133378509500	0.000000000000	2.856558967600
N	0.828598643800	0.131423244500	4.181582671000
C	-0.555830885400	0.223588607600	4.316346393800
C	-1.060933104500	0.137826877000	3.042756565100
H	2.129806820100	-0.063636191600	2.433585292200
H	1.502837181800	0.198915730500	4.926541615700
H	-1.035691676400	0.344827073700	5.271546783300
H	-2.077948907700	0.182071817200	2.694497105700
N	-0.588182618800	-2.118066386500	0.240157119600
C	-1.808265676500	-2.588425062200	0.500080021000
N	-1.748064787000	-3.941665586500	0.691956649200
C	-0.421473628200	-4.346155304900	0.541770542800
C	0.287586062000	-3.204843791200	0.261909380100
H	-2.700730952500	-1.989719319000	0.541078585300
H	-2.530743763900	-4.542452577700	0.893168314300
H	-0.117896614700	-5.373957063300	0.639096613700
H	1.334285058000	-3.059350758200	0.070359803700
O	-0.872010002200	0.088193900900	-1.949067412300
C	-2.075383025100	0.281449647600	-1.491717499200
O	-2.263269726200	0.184488634600	-0.212408005700

C	-3.180653687900	0.654948631800	-2.431331277000
H	-4.155456521700	0.443729954200	-1.988277522600
H	-3.066632786500	0.128050390700	-3.381726454400
H	-3.113367107700	1.732377825700	-2.626208279700
C	0.497521493600	2.362353672100	-3.162082478000
O	1.447456634300	1.699400033400	-3.420122691700
O	-0.421538619200	3.084057692500	-2.951178356000
C	3.033074195400	-0.390225550100	-0.268428666000
O	1.743308217500	-0.732997873900	-0.334399931000
C	3.756712486400	-0.427854763500	-1.595028104200
H	3.651820429200	-1.419854095900	-2.047502274700
H	4.812951300800	-0.190376257600	-1.459231864200
H	3.292768876400	0.288620628800	-2.281024129700
O	0.363068448400	1.820087974400	-0.024818321700
O	3.597872833300	-0.087830497100	0.809424920300
N	1.510144240900	3.575237840600	2.641525941400
C	0.167533894500	3.773827380900	2.762922897900
C	-0.583737361500	4.202088832000	3.872405704300
N	-0.491757828100	3.538248148800	1.524718266800
C	-1.931152112000	4.393379346200	3.707750436200
H	-0.090009050700	4.390643085500	4.814906349000
C	-1.835927652600	3.771128344600	1.301203608500
N	-2.522919811700	4.174267921000	2.461774959600
H	-2.590775483700	4.726752988300	4.496612516600
O	-2.416689644900	3.664130734000	0.208394190400
H	-3.507615501400	4.344149653300	2.322327038800
C	0.514919643300	3.114778198300	0.504394142100
H	0.473771870500	3.822514163400	-0.334810251800
C	1.763912540500	3.233676544600	1.376290787800
H	2.752638351600	2.969826335100	1.033364333700

Cytosine: ***Part 2: Hydroxylation (DFT calculations in UB3LYP/LANL2DZ)***

$^{1}RE_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.955093950400
C	1.020921866500	0.000000000000	2.811177207900
N	0.522930973700	0.057462124900	4.083193991500
C	-0.870443510400	0.089641666500	4.019843211900
C	-1.186245418600	0.058626037900	2.684532543300
H	2.061572841400	0.030803843800	2.528676256600
H	1.076095290000	0.010883205900	4.924674882300
H	-1.488782776800	0.109328785300	4.900269464400
H	-2.140966205500	0.077774226400	2.188219130800
N	-0.330190695900	-2.021143893600	0.019054327000
C	-1.494137938400	-2.668007990400	0.133202818300
N	-1.274150979900	-4.011900286800	0.053016165500
C	0.090497475500	-4.226486018400	-0.124266126300
C	0.668029893100	-2.983011943200	-0.144966746200
H	-2.457458039700	-2.208311224300	0.258801604200
H	-1.982698455500	-4.726914475100	0.101543612600
H	0.511868024100	-5.211168706000	-0.226335586400
H	1.688732794900	-2.683724634900	-0.285015486300
O	-0.566505619800	-0.090500701000	-1.967204047400
C	-1.804383294700	0.079116026700	-1.623435133900
O	-2.010925473700	0.180906399500	-0.331860385500
C	-2.898330803000	0.176513551600	-2.628687311500
H	-3.874011664100	0.046756151900	-2.158173649200
H	-2.752755014700	-0.566775767300	-3.416933891800
H	-2.856933751900	1.167680781700	-3.095755167900
C	0.552365479100	1.997610358200	-2.787551246200
O	1.598486132700	1.459769798700	-2.923371968200
O	-0.481246858600	2.579876911700	-2.691512571800
C	2.964460655800	0.173403319800	-0.005755677300
O	1.824605921800	-0.463994895700	-0.247041390800
C	4.069545667300	-0.213861661800	-0.964851787700
H	4.089168252000	-1.297299710000	-1.113130486900
H	5.035809405900	0.134628677000	-0.597379239800
H	3.856110840800	0.245093393500	-1.937004981200
O	0.259340232700	1.723580358400	0.040929100000
O	3.128324644300	1.005788911600	0.926894159000
H	-1.068957448500	3.793968729900	2.241086297400
N	-0.097319004800	3.724756232300	2.513577917700
C	0.295384624400	4.224496732200	3.687233672300
H	0.474462939200	3.203296044500	1.845672147400
C	-0.641054825100	4.850223460200	4.578204639300
N	1.613435265300	4.147978394800	4.066118704100
C	-0.203095771500	5.325437396500	5.776624917000
H	-1.678159894100	4.940216825100	4.290036289100
C	2.084506627900	4.604742637400	5.331783452600
N	1.107608410100	5.195729852900	6.137460865200
H	-0.857500789500	5.812282822500	6.487172073800
O	3.256640432500	4.491682755900	5.695844645300
H	1.445455504800	5.542001589500	7.026821747200
H	2.687835065600	4.259281391600	2.241558765300

C	2.638445179100	3.616071692300	3.124547515600
H	3.596166289900	3.631021929600	3.638638130100
H	2.411059513200	2.593767705500	2.812361005800

$^{3}RE_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.948666550300
C	1.071026457800	0.000000000000	2.738555882800
N	0.663224496500	-0.154878345600	4.032208728400
C	-0.728747050200	-0.257572191000	4.050860839400
C	-1.133021550400	-0.154547926600	2.742251498500
H	2.087945850200	0.091221130700	2.404056787800
H	1.272009195500	-0.245673748800	4.830273377400
H	-1.283017083200	-0.409514464100	4.960134981700
H	-2.114933934400	-0.199475997100	2.304025540400
N	0.882776592000	-1.850695788400	0.100980439400
C	0.284178050300	-2.999761117800	0.430328278500
N	1.203285024700	-4.007457290000	0.416126703200
C	2.438810169600	-3.474699581700	0.053945495300
C	2.228160409600	-2.132510165000	-0.140095172400
H	-0.760383783900	-3.117279900600	0.656834902900
H	1.012895799100	-4.978586317600	0.608441624900
H	3.322574001700	-4.080849322700	-0.042227491300
H	2.902094965700	-1.349888869400	-0.435521470200
O	-0.412200812800	-0.415350347400	-1.987161643400
C	-1.521393581000	-0.974162860200	-1.611706173900
O	-1.716031503400	-1.008030551000	-0.311608639300
C	-2.522078468900	-1.511259273700	-2.573202976800
H	-3.227427219000	-2.172081993300	-2.066884037900
H	-2.019667233400	-2.040120482400	-3.387698561700
H	-3.072259160200	-0.670561274500	-3.012085731800
C	-1.049168693200	2.186813913700	-3.257274996900
O	0.072294788400	2.574595243900	-3.278044419500
O	-2.182325751200	1.829142824700	-3.262969501300
C	2.194878068900	1.970958766900	-0.006455234500
O	1.799258662700	0.710536920300	-0.092736042200
C	3.140754535500	2.413648368000	-1.093912654700
H	3.870222904600	1.630503169600	-1.315687803400
H	3.644667308000	3.339796793700	-0.815664479500
H	2.552749047500	2.581384867700	-2.004916694800
O	-0.741962795300	1.476042486700	-0.109805172200
O	1.840788493100	2.777292415000	0.902929001900
H	1.647118247400	3.137004699300	3.929391955800
N	0.863020768400	3.244557990900	3.300524663500
C	-0.351057133500	3.368285603400	3.824930068800
H	1.094835979400	3.108351208500	2.280737650700
C	-0.581013194700	3.205642582800	5.235969965800
N	-1.419490612600	3.663537679900	3.015382449500
C	-1.856024130600	3.236797122100	5.706904378200
H	0.256176186500	3.042257245300	5.899180964600
C	-2.758621683500	3.664711584500	3.477962172200
N	-2.904239412600	3.428052749400	4.850303989700
H	-2.099653427600	3.105748516800	6.753040544900
O	-3.728679450500	3.868614562700	2.744708895700
H	-3.859858577100	3.448661077900	5.182922474900
H	-0.322692898800	4.637993994700	1.499378830100
C	-1.216364495100	4.017571152600	1.582310380400
H	-1.104147446700	3.117983530000	0.968252476400
H	-2.095345007000	4.570944624700	1.258239607200

$^{5}RE_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.101125676100
C	1.100505459500	0.000000000000	2.851787027000
N	0.742306921800	-0.065378691300	4.169241904700
C	-0.650058880000	-0.114222424100	4.246932324300

C	-1.102169090500	-0.069329629700	2.950325278500
H	2.106200440000	0.069015798700	2.479148746600
H	1.377987703000	-0.131349941600	4.948372317500
H	-1.172864566000	-0.188486413400	5.184553964300
H	-2.102475427200	-0.089334802400	2.553959744200
N	0.315929181700	-2.020367366800	0.101367276400
C	-0.601692170400	-2.950144080800	0.389835695300
N	-0.006058357900	-4.174568553300	0.412160896600
C	1.347829899100	-4.017551638000	0.122412537800
C	1.538315950900	-2.672647021100	-0.068994652300
H	-1.643621369900	-2.757650329000	0.572144202900
H	-0.473719393400	-5.049537891200	0.590791304200
H	2.027735224300	-4.849772072200	0.071807891800
H	2.424651199500	-2.117846782900	-0.315076991700
O	-0.974210481500	-0.283362973100	-1.833947712200
C	-2.136368126000	-0.505873207300	-1.285477254800
O	-2.178382023600	-0.552736524300	0.010153911200
C	-3.356627698000	-0.666586019600	-2.133667541300
H	-4.190252986800	-1.044341135300	-1.541623759500
H	-3.150673630600	-1.336097330700	-2.972799965600
H	-3.623103148800	0.311127412500	-2.551030956600
C	-0.879011910200	2.545923382200	-2.981294365200
O	0.300897100100	2.633962936100	-3.072159202700
O	-2.063080410500	2.494695966500	-2.916380775200
C	2.681067599100	1.300053943900	-0.142270260800
O	1.941843493700	0.196984109300	-0.146872725700
C	3.425791035600	1.598633379600	-1.416028162900
H	3.883188167800	0.689615533300	-1.816842883000
H	4.184295355600	2.364415360900	-1.248660095700
H	2.704245192000	1.956569871200	-2.161793577600
O	-0.308582316600	1.617888392900	-0.097644003200
O	2.773020139500	2.056747319800	0.866936963000
H	2.966676297300	3.134110728500	3.756935063800
N	2.184783350500	3.322014262500	3.144840669600
C	1.117224063300	3.934209114900	3.650647253200
H	2.275451062800	2.924093836300	2.184877915400
C	1.006989589100	4.203903806800	5.057419114700
N	0.095915475300	4.328912541100	2.824773003500
C	-0.137266423000	4.762205282800	5.536961170200
H	1.823269699200	3.949885938200	5.717528707900
C	-1.126572235000	4.862853202500	3.308141490800
N	-1.169594244900	5.058466811400	4.692704513400
H	-0.287260723100	4.983324112500	6.585472432300
O	-2.075411482100	5.147119769600	2.574651317200
H	-2.032770837400	5.459953574000	5.036523968300
H	1.239837677000	4.492558557400	1.060055062300
C	0.221936059300	4.224220057600	1.346727509300
H	-0.010667097100	3.213174637700	0.999091958900
H	-0.489357347200	4.922138946100	0.909985005800

$^{7}RE_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.120062610800
C	1.103284123700	0.000000000000	2.874597883100
N	0.739834053400	-0.087908634000	4.188822026700
C	-0.655232199100	-0.150352174700	4.263461397400
C	-1.103828831400	-0.087189801200	2.968287810200
H	2.108767336400	0.113722065300	2.494034155500
H	1.375294394900	-0.169942949600	4.966698725000
H	-1.178840741800	-0.245810645500	5.198781218300
H	-2.103622352500	-0.094285134500	2.569814698300
N	-0.123604806000	-2.156267209600	-0.158601738300
C	-1.210729597200	-2.912643638500	0.033051621600
N	-0.912450147300	-4.214278517200	-0.239810976500
C	0.426162883500	-4.291803502400	-0.622638174300
C	0.907003118800	-3.007725972800	-0.566224443400

H	-2.175888639500	-2.544523990400	0.330696815800
H	-1.555906741600	-4.988095853600	-0.184384550500
H	0.894565430700	-5.221375493500	-0.894728848000
H	1.884891162900	-2.618155544200	-0.784089076200
O	-1.035370983800	0.280322606400	-1.775206762900
C	-2.229525467200	-0.005898944100	-1.298998714200
O	-2.316085235300	-0.304739019600	-0.049632093100
C	-3.411612036800	0.005716498600	-2.214714532300
H	-4.300934311700	-0.356453108100	-1.697958658000
H	-3.209124564700	-0.613286324800	-3.094280549200
H	-3.583251335800	1.027712276900	-2.569493862200
C	-0.714291621800	2.853501158000	-2.769302728700
O	0.460850060100	2.734036736300	-2.882950550200
O	-1.886510057300	3.024657963900	-2.685165079700
C	2.896468175600	0.808935909000	-0.150228461400
O	1.921187953100	-0.092380288400	-0.263301058500
C	3.542095585800	1.221697897000	-1.449077201000
H	3.794392564500	0.339166393100	-2.044128288400
H	4.437242903200	1.816644110600	-1.263050833200
H	2.820882661500	1.807934507300	-2.031654685000
O	-0.140775350200	1.927030462000	0.183918687800
O	3.248875861200	1.288987609500	0.963812322600
H	4.074465503300	4.369358646600	4.811904923700
N	3.378966327600	4.186686288100	4.104057171000
C	2.076997806300	4.349388156000	4.375535425800
H	3.705935923500	3.866785850700	3.201670075700
C	1.638452136600	4.759319422000	5.674101251300
N	1.156989191800	4.120771504100	3.391443219100
C	0.300566661600	4.902249073700	5.897213836700
H	2.359334388500	4.953726281500	6.454307441500
C	-0.245953768600	4.264267434500	3.601891148600
N	-0.596585140700	4.654192018200	4.903247570400
H	-0.102072690200	5.212197631700	6.852164294900
O	-1.084997104100	4.069671215300	2.727011129900
H	-1.592109309600	4.765755011100	5.053576155300
H	2.224332935100	2.847657183300	2.026346434200
C	1.584114568600	3.736406080300	2.015603966400
H	0.698928269300	3.477173058700	1.430232169000
H	2.098318950000	4.583618311400	1.549157191600

$^{1}TS_{H,3\text{-}meC}$

Fe	0.002870135000	0.009316654000	0.001002404000
N	0.001440543000	0.004010885000	1.950997076000
C	1.049163804000	-0.004009269000	2.774316931000
N	0.600433587000	0.061914034000	4.062718574000
C	-0.793281791000	0.121150677000	4.047231003000
C	-1.157261415000	0.086103307000	2.721000328000
H	2.075711779000	-0.046887898000	2.460720708000
H	1.182982673000	0.079055728000	4.886376974000
H	-1.383031238000	0.190727881000	4.944714068000
H	-2.130394046000	0.129030050000	2.262943875000
N	0.421589529000	-1.973389053000	-0.028295801000
C	-0.102067886000	-2.928988108000	0.744801058000
N	0.414075976000	-4.140196412000	0.381797968000
C	1.303502573000	-3.942562917000	-0.675456925000
C	1.298536736000	-2.590507060000	-0.924998829000
H	-0.830622371000	-2.781023141000	1.522959275000
H	0.182111619000	-5.028008300000	0.802009231000
H	1.840173283000	-4.749826373000	-1.143871970000
H	1.833694683000	-2.034922205000	-1.675382448000
O	-0.524650809000	-0.152699556000	-1.979950611000
C	-1.725077158000	-0.506474045000	-1.609170464000
O	-1.911669739000	-0.546673890000	-0.315355689000
C	-2.808393469000	-0.856842825000	-2.576319371000
H	-2.888351856000	-1.948213490000	-2.662757951000
H	-2.585113583000	-0.440950297000	-3.561219125000

H	-3.770890346000	-0.482694689000	-2.214483595000
C	1.424824740000	0.308988877000	-3.977799391000
O	2.043135193000	-0.628325431000	-3.594545104000
O	0.822660856000	1.237194491000	-4.406805187000
C	2.615250385000	1.060186379000	-0.749355466000
O	1.901801533000	0.273273384000	0.027314545000
C	4.115344100000	0.975446441000	-0.527572485000
H	4.412889333000	1.756059936000	0.185730829000
H	4.644791747000	1.156292899000	-1.466470297000
H	4.394489754000	0.004235156000	-0.114818867000
O	2.143521215000	1.855454236000	-1.613526566000
H	2.082760593000	4.714067462000	-2.267464608000
N	1.203481785000	4.225971680000	-2.164740366000
C	0.093490945000	4.950418079000	-2.110728821000
H	1.313383760000	3.202726004000	-1.991665554000
C	0.139510751000	6.386365060000	-2.135775964000
N	-1.134703868000	4.329932975000	-2.038925707000
C	-1.019397735000	7.088352794000	-2.018586254000
H	1.090566750000	6.889799205000	-2.224091624000
C	-2.353541825000	5.047321835000	-1.899543016000
N	-2.216775306000	6.437076757000	-1.889391943000
H	-1.048909788000	8.168761956000	-2.012744546000
O	-3.453687833000	4.496648090000	-1.803906090000
H	-3.088127069000	6.943717162000	-1.794603438000
O	-0.400655093000	1.713886539000	0.075444231000
H	-0.786501589000	2.289073215000	-0.960346425000
C	-1.235087188000	2.872143668000	-2.080389477000
H	-2.278524769000	2.605639712000	-2.233201612000
H	-0.606639588000	2.467809228000	-2.875405453000

^{3}TS$_{H,3\text{-}meC}$

Fe	0.031626084000	0.021958507000	0.002793778000
N	-0.081139688000	0.010175569000	2.005350852000
C	0.925870291000	0.008621567000	2.879274629000
N	0.418193656000	0.066826737000	4.144674058000
C	-0.973000127000	0.113315235000	4.065265942000
C	-1.274682247000	0.080311623000	2.725848420000
H	1.968814856000	-0.023178164000	2.619599755000
H	0.960871003000	0.087014467000	4.994144367000
H	-1.600505382000	0.173626236000	4.937240228000
H	-2.225360280000	0.116425865000	2.223118798000
N	0.474842989000	-1.958510932000	-0.012399261000
C	-0.039933593000	-2.909034179000	0.771568802000
N	0.478331787000	-4.118173131000	0.414071128000
C	1.355161850000	-3.925646872000	-0.652092656000
C	1.342098272000	-2.578831954000	-0.915050089000
H	-0.766511355000	-2.758483035000	1.549621217000
H	0.253815328000	-5.002898568000	0.841888693000
H	1.889012824000	-4.735940230000	-1.116770668000
H	1.857382623000	-2.029739781000	-1.682467152000
O	-0.559914854000	-0.186896898000	-1.995644040000
C	-1.745874323000	-0.554354250000	-1.599250872000
O	-1.923231761000	-0.583948951000	-0.310204439000
C	-2.828584635000	-0.941350387000	-2.553186910000
H	-2.888880360000	-2.034634597000	-2.620007401000
H	-2.622210720000	-0.543745901000	-3.548371359000
H	-3.794723680000	-0.579690787000	-2.191793112000
C	1.390444387000	0.271929992000	-4.018209868000
O	2.022009318000	-0.652295083000	-3.626370821000
O	0.779532300000	1.187985509000	-4.460896291000
C	2.672186286000	1.072312039000	-0.878045121000
O	1.969042283000	0.307573150000	-0.075275856000
C	4.177359388000	0.982223528000	-0.714051755000
H	4.511938977000	1.766536360000	-0.022149752000
H	4.670645623000	1.149910281000	-1.674225424000
H	4.466770249000	0.014031459000	-0.302811156000

O	2.172824401000	1.857378558000	-1.738207647000
H	2.074211501000	4.721669651000	-2.356560762000
N	1.200411503000	4.226338074000	-2.239912398000
C	0.086114590000	4.937036145000	-2.150398666000
H	1.322899133000	3.202511656000	-2.080384919000
C	0.116109408000	6.372344889000	-2.157029098000
N	-1.136967636000	4.301936906000	-2.053162199000
C	-1.043336596000	7.063420426000	-1.998279480000
H	1.060509316000	6.885658341000	-2.262290510000
C	-2.358148913000	5.011191695000	-1.869012729000
N	-2.230446326000	6.400137798000	-1.844449977000
H	-1.082782362000	8.143996625000	-1.975693825000
O	-3.449472522000	4.448199379000	-1.750997628000
H	-3.100796916000	6.900661675000	-1.718207193000
O	-0.381692350000	1.754483015000	0.072506850000
H	-0.777664895000	2.291030878000	-0.954492014000
C	-1.233730252000	2.852646105000	-2.098644291000
H	-2.275429562000	2.568556149000	-2.214176931000
H	-0.603919612000	2.437199641000	-2.885941855000

$^{5}TS_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.083532326100
C	1.066917542300	0.000000000000	2.885640204500
N	0.647060775500	0.060631461200	4.181491149800
C	-0.746733376000	0.103195836600	4.197164553900
C	-1.142073420700	0.065976318800	2.883194804300
H	2.092380734000	-0.037180161900	2.562549460500
H	1.245397933900	0.080350643200	4.992758458000
H	-1.310807903500	0.160399169600	5.111527646300
H	-2.122164316500	0.088043323300	2.439601586700
N	0.144306613700	-2.140630330200	-0.052064241600
C	-0.420294151700	-3.003852355300	0.795715842400
N	-0.136869385800	-4.278973453100	0.402482460400
C	0.638380099500	-4.221041363700	-0.755060669800
C	0.806466384500	-2.887592900600	-1.029865746100
H	-1.021095352400	-2.746304637600	1.649190738200
H	-0.442071099000	-5.120108179800	0.866384803300
H	0.983793779400	-5.104609434200	-1.262345194200
H	1.317862870600	-2.413067096000	-1.847325051500
O	-1.093291823100	-0.294718983100	-1.870613219500
C	-2.207350062200	-0.522248843400	-1.234042546500
O	-2.187090219200	-0.458454662300	0.058468051900
C	-3.459669021400	-0.876053354500	-1.978018418100
H	-3.590951809800	-1.965327080400	-1.975070902700
H	-3.398736349100	-0.539943587600	-3.014315548800
H	-4.329447815400	-0.434943917300	-1.485383201700
C	0.637607600400	-0.070051746100	-4.119330442600
O	1.140752586900	-1.110831901700	-3.856026296300
O	0.148573147900	0.964727950000	-4.433726109500
C	2.714163436200	0.561757831200	-1.233300527300
O	1.943541815200	-0.029644880300	-0.346644645700
C	4.194774488600	0.273161845900	-1.100827110100
H	4.633000647400	0.952969599100	-0.358487184200
H	4.696729946100	0.437208364000	-2.055849906000
H	4.358511783200	-0.750009175300	-0.756503300100
O	2.288656134000	1.329597950400	-2.146533712100
H	2.572103193000	4.136500351400	-2.577415974200
N	1.616211197700	3.854482194200	-2.407212974800
C	0.696145569900	4.797410665900	-2.257571038300
H	1.517959254900	2.826648149100	-2.281407588600
C	1.048233042000	6.188920960000	-2.277978139400
N	-0.627909641800	4.453151426000	-2.085496276700
C	0.082725364700	7.123557674100	-2.075375624600
H	2.077712774500	6.474974101000	-2.436116045300
C	-1.645956453300	5.417411218700	-1.834208376900

N	-1.212724841200	6.742886720800	-1.852848474100
H	0.285015399900	8.186126141700	-2.070589053000
O	-2.823126936100	5.111329677600	-1.629174519000
H	-1.939815796500	7.427064580400	-1.687945012900
O	-0.211741774000	1.725778263600	-0.154427433500
H	-0.670285848200	2.465406370100	-1.112321610300
C	-1.045499485200	3.061086414000	-2.120012353900
H	-2.129635197300	3.005156714100	-2.115061269900
H	-0.584933860300	2.506564899600	-2.937862662300

$^{7}TS_{H,3\text{-}meC}$

Fe	0.028609951000	0.021408852000	0.037500483000
N	-0.079261073000	0.027044569000	2.053216086000
C	0.953341533000	0.034841634000	2.899254575000
N	0.484976656000	0.064344976000	4.177696493000
C	-0.909596799000	0.100336449000	4.143382462000
C	-1.251745681000	0.085861101000	2.812951576000
H	1.986847958000	0.008501425000	2.605524515000
H	1.055236087000	0.071226202000	5.008413173000
H	-1.509588088000	0.138405739000	5.035838831000
H	-2.219154846000	0.111804965000	2.345654887000
N	0.487942274000	-2.013505366000	-0.030932478000
C	-0.013925902000	-2.982733203000	0.743042134000
N	0.486038936000	-4.190020505000	0.350760477000
C	1.341304764000	-3.980957591000	-0.730879671000
C	1.331193776000	-2.627256198000	-0.964075425000
H	-0.725390808000	-2.847278322000	1.538536599000
H	0.264020413000	-5.082506346000	0.765041545000
H	1.860275711000	-4.783942482000	-1.225300289000
H	1.835375625000	-2.078818083000	-1.740887104000
O	-0.541194974000	-0.115700244000	-1.985229240000
C	-1.728683869000	-0.525523474000	-1.621827738000
O	-1.927553874000	-0.599667559000	-0.339210760000
C	-2.783537178000	-0.906526946000	-2.612068468000
H	-2.821573112000	-1.997496996000	-2.708655281000
H	-2.558256174000	-0.480680880000	-3.591477985000
H	-3.765265381000	-0.570378827000	-2.266720345000
C	1.328534527000	0.229761716000	-4.031835463000
O	1.970261524000	-0.704482084000	-3.682488488000
O	0.720570113000	1.163773443000	-4.437563951000
C	2.669411586000	1.076832849000	-0.816026826000
O	1.961883229000	0.316464456000	-0.008081557000
C	4.169708747000	1.006561351000	-0.629641924000
H	4.486218322000	1.802850244000	0.060063846000
H	4.677689844000	1.179829014000	-1.581742920000
H	4.458749575000	0.041755523000	-0.211914342000
O	2.177870084000	1.851348205000	-1.690348464000
H	2.102169627000	4.710782144000	-2.324157163000
N	1.215100809000	4.227713407000	-2.199943953000
C	0.113041409000	4.960954064000	-2.127236308000
H	1.331372076000	3.201600409000	-2.036134113000
C	0.177030207000	6.395431594000	-2.167439414000
N	-1.131892039000	4.351712357000	-2.025047883000
C	-0.971991191000	7.109749317000	-2.037467852000
H	1.136334144000	6.894258829000	-2.283497723000
C	-2.340460825000	5.085285885000	-1.860449657000
N	-2.180527528000	6.471898612000	-1.873158305000
H	-0.984321987000	8.191392409000	-2.050145974000
O	-3.450403227000	4.547705893000	-1.739486258000
H	-3.042200504000	6.991641260000	-1.769798788000
O	-0.383637265000	1.827021041000	0.071883952000
H	-0.748837405000	2.376008913000	-0.956329528000
C	-1.248400362000	2.910615706000	-2.082797367000
H	-2.291568575000	2.627859678000	-2.209143173000
H	-0.607609271000	2.510889512000	-2.870407284000

^{1}**IM$_{H,3\text{-}meC}$**

Fe	-0.135215087300	-0.019539365700	0.083115218700
N	0.079986529700	0.033544243200	2.041387049300
C	1.230310713700	0.023879468800	2.712988713900
N	0.961823387800	-0.007633270500	4.053443182000
C	-0.422433926900	-0.033393649400	4.228640361000
C	-0.960423534200	-0.002783665700	2.964353846700
H	2.208741467100	0.037217216000	2.268500760100
H	1.651037256800	-0.071702306000	4.787244925900
H	-0.879694767300	-0.089744778300	5.201387122900
H	-1.987892958100	-0.009534195200	2.645292990000
N	0.323881849900	-1.981345884000	0.263296616500
C	-0.526515299800	-2.948340700100	0.622055475100
N	0.163632687300	-4.111972005800	0.791920771500
C	1.509221583200	-3.873153948100	0.521570722800
C	1.598828944100	-2.543169791700	0.193912652800
H	-1.586224902000	-2.828264250800	0.757868839800
H	-0.238070439000	-5.000901947200	1.047056447900
H	2.253866004300	-4.648460471000	0.571282866300
H	2.442684497800	-1.943507385400	-0.093581061100
O	-0.684949779300	-0.269129606500	-1.856810513200
C	-1.874792467500	-0.623440193400	-1.476198195600
O	-2.058243095700	-0.617219962000	-0.175961177900
C	-2.954191727900	-0.982461141000	-2.436856162800
H	-3.789716675000	-1.456549751200	-1.919397275900
H	-2.562435708900	-1.646452429100	-3.212767769600
H	-3.312688057300	-0.072397741600	-2.933495406600
C	-0.605576015500	2.698242073100	-3.061276730700
O	0.523987831700	2.849739978700	-3.383669217300
O	-1.744416531200	2.568559351100	-2.741978157300
C	2.414979549500	1.467552574500	-0.362101832700
O	1.754126455400	0.342560361500	-0.164367653000
C	3.368764457200	1.462195478800	-1.531782952400
H	3.869702905900	0.494536938400	-1.619304165900
H	4.100438644100	2.266101430900	-1.434910199500
H	2.788916423700	1.619557361800	-2.450122893900
O	2.305437770000	2.503533436000	0.363739602800
H	1.006524535200	2.776668116900	3.246762312900
N	0.714330924900	3.188688540400	2.372214459300
C	-0.542418308600	3.616970080300	2.291814840700
H	1.312287502000	2.938118819700	1.536062805100
C	-1.480515362400	3.429521457700	3.353527114500
N	-0.950871464200	4.320652274500	1.160061421400
C	-2.772514927000	3.822303840500	3.202740735200
H	-1.158305958800	2.924708793500	4.251790435200
C	-2.327763931900	4.703393873500	0.970797791500
N	-3.169579858000	4.422647461000	2.034070670500
H	-3.531208995900	3.681080422800	3.959304370200
O	-2.713800483400	5.253949137900	-0.065064146200
H	-4.130649236100	4.706095250200	1.892698439400
O	-0.645766506900	1.727563438600	0.060946177500
H	-1.423350187800	1.854123583300	-0.522527979000
C	-0.089549770700	4.636144200000	0.126736570300
H	-0.518879849500	5.187962716300	-0.693616250600
H	0.932660148600	4.296773035700	0.147658867400

^{3}**IM$_{H,3\text{-}meC}$**

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.205142834800
C	1.150841471500	0.000000000000	2.878380833000
N	0.894695565600	-0.064434950100	4.221928555800
C	-0.486703091900	-0.124038826100	4.403122366000
C	-1.030200835400	-0.081392526600	3.140447182200
H	2.128821279700	0.046659918300	2.432707604100
H	1.588241099800	-0.126627978700	4.951659769800
H	-0.936957427800	-0.208868631600	5.377192762700

H	-2.061150983000	-0.110386360300	2.833997914000
N	0.396804420200	-1.956856339400	0.238529183100
C	-0.520079128500	-2.860680884100	0.601126435800
N	0.095212001200	-4.053687834700	0.825525979400
C	1.460344335900	-3.902844580200	0.586539878700
C	1.637073041100	-2.591807792600	0.220261855500
H	-1.573366930700	-2.670557724300	0.703867251100
H	-0.364657310800	-4.909501550100	1.095128202800
H	2.155566913200	-4.718092796600	0.683550129800
H	2.525241735500	-2.052498899300	-0.054528332800
O	-0.739079067100	-0.495974784700	-2.098481051600
C	-1.895735161200	-0.637852336400	-1.566955364400
O	-1.986586629100	-0.452768744000	-0.259634372600
C	-3.117052198000	-0.962708016900	-2.368190266000
H	-3.919029726900	-1.333457209800	-1.728320650400
H	-2.874681083000	-1.696548601300	-3.140836207200
H	-3.463457794500	-0.052572914400	-2.872934948600
C	-0.705738663300	2.639863583800	-3.108821076100
O	0.405307469700	2.729871674200	-3.511667533200
O	-1.828565127900	2.578532047400	-2.720476629200
C	2.499944726300	1.528669485200	-0.312351230000
O	1.887459739800	0.365308414100	-0.107810551900
C	3.346182997200	1.615289518600	-1.554060803200
H	3.869466152700	0.673076739300	-1.732226618900
H	4.055964348300	2.439774942800	-1.476764857200
H	2.685327279100	1.795090369600	-2.411824299100
O	2.408684852000	2.510684470200	0.481225176800
H	0.943086565800	2.753108505200	3.277362253400
N	0.672966438100	3.179041453400	2.402270610800
C	-0.582694318800	3.604367025200	2.299516652200
H	1.311558168400	2.956226224100	1.594746278600
C	-1.538178145800	3.398864432100	3.341879770500
N	-0.977846466300	4.310174087600	1.163057393600
C	-2.827808768600	3.798119761300	3.180364495500
H	-1.230000724200	2.877617723500	4.235565807800
C	-2.352284402300	4.716661459400	0.969061589900
N	-3.207670311100	4.419402302900	2.017294527000
H	-3.597166019700	3.645204130400	3.924286519300
O	-2.718640591000	5.294228785100	-0.057101519900
H	-4.165172450200	4.712804160000	1.871200749500
O	-0.404434427000	1.759977149000	-0.216635967900
H	-1.355073034900	1.840927247700	-0.450325912900
C	-0.101867225200	4.646676369400	0.149302625700
H	-0.522030607500	5.193969385700	-0.678169815700
H	0.920509911500	4.312587862800	0.183735862900

$^{5}IM_{H,3\text{-}meC}$

Fe	-0.035919362100	-0.005228438200	0.279442467900
N	-0.014010262800	-0.333856379000	2.371786756200
C	1.048265652200	-0.233673109000	3.175089957600
N	0.688312046600	-0.594683286100	4.441345194300
C	-0.662762515400	-0.943919894900	4.435657513000
C	-1.091126534600	-0.776470736200	3.141960504000
H	2.033890518600	0.075323392700	2.874504892600
H	1.305355790200	-0.641012500800	5.237647144700
H	-1.174855712100	-1.274283531200	5.322507566000
H	-2.052775535200	-0.943939669600	2.690211861300
N	0.683230462400	-2.011705289100	-0.135483078900
C	0.016330140500	-3.153966371400	0.062905255900
N	0.786240385100	-4.206611641400	-0.336099725200
C	1.998419079800	-3.712206634600	-0.813563170900
C	1.924263829400	-2.348427815800	-0.682885388100
H	-0.977795084800	-3.230499162000	0.465251658800
H	0.518584196000	-5.177758107600	-0.299660886600
H	2.773601601300	-4.354431608800	-1.193186308000
H	2.640258948700	-1.585439921400	-0.922781350400

O	-1.195366863100	-0.282685123500	-1.591163566100
C	-2.168641261700	-0.856697251300	-0.949348775900
O	-2.025176894500	-1.039527823400	0.328534663800
C	-3.415892806100	-1.279929672300	-1.664776610800
H	-4.030707453200	-1.912386267000	-1.023082452400
H	-3.160646445000	-1.809279652400	-2.587271015000
H	-3.998176867500	-0.395067694100	-1.948401000100
C	-1.233654505500	1.688992162000	-3.541705716800
O	-1.377344521100	0.965659360500	-4.465947886700
O	-1.092815610000	2.463900883500	-2.647843874000
C	2.604799831200	1.578274379500	0.195468335200
O	1.906106891700	0.466102970400	0.121250359200
C	3.774225200100	1.690307929900	-0.755360024100
H	4.483552440600	0.875622496800	-0.572754125300
H	4.280214549500	2.647502888700	-0.628000418400
H	3.423719354900	1.589251699600	-1.788326898600
O	2.359766847200	2.511922071200	1.020082845000
H	0.464827547800	3.076717842200	3.545792487000
N	0.389614627600	3.428515715800	2.602141837300
C	-0.673181406700	4.169064118700	2.303768154500
H	1.071430666100	3.025651730000	1.919116225500
C	-1.685467805000	4.451083083800	3.273111041400
N	-0.796707357200	4.725610946500	1.030945936900
C	-2.773627863600	5.192383138500	2.933174272200
H	-1.582379079300	4.048855245500	4.270511995600
C	-1.971159849300	5.476442083900	0.646782435400
N	-2.900037245200	5.673930210500	1.654579552300
H	-3.572183325700	5.426885210600	3.622868540200
O	-2.114431077000	5.916056698700	-0.497275450400
H	-3.709927165200	6.214030370400	1.378395126200
O	-0.668412611900	1.729915074000	0.203581247600
H	-0.997452311900	2.095758915100	-0.643409265800
C	0.165267834800	4.576341692800	0.047955856200
H	-0.074842631200	4.990986199400	-0.917262709700
H	1.092669125400	4.076276954700	0.271354734400

$^{7}IM_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.210808265000
C	1.134382561900	0.000000000000	2.916496649800
N	0.844065756600	-0.020488280100	4.252498163900
C	-0.541288317900	-0.052705597500	4.402167367400
C	-1.053188379600	-0.040986153600	3.125592887300
H	2.126194879000	0.023103109800	2.505465890100
H	1.520737497400	-0.061609616100	4.999862721500
H	-1.016569630800	-0.100624386000	5.366911797000
H	-2.077921603900	-0.066932733300	2.798315613100
N	-0.264498358600	-2.121185735900	0.292586502300
C	-1.435947322000	-2.755278569000	0.415751203600
N	-1.213229783500	-4.077099097100	0.662480478600
C	0.161338173400	-4.296908988300	0.695454539600
C	0.742293531200	-3.073860880900	0.466056096400
H	-2.401799750200	-2.293857671700	0.315157759900
H	-1.925944990800	-4.780613139700	0.778929620200
H	0.585685731200	-5.271560392000	0.862333050200
H	1.781173811900	-2.803962027200	0.395918586500
O	-0.509917835700	-0.364735781300	-2.048351609300
C	-1.798426811100	-0.396430760300	-1.848826238200
O	-2.231297203200	-0.256297608400	-0.634341933100
C	-2.734990813200	-0.572181388000	-3.004424536000
H	-3.761159135500	-0.691163444000	-2.654517333400
H	-2.436959483100	-1.439607971400	-3.601447483500
H	-2.675451828800	0.305954724900	-3.657948230900
C	0.692804271200	2.239863314700	-3.235297093200
O	1.821085748700	1.879871983000	-3.240489304100
O	-0.427511421300	2.636280143600	-3.239275521800

C	2.804475231500	1.064994800200	0.086732632300
O	1.941481251700	0.048000148800	0.045135178000
C	4.063217126900	0.881261835700	-0.717043966700
H	4.454595398900	-0.131503949100	-0.588885653200
H	4.811605397800	1.620834969600	-0.429205801000
H	3.819697527500	1.007430493600	-1.778796155600
O	2.594338930800	2.109716243000	0.766621739800
H	0.617617054300	2.718164553800	3.101786502900
N	0.502709430200	3.175469241600	2.208644837200
C	-0.719484605500	3.617036782500	1.910579531500
H	1.223695918400	2.898561995800	1.510420890600
C	-1.839158275900	3.363508634000	2.758339343100
N	-0.912539005300	4.393917353300	0.770100380900
C	-3.083713526700	3.772712801200	2.391836438200
H	-1.691450422500	2.782153375200	3.655808686200
C	-2.230986693200	4.826560472800	0.364461672400
N	-3.257190332200	4.465418206800	1.221756027500
H	-3.971910803300	3.572135685500	2.974272946100
O	-2.413664787700	5.479624720500	-0.666022675200
H	-4.176216839000	4.768464248000	0.925871583800
O	-0.345884887600	1.814116551300	-0.246984935900
H	-1.021742246300	2.089992454000	-0.894749973600
C	0.125357679400	4.762460552500	-0.062981020900
H	-0.137116198700	5.335646660900	-0.936535872800
H	1.128856584700	4.453053521900	0.167123797800

$^{1}TS_{reb,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.958566223500
C	1.046628800000	0.000000000000	2.785958297500
N	0.591739853500	-0.057008772300	4.070329633900
C	-0.801703537800	-0.093930149900	4.051683682800
C	-1.162549383700	-0.058928320600	2.727853935000
H	2.075722322700	0.036113187300	2.479762645400
H	1.169811719900	-0.071600881600	4.896042715900
H	-1.389880442100	-0.135445768000	4.951593738000
H	-2.134212865300	-0.063931744200	2.266112514300
N	0.669210701400	-1.889436879900	-0.002557536500
C	-0.047601464700	-2.975810687100	0.304183961100
N	0.730439577300	-4.083617429400	0.145969801900
C	1.992773909600	-3.682647105400	-0.285597010200
C	1.945484057200	-2.314138725500	-0.373300292900
H	-1.077984364100	-2.978967745900	0.610406168700
H	0.435376256600	-5.034277152500	0.305130758200
H	2.781687357500	-4.383880501800	-0.492981282100
H	2.696266207600	-1.609121356700	-0.674675626800
O	-0.460549080300	-0.182268966100	-1.982500612200
C	-1.628526319000	-0.648685439300	-1.640794121500
O	-1.812554808600	-0.782399314800	-0.354297688700
C	-2.696929576800	-0.965020207500	-2.628948895800
H	-3.247006353500	-1.858002382700	-2.321649509800
H	-2.272753780200	-1.101907728900	-3.624575677500
H	-3.414176837600	-0.134394651400	-2.661842626900
C	1.692607392900	0.684495971000	-3.764603017100
O	2.467005309400	-0.070124258700	-3.272638344100
O	0.947197377400	1.451934475300	-4.276178701600
C	2.504430010400	1.553166152000	-0.505950514100
O	1.853680670700	0.572555162300	0.086814502100
C	4.013955590700	1.450339826400	-0.438208301500
H	4.336170574300	0.927549733600	0.464519608600
H	4.463859880300	2.443883060900	-0.484968193900
H	4.362511725000	0.877705359400	-1.306882085900
O	1.961004752600	2.513349953100	-1.125673464300
H	1.175340658800	5.694927942100	-0.954939976800
N	0.583152838100	4.898380198800	-1.134300541800
C	-0.753743375500	5.084676210600	-1.136561546400

H	1.057957072700	3.990872353000	-1.212352498700
C	-1.355115480300	6.325362202300	-0.824260851200
N	-1.576284210300	3.993620789800	-1.473461930100
C	-2.717681661500	6.455999941700	-0.807305358000
H	-0.722855563800	7.169207231400	-0.585645192600
C	-3.026212798600	4.109807081200	-1.431608293500
N	-3.502513261700	5.354727353700	-1.093435778100
H	-3.232828125100	7.375514511600	-0.573802952500
O	-3.754318802400	3.146730479100	-1.702114011000
H	-4.511485213500	5.426953614900	-1.083708451800
O	-0.776548365900	1.689930991700	0.002234314000
H	-0.257277241300	2.310489345800	0.556201438300
C	-1.089208623900	2.760535066600	-1.804175284800
H	-1.828788408800	2.052660054000	-2.125453066700
H	-0.063133192700	2.642860236400	-2.104487480400

$^{3}TS_{reb,3\text{-}meC}$

Fe	-0.003897462000	0.001280342000	0.000681992000
N	0.000224388000	-0.007298716000	1.955317680000
C	1.046304665000	-0.007803702000	2.790400556000
N	0.591860478000	-0.056934548000	4.080215565000
C	-0.805444903000	-0.087503225000	4.059644319000
C	-1.164321975000	-0.056574422000	2.727458132000
H	2.078521254000	0.025294583000	2.487965227000
H	1.173307882000	-0.067687719000	4.907697007000
H	-1.401458579000	-0.123006779000	4.956204337000
H	-2.140753783000	-0.057534851000	2.271642737000
N	0.667378448000	-1.897562802000	-0.044170582000
C	-0.040892528000	-2.991921227000	0.269158576000
N	0.734405589000	-4.102564089000	0.079315365000
C	1.988512074000	-3.693649780000	-0.381733815000
C	1.935731011000	-2.316901406000	-0.453503582000
H	-1.063802261000	-2.999792883000	0.605298401000
H	0.442040135000	-5.057420537000	0.238981794000
H	2.777478445000	-4.387049205000	-0.620060917000
H	2.683171281000	-1.611896658000	-0.769195680000
O	-0.492743312000	-0.160410641000	-1.980641410000
C	-1.660616437000	-0.626866395000	-1.632077506000
O	-1.819781752000	-0.756216236000	-0.333380192000
C	-2.745481903000	-0.954512646000	-2.607816937000
H	-3.286409556000	-1.850611606000	-2.289438605000
H	-2.331832933000	-1.092826896000	-3.609249029000
H	-3.468199168000	-0.127679641000	-2.634591398000
C	1.509867619000	0.810667432000	-3.851324051000
O	2.310250242000	0.053308785000	-3.400051863000
O	0.731418668000	1.576793044000	-4.322346368000
C	2.480762899000	1.568929153000	-0.555062445000
O	1.845076196000	0.578151717000	0.053083434000
C	3.996016057000	1.451061848000	-0.551086920000
H	4.347840940000	0.904661970000	0.327949724000
H	4.452917435000	2.443154028000	-0.593583429000
H	4.303048338000	0.895861809000	-1.447094162000
O	1.917511022000	2.551049156000	-1.125315088000
H	1.177720600000	5.733940095000	-0.933094423000
N	0.570885531000	4.938855290000	-1.082029756000
C	-0.771269498000	5.150741451000	-1.025211906000
H	1.034306705000	4.024401071000	-1.184148570000
C	-1.337632934000	6.400486892000	-0.678598376000
N	-1.632146335000	4.070847513000	-1.338701733000
C	-2.704522413000	6.560168211000	-0.608777810000
H	-0.682878295000	7.234279857000	-0.459271264000
C	-3.081912686000	4.215582840000	-1.238682752000
N	-3.524112656000	5.468536648000	-0.875154057000
H	-3.191575439000	7.490317416000	-0.351048510000
O	-3.838681623000	3.263080241000	-1.490325430000
H	-4.533820051000	5.559888402000	-0.830652205000

O	-0.736864466000	1.739094924000	-0.002347874000
H	-0.192662989000	2.348064844000	0.543110923000
C	-1.176230616000	2.832564670000	-1.712202511000
H	-1.942100092000	2.148039838000	-2.035096510000
H	-0.172429149000	2.724388100000	-2.089377881000

^{5}TS$_{reb,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.141060259000
C	1.040477181600	0.000000000000	2.976331527400
N	0.585146110200	0.012653362900	4.263988908000
C	-0.808592934100	0.019365685900	4.240491238500
C	-1.163702656100	0.011812051200	2.913924638600
H	2.076884285800	-0.007661005000	2.687669200500
H	1.160045722200	0.013608157800	5.092246207400
H	-1.399802238800	0.031720362600	5.139573227000
H	-2.133270956700	0.014089494000	2.446956517000
N	0.484934144600	-2.114417229900	0.021421060300
C	-0.218575877300	-3.077097173600	0.624757071400
N	0.365019083600	-4.286809097100	0.385980529500
C	1.487026707500	-4.084351375300	-0.416855027200
C	1.550263257800	-2.731584926200	-0.638823048600
H	-1.117183329400	-2.928573553700	1.196413956100
H	0.033938624500	-5.177109044700	0.723354563600
H	2.110802150500	-4.895247301000	-0.749647131600
H	2.251210937200	-2.158435206700	-1.215988670600
O	-0.997494869200	-0.305872855200	-1.895133187900
C	-2.097918310600	-0.671786245200	-1.295269698200
O	-2.078304123600	-0.732943222300	0.000688527200
C	-3.339455086100	-0.977297224800	-2.071448748300
H	-3.863060925300	-1.828374627800	-1.628725884800
H	-3.101647040200	-1.178757217100	-3.116759402900
H	-4.016596845100	-0.115040573400	-2.025643215700
C	1.073550806200	0.025991736000	-3.999921131500
O	1.800582964800	-0.812893745600	-3.576202974600
O	0.384942514400	0.880717329900	-4.448331852500
C	2.721220681500	1.089161861700	-0.986402906800
O	1.957113255700	0.298590469100	-0.266131322200
C	4.169760619400	0.674157306800	-1.116628014500
H	4.492184246900	0.095434898900	-0.249403108000
H	4.808702869000	1.548889957000	-1.254445144900
H	4.268476140300	0.040490914900	-2.007292762900
O	2.298614222200	2.118003077000	-1.594111239200
H	2.095900712800	5.305632257900	-1.564671305100
N	1.343773827400	4.634410912000	-1.627313834800
C	0.087100707000	5.096624118200	-1.573229464700
H	1.632712710300	3.640074951200	-1.646009410500
C	-0.209126442900	6.467006245000	-1.339207949800
N	-0.973217484200	4.198314642900	-1.757557386800
C	-1.503822097600	6.886105729800	-1.238855819000
H	0.605261781200	7.167712363400	-1.222007815700
C	-2.354248112900	4.625716156300	-1.615726427100
N	-2.525409736000	5.973209348100	-1.365382604600
H	-1.787166802100	7.911573238300	-1.051546972200
O	-3.290677519900	3.830633382500	-1.729158848300
H	-3.491352022300	6.263248547900	-1.282042129000
O	-0.533317576900	1.830112045400	-0.029648197200
H	-0.083139768900	2.491016369900	0.532168969700
C	-0.787580505000	2.864829426100	-2.032102403700
H	-1.671318042100	2.278936703900	-2.206087596600
H	0.181706419500	2.504819655800	-2.328135748300

^{7}TS$_{reb,3\text{-}meC}$

Fe	0.183162194000	0.084133208000	-0.056102872000
N	-0.282388977000	0.025953441000	1.979508551000
C	0.583574386000	0.031967235000	2.998404508000
N	-0.109459049000	0.016888472000	4.169607846000

C	-1.473258786000	0.002702160000	3.881818255000
C	-1.572594943000	0.009386652000	2.513380645000
H	1.656212858000	0.051669079000	2.915426388000
H	0.297425503000	0.026404008000	5.092491656000
H	-2.223776921000	-0.004816578000	4.652482855000
H	-2.439640360000	0.014351641000	1.876378921000
N	0.556538404000	-2.031566492000	-0.021111865000
C	-0.365637173000	-3.001711340000	0.004129514000
N	0.256284765000	-4.212270341000	0.052358458000
C	1.634385842000	-4.006544323000	0.059341496000
C	1.811538298000	-2.647215406000	0.013261537000
H	-1.430633001000	-2.850658905000	-0.008642716000
H	-0.205282583000	-5.108596897000	0.073719344000
H	2.339189028000	-4.819075533000	0.088456477000
H	2.711685502000	-2.061420546000	-0.007861709000
O	-0.316208093000	-0.076894319000	-2.174471178000
C	-1.538461602000	-0.412398848000	-1.883953513000
O	-1.836152720000	-0.468131227000	-0.614294245000
C	-2.542391318000	-0.726731341000	-2.942561745000
H	-2.255253536000	-1.647299984000	-3.464260048000
H	-2.559948467000	0.073672515000	-3.689703708000
H	-3.534460838000	-0.849029481000	-2.507224940000
C	1.420330426000	1.028063326000	-4.162021224000
O	2.193444310000	0.130741209000	-4.099618192000
O	0.672344383000	1.947640520000	-4.233883458000
C	2.884850406000	1.224508544000	-0.761876989000
O	2.132567119000	0.315363387000	-0.139264968000
C	4.275425106000	0.797908096000	-1.138597506000
H	4.718907884000	0.183697609000	-0.351149293000
H	4.899513708000	1.669954523000	-1.336849879000
H	4.220653759000	0.188932217000	-2.050296076000
O	2.441246090000	2.375839452000	-1.039923424000
H	1.674237553000	5.514072223000	-2.227741460000
N	1.039789065000	4.806592905000	-1.894559567000
C	-0.133646782000	5.229483321000	-1.315916800000
H	1.453967957000	3.896409318000	-1.727693820000
C	-0.414801710000	6.559903957000	-1.007485015000
N	-1.155152892000	4.243728505000	-1.100564530000
C	-1.626325583000	6.932886999000	-0.456503300000
H	0.345937669000	7.308176423000	-1.185517034000
C	-2.394392146000	4.597321166000	-0.428511823000
N	-2.559311857000	5.926601122000	-0.169999574000
H	-1.903372409000	7.942971916000	-0.202145823000
O	-3.245161359000	3.728350977000	-0.169035314000
H	-3.445103184000	6.163115088000	0.254763826000
O	-0.082592946000	2.044898419000	-0.175226845000
H	0.836863450000	2.423833764000	-0.268802573000
C	-1.013878380000	2.928288121000	-1.443015992000
H	-1.929114567000	2.364798250000	-1.343449599000
H	-0.364307255000	2.708735837000	-2.279229437000

^{1}P$_{H,3\text{-meC}}$

Fe	0.006329069000	-0.001217410700	0.023262197600
N	0.027918467300	-0.023217028500	2.020261386500
C	1.090806482100	-0.116764100600	2.820695982500
N	0.678791708400	-0.155328610000	4.126107452800
C	-0.712043371000	-0.093368477900	4.148952757000
C	-1.106221654400	-0.011313477600	2.834135684500
H	2.112587266600	-0.179263513400	2.492492239000
H	1.278546800300	-0.260993395500	4.929102513600
H	-1.274972276800	-0.130088032200	5.065564172300
H	-2.091694816500	0.033853210300	2.403172442600
N	0.057875960700	-1.982374860300	-0.004238564300
C	-1.010872345500	-2.781846656700	0.056272012200
N	-0.603298379000	-4.086391042300	0.039730064700
C	0.786249744700	-4.113099095300	-0.036707975300

C	1.187388753200	-2.799797359800	-0.063295235500
H	-2.032231808700	-2.449096584000	0.102335673800
H	-1.209164528700	-4.890836081400	0.062346917700
H	1.344455764500	-5.032255748000	-0.072222018100
H	2.170114133600	-2.370872449300	-0.131735519400
O	-0.512933599300	0.064954724600	-2.002970403300
C	-1.760371903400	0.015435508400	-1.666263297200
O	-2.026937413400	-0.027165186400	-0.381435036100
C	-2.857276156300	0.015070566700	-2.687429588900
H	-3.824919613400	-0.149844091000	-2.211121606700
H	-2.669838173000	-0.761400111500	-3.436450839500
H	-2.876838560400	0.974514058700	-3.218301810700
C	2.347417867600	3.148063450000	-2.971195264600
O	3.191741073500	2.411270864700	-3.358931100500
O	1.496296492100	3.897352917600	-2.614134256200
C	2.867165873200	1.098198194000	-0.263385183500
O	2.097361852100	0.097411924900	-0.036763508400
C	4.331564702500	0.894328111000	-0.520995089800
H	4.654808934700	-0.094620287900	-0.194347269500
H	4.916657171600	1.673757105800	-0.025421329900
H	4.509621321000	0.987408344000	-1.599062353900
O	2.419027261200	2.335296252400	-0.324447931000
H	1.715696625500	4.326084783000	2.431882233000
N	1.054711557500	3.965118196600	1.758131779100
C	-0.247035045200	4.052730555200	2.043537111200
H	1.469497985300	3.472476029800	0.965007196800
C	-0.655758983100	4.580746172600	3.314864556800
N	-1.218265878200	3.672592126300	1.150627691200
C	-1.981006372200	4.664691714500	3.609067401400
H	0.092322935800	4.893127090000	4.028789099600
C	-2.608175659400	3.778865003500	1.427915426400
N	-2.917434493500	4.266159408300	2.700189183400
H	-2.348247881600	5.043540449100	4.553456271400
O	-3.482446860400	3.478155416100	0.612787810400
H	-3.907824718900	4.336020879000	2.897961168700
O	0.041557402400	2.028516550000	-0.022189579400
H	1.049643970900	2.239146831900	-0.301177645700
C	-0.882228993900	3.061805121200	-0.199315393200
H	-1.827730063400	2.695183043400	-0.586770871600
H	-0.471854831900	3.852991813300	-0.837279322800

$^{3}P_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.054376816300
C	1.059728795900	0.000000000000	2.861887668200
N	0.640261344300	-0.053711699100	4.163433725800
C	-0.752209530800	-0.094484029900	4.174739569300
C	-1.140942487700	-0.061443607700	2.856413979100
H	2.085533191900	0.009118473000	2.539313525800
H	1.238536497000	-0.111764417200	4.972665441700
H	-1.318321302400	-0.161463035500	5.087603587900
H	-2.123016779200	-0.098122772100	2.415382780800
N	0.031496103200	-1.979125801100	-0.058976974900
C	-1.015949914200	-2.809254033000	-0.079262056700
N	-0.565591356100	-4.097231836400	-0.088927423500
C	0.827129361100	-4.083430559400	-0.077704582400
C	1.190270430800	-2.760206624300	-0.059578816100
H	-2.046513502200	-2.500047942100	-0.087503100500
H	-1.147288811900	-4.919617293200	-0.113411826600
H	1.413192514400	-4.985636040300	-0.089162959800
H	2.161017318700	-2.298142867200	-0.055676697600
O	-0.781978454200	0.178226372200	-1.848343848800
C	-2.049888515600	-0.050584549000	-1.601544986500
O	-2.435151434100	-0.231448123000	-0.386779618200
C	-3.013286780300	-0.095959922800	-2.757561199300
H	-4.004504300400	-0.397544153000	-2.416249739400

H	-2.649266838500	-0.791545746000	-3.520585283900
H	-3.080517946700	0.890832135300	-3.229130227000
C	2.258995603800	3.167730782700	-2.904580225000
O	3.055230898100	2.412726715500	-3.353077087100
O	1.450185391700	3.935332928400	-2.489330577200
C	3.048038999300	1.073735967600	-0.270333767400
O	2.297677002500	0.077203383300	0.012060513000
C	4.501874535400	0.880275654700	-0.598434708200
H	4.841920425500	-0.107156830800	-0.283846662800
H	5.108995202700	1.661165463300	-0.132810895700
H	4.629484020400	0.971938229900	-1.684051277700
O	2.572700055700	2.305045629100	-0.328127948200
H	1.772958032200	4.396938072900	2.476922583000
N	1.126636004400	4.009399406000	1.804421403300
C	-0.182929397700	4.083099119900	2.061985028100
H	1.551680626500	3.510673402400	1.024533670000
C	-0.628228621600	4.629721445400	3.312210831800
N	-1.123218424000	3.666935508700	1.153537690400
C	-1.962460231800	4.695371630900	3.574135146700
H	0.097721978500	4.970449743400	4.035844689400
C	-2.522515508800	3.748962047700	1.398079660600
N	-2.869254545600	4.259201222800	2.653375687600
H	-2.358392679100	5.087477938400	4.501794842700
O	-3.373697377100	3.413758873600	0.573430626100
H	-3.865376843300	4.311687191100	2.828009656200
O	0.185648621300	2.017159684600	0.033496808800
H	1.225437207500	2.203646875100	-0.233077162600
C	-0.730577266800	3.056774996000	-0.182109190500
H	-1.657599715000	2.692113920600	-0.615841354400
H	-0.293599401800	3.846683031300	-0.800737468300

$^{5}P_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.147010042900
C	1.069179169200	0.000000000000	2.944173246500
N	0.673689111200	-0.185863071100	4.240992195000
C	-0.715073266300	-0.318826860800	4.259458698600
C	-1.122593992300	-0.201854414000	2.951908038200
H	2.090060331000	0.108277198300	2.621612955200
H	1.285591463800	-0.275260235500	5.037569889200
H	-1.262273993600	-0.504069898800	5.167665101800
H	-2.102477272400	-0.281728644300	2.511358901500
N	0.665320170700	-2.039652454000	-0.091762339100
C	-0.150959565700	-3.084496699400	0.078469491500
N	0.576925673700	-4.239551355200	0.063626720700
C	1.918672527100	-3.914153937400	-0.125739769900
C	1.960586292800	-2.545097490200	-0.222885760900
H	-1.218424504800	-3.016636406900	0.201577327900
H	0.203343218500	-5.171356739200	0.153231126400
H	2.690567103700	-4.661736171600	-0.180708544000
H	2.795711737600	-1.885854803600	-0.379678809900
O	-1.109928392000	0.134922477200	-1.749147188300
C	-2.187241912900	-0.456009539000	-1.292523848100
O	-2.194210583800	-0.850225905400	-0.062185745200
C	-3.363702660200	-0.647769077500	-2.202552920400
H	-4.124967287500	-1.266809033300	-1.726615797400
H	-3.039335038400	-1.103376576900	-3.143446987400
H	-3.793624144000	0.330436116000	-2.447894864600
C	-1.076185445700	2.947524396300	-2.919552184800
O	0.031177444900	2.813171455900	-3.317204947800
O	-2.181475361200	3.144483478200	-2.527751068700
C	2.524855858100	1.932828217300	-0.090371618200
O	1.969370261500	0.769066766500	-0.073318377700
C	3.914120604500	2.077939472000	-0.647325574000
H	4.460212831100	1.135048572800	-0.581282802800
H	4.454344258100	2.876717702400	-0.135300921100

H	3.837552200500	2.354756078900	-1.706377597500
O	1.914894679300	3.008414692800	0.322701992700
H	1.413437560700	4.045472312400	3.330354790400
N	0.707627470300	3.821986942000	2.641614049100
C	-0.557219002300	3.744367024900	3.052993403200
H	1.087949440400	3.559717460800	1.712812677700
C	-0.865600674100	3.879640426500	4.449983293200
N	-1.591270304900	3.559343484900	2.164789577600
C	-2.157021482100	3.772036072600	4.862372650100
H	-0.068008649400	4.051118141300	5.158166833100
C	-2.947369307000	3.426970416100	2.579997078200
N	-3.153436162300	3.540971604500	3.958451411900
H	-2.450453439500	3.857454434100	5.900461128400
O	-3.882774719000	3.248829608300	1.798232321000
H	-4.120501307700	3.461478827700	4.248190381200
O	-0.565568202800	2.425562057100	0.262918596100
H	0.416470608800	2.691004415200	0.169671223400
C	-1.363815792300	3.516372982400	0.664783276800
H	-2.352653212300	3.432677029200	0.224105582400
H	-0.898512039500	4.473136423600	0.399481278700

$^{7}P_{H,3\text{-}meC}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.085901231200
C	1.076826180400	0.000000000000	2.888881984800
N	0.664271342900	-0.076794161700	4.179615942100
C	-0.729335230500	-0.122853227300	4.208767702700
C	-1.136643525900	-0.074282236800	2.902109554300
H	2.100071464600	0.095072539700	2.562428935300
H	1.271170687200	-0.077059122800	4.985256859600
H	-1.285569160100	-0.180021717900	5.127874808200
H	-2.122791019600	-0.087735148100	2.475679191400
N	0.026247275900	-2.092292988200	-0.300247660500
C	-0.911641710400	-2.975334878300	0.067636340300
N	-0.510607211200	-4.225897238200	-0.285830607500
C	0.733297210000	-4.139330003700	-0.908708196500
C	1.059667779700	-2.808311815800	-0.912350975600
H	-1.837569862000	-2.733365404700	0.557692416400
H	-1.030291466500	-5.075458943800	-0.125097337400
H	1.253399783100	-5.004050965600	-1.281882102100
H	1.928038222200	-2.307435388100	-1.296218887400
O	-1.306568941800	0.210463877300	-1.701535652800
C	-2.381625188800	-0.085605836300	-1.016988856400
O	-2.206977318100	-0.342516997900	0.240991954100
C	-3.729830548900	-0.096010167000	-1.657326693000
H	-4.425664053400	-0.699248321700	-1.071890015800
H	-3.665131721800	-0.471327513200	-2.681309287400
H	-4.124044568500	0.927390576300	-1.700301110000
C	-1.979710830100	2.927493036300	-3.512789167000
O	-1.080626261400	3.086997930300	-2.749786916200
O	-2.872968899500	2.768709983800	-4.271144144600
C	3.084366338700	0.439988226300	-0.056538083400
O	1.858663177600	-0.025774786300	-0.348714930400
C	4.133140197200	0.157538103000	-1.099360004100
H	4.306884303200	-0.923053916300	-1.168032749000
H	5.067701293200	0.652974568200	-0.836288594100
H	3.790836582500	0.497230266700	-2.081898140500
O	3.320678147700	1.033045802500	1.021014577500
H	2.532817811300	3.877053610300	3.244615965000
N	1.870240503400	3.378167850500	2.673473657900
C	0.530585943600	3.739509263900	2.721700324500
H	2.217576639500	2.556263344100	2.194553167200
C	-0.106946619400	4.270785110400	3.837345253900
N	-0.204833472000	3.731661742700	1.472638436800
C	-1.402089761600	4.767806856800	3.770817517200
H	0.428471994100	4.300566624000	4.778039506300

C	-1.544132162700	4.175579395900	1.384854430000
N	-2.086676448000	4.679284912500	2.538283137100
H	-1.940113336200	5.204274552100	4.596987447400
O	-2.171117626100	4.114204489100	0.301555181500
H	-3.038441004800	5.005145997100	2.456364638100
O	-0.145808515900	2.049972541400	-0.284109009400
H	-0.712195944900	2.227522802500	-1.068139853800
C	0.395952546300	3.348337275700	0.237537000500
H	0.166617115300	4.067700259700	-0.548802684400
H	1.464913735100	3.225272688800	0.365071787600

Adenine: ***Part 1: Epoxidation (DFT calculations in UB3LYP/LANL2DZ)***

$^{5}\mathbf{RE}_{\mathbf{E,\varepsilon A}}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.092250105600
C	1.099050008300	0.000000000000	2.850972886800
N	0.727806862400	0.127145677900	4.159989524700
C	-0.661951981700	0.219063098900	4.226417121600
C	-1.105571162400	0.137473741000	2.930564478300
H	2.112472756800	-0.019423591400	2.466643028300
H	1.362297364700	0.212775521700	4.938152952200
H	-1.189432462500	0.345766592700	5.156015725600
H	-2.099512534700	0.202115614400	2.526442688900
N	-0.397618276300	-2.023520361100	0.009120054200
C	-1.537421174300	-2.623384978700	0.361082131900
N	-1.399317159900	-3.973657437400	0.221604632400
C	-0.111945385600	-4.240054402400	-0.242308331000
C	0.502253606100	-3.019652942900	-0.369636269500
H	-2.425460192400	-2.117367422100	0.689391123100
H	-2.110878051700	-4.658710189800	0.418779800500
H	0.235056498100	-5.239714701200	-0.433736358300
H	1.494080008300	-2.756478372600	-0.687568312200
O	-1.190221148800	0.120120850800	-1.772660096500
C	-2.308165469900	0.256160018800	-1.118505394800
O	-2.275436671300	0.150042086100	0.167708201200
C	-3.580049383200	0.563113487900	-1.847204016900
H	-4.443977933400	0.370596084300	-1.210269700300
H	-3.644005153500	-0.022122154600	-2.767095628700
H	-3.571069954400	1.623178111800	-2.125119423400
C	-0.261472660900	2.578319220600	-2.772562194200
O	0.807255957800	2.174240993800	-3.088181914800
O	-1.325526254800	3.042041907500	-2.515286039800
C	2.952993753500	0.201493974200	-0.171638849100
O	1.821582670500	-0.503572325700	-0.339370994000
C	3.664818950900	0.570359905100	-1.448238390500
H	3.851479301800	-0.327188425700	-2.049330258700
H	4.607429082600	1.070873679400	-1.223053150200
H	3.019513694100	1.229958568700	-2.038480995300
O	0.276021376600	1.628292563000	-0.076045015400
O	3.390629553000	0.509729809700	0.959952240500
N	-0.026319696800	4.116563663000	7.220179988900
C	-1.335788646300	4.511660470700	7.450739232300
C	0.119766361000	4.007990914500	5.847704630900
H	-1.723668015500	4.678726551300	8.442155660600
N	-2.031102342400	4.655300677100	6.326593808900
C	-1.130585162800	4.348722580100	5.308184575200
N	1.246423827000	3.637931589200	5.170163922800
C	-1.259295260400	4.320732128000	3.898747457400
C	1.128736905100	3.618703674900	3.859585037300
N	-2.235402033600	4.547959900000	3.032064396700
N	-0.049024731900	3.938365534700	3.212714772800
H	1.970604044700	3.335221340700	3.242655912900
H	0.703105628900	3.968877217000	7.898970358600

C	-0.358295947300	3.943804109000	1.851940652300
H	0.341959671100	3.611944278200	1.105277535700
C	-1.679719414400	4.312017051400	1.772561349600
H	-2.273789682500	4.409017941900	0.881329193100

^{5}**TS$_{E,\varepsilon A}$**

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.125672828400
C	1.113193855900	0.000000000000	2.860246133200
N	0.774787697300	0.165393207400	4.175599405600
C	-0.612820648200	0.278598081400	4.268941788900
C	-1.083678704200	0.173929954200	2.983611010000
H	2.116791240200	-0.063666432700	2.460196788500
H	1.425969116600	0.220863198900	4.941365428700
H	-1.117042034700	0.438030937200	5.205824950900
H	-2.085470736400	0.244423827900	2.598295578500
N	-0.739958785100	-2.074389871400	0.082568146300
C	-1.980522308000	-2.488344628200	0.342923035600
N	-2.018547148500	-3.856156356600	0.349198353400
C	-0.734697782800	-4.329398916000	0.077774233700
C	0.048646048700	-3.213476432200	-0.085323697000
H	-2.822032564500	-1.841422134300	0.516129169000
H	-2.835203221400	-4.421325285900	0.515822419100
H	-0.508523762800	-5.380026574200	0.024506898200
H	1.094836776600	-3.113348978900	-0.308538183800
O	-1.091538285200	0.154577936000	-1.850726473800
C	-2.221904183600	0.436788392500	-1.271856145500
O	-2.280368877900	0.405838096500	0.019247673900
C	-3.420228492000	0.797572844900	-2.104941167200
H	-4.296858354200	0.943654201500	-1.472158662800
H	-3.615075700900	0.014198394400	-2.844613916000
H	-3.210600157700	1.716311511300	-2.663107677500
C	-0.006712060900	0.880416635200	-4.189793788000
O	1.039298216200	0.382979401600	-3.932004536200
O	-1.013332937100	1.406889669900	-4.539478429000
C	2.975278172300	-0.362440369800	-0.288474922000
O	1.734625972400	-0.836013714900	-0.317959406000
C	3.777738571500	-0.614910083600	-1.546874029000
H	3.858577521500	-1.693607100600	-1.722227713200
H	4.776494026100	-0.184616014100	-1.457494997500
H	3.250783166000	-0.188500629800	-2.406706657300
O	0.495042775900	1.648965453400	-0.108390598700
O	3.467696440700	0.224894495000	0.710884974500
N	2.859561193000	3.682246216800	5.468754150700
C	1.717732597800	4.253516890000	6.015601256300
C	2.621247337000	3.534344621900	4.114839903700
H	1.634450918600	4.488175263000	7.063922794100
N	0.771587119000	4.469885531200	5.107835827200
C	1.323590410200	4.030574197100	3.904258813400
N	3.462302795900	2.990485013800	3.190609193500
C	0.847258138800	4.025112272500	2.577188180300
C	3.006826846900	2.963116473900	1.954015864100
N	-0.272311358500	4.441554861800	1.972132269200
N	1.770776102400	3.487466063700	1.618385247600
H	3.573928865900	2.468243117700	1.178735332900
H	3.722743493600	3.454634839300	5.936433812800
C	1.131884366200	3.552435886800	0.369530660600
H	1.690368664100	3.472906861400	-0.544536387200
C	-0.092040573500	4.193747850100	0.633861175700
H	-0.857020901700	4.431049021100	-0.085801495800

Adenine: *Part 2: Hydroxylation*

^{5}**RE$_{H,1\text{-}meA}$**

Fe	1.871721000000	0.242769000000	0.176629000000

N	2.086584000000	2.294629000000	0.116419000000
C	1.785816000000	3.098652000000	-0.909344000000
N	1.996015000000	4.403307000000	-0.539412000000
C	2.448308000000	4.417893000000	0.784754000000
C	2.498873000000	3.094578000000	1.184283000000
H	1.426827000000	2.778457000000	-1.873537000000
H	1.849494000000	5.213569000000	-1.127590000000
H	2.684641000000	5.328470000000	1.310054000000
H	2.782317000000	2.657716000000	2.127708000000
N	3.748128000000	0.075107000000	-0.661172000000
C	4.915510000000	0.414768000000	-0.092398000000
N	5.945100000000	0.112346000000	-0.943829000000
C	5.405705000000	-0.446626000000	-2.107557000000
C	4.036823000000	-0.463425000000	-1.919216000000
H	5.028661000000	0.840469000000	0.890189000000
H	6.927735000000	0.261589000000	-0.754016000000
H	6.014399000000	-0.775586000000	-2.933421000000
H	3.247334000000	-0.807522000000	-2.563295000000
O	2.272943000000	-1.552763000000	1.149756000000
C	2.881580000000	-1.029432000000	2.189310000000
O	3.053094000000	0.255378000000	2.184854000000
C	3.326982000000	-1.905943000000	3.329862000000
H	4.289843000000	-1.561509000000	3.719819000000
H	3.388966000000	-2.949145000000	3.012521000000
H	2.593935000000	-1.830509000000	4.143923000000
C	1.760935000000	-4.040468000000	0.203945000000
O	1.195606000000	-3.595302000000	-0.747494000000
O	2.315044000000	-4.544000000000	1.131759000000
C	-0.008922000000	-0.465192000000	-2.091084000000
O	1.202253000000	-0.177396000000	-1.608689000000
C	-0.000863000000	-1.489847000000	-3.214362000000
H	0.702788000000	-1.187338000000	-3.998349000000
H	-1.000656000000	-1.604353000000	-3.639943000000
H	0.343414000000	-2.447778000000	-2.806900000000
O	0.421307000000	0.363892000000	0.946217000000
O	-1.081902000000	0.053800000000	-1.671149000000
N	-7.546645000000	-0.261075000000	-1.237392000000
C	-8.313187000000	-0.167732000000	-0.070746000000
C	-6.225228000000	-0.103300000000	-0.869468000000
H	-9.388819000000	-0.256672000000	-0.073722000000
N	-7.565126000000	0.039074000000	1.014488000000
C	-6.258041000000	0.081188000000	0.527185000000
N	-5.101234000000	-0.118538000000	-1.640551000000
C	-5.034370000000	0.269555000000	1.209198000000
C	-3.972126000000	0.062999000000	-0.970204000000
N	-4.978081000000	0.448285000000	2.546013000000
N	-3.901432000000	0.258832000000	0.419285000000
H	-3.011597000000	0.054992000000	-1.484802000000
H	-4.112601000000	0.571155000000	3.053666000000
H	-5.852286000000	0.443081000000	3.060718000000
H	-7.888070000000	-0.417460000000	-2.178961000000
C	-2.555692000000	0.453271000000	1.042614000000
H	-1.789499000000	0.437699000000	0.265392000000
H	-2.343880000000	-0.361115000000	1.743816000000
H	-2.520215000000	1.421533000000	1.554794000000

$^{5}TS_{H,1\text{-}meA}$

Fe	1.512772000000	-0.116101000000	-0.116625000000
N	2.319753000000	-1.975252000000	-0.640898000000
C	2.260516000000	-3.084467000000	0.112337000000
N	2.873640000000	-4.113297000000	-0.552986000000
C	3.335141000000	-3.635155000000	-1.785495000000
C	2.980107000000	-2.300093000000	-1.830183000000
H	1.762605000000	-3.154732000000	1.069462000000
H	2.975262000000	-5.058330000000	-0.205111000000
H	3.850143000000	-4.258800000000	-2.497379000000

H	3.112301000000	-1.573525000000	-2.614370000000
N	3.481526000000	0.673148000000	0.251333000000
C	4.443080000000	0.941147000000	-0.647708000000
N	5.545312000000	1.447021000000	-0.010384000000
C	5.273292000000	1.505209000000	1.360406000000
C	3.988057000000	1.019991000000	1.510032000000
H	4.361645000000	0.794923000000	-1.711353000000
H	6.406130000000	1.733181000000	-0.459054000000
H	5.984076000000	1.874046000000	2.081262000000
H	3.391970000000	0.896170000000	2.396792000000
O	0.921394000000	1.836466000000	-0.719631000000
C	1.372244000000	1.699206000000	-1.946829000000
O	1.959160000000	0.575908000000	-2.227147000000
C	1.192007000000	2.796676000000	-2.959232000000
H	1.839294000000	2.630958000000	-3.823366000000
H	1.401875000000	3.770025000000	-2.504422000000
H	0.148862000000	2.805380000000	-3.301758000000
C	-0.439008000000	3.950001000000	0.460070000000
O	0.412691000000	4.722507000000	0.159315000000
O	-1.326046000000	3.216662000000	0.778148000000
C	0.650709000000	-0.993395000000	2.651665000000
O	1.379153000000	-0.225501000000	1.828182000000
C	0.418930000000	-0.399535000000	4.030523000000
H	1.378118000000	-0.303938000000	4.554608000000
H	-0.246706000000	-1.040178000000	4.613142000000
H	-0.005462000000	0.607061000000	3.941516000000
O	-0.193672000000	-0.641313000000	-0.445256000000
O	0.211655000000	-2.132390000000	2.322282000000
N	-6.947291000000	0.147683000000	-0.479596000000
C	-6.611462000000	1.432936000000	-0.044753000000
C	-5.790524000000	-0.603445000000	-0.446246000000
H	-7.335727000000	2.229248000000	0.031831000000
N	-5.315077000000	1.543456000000	0.255075000000
C	-4.792798000000	0.273796000000	0.013467000000
N	-5.596166000000	-1.910405000000	-0.806630000000
C	-3.451530000000	-0.194730000000	0.123551000000
C	-4.359015000000	-2.331511000000	-0.652783000000
N	-2.419157000000	0.574327000000	0.453801000000
N	-3.285441000000	-1.558166000000	-0.171697000000
H	-4.116624000000	-3.360236000000	-0.891250000000
H	-1.435192000000	0.271156000000	0.263395000000
H	-2.576317000000	1.558543000000	0.663149000000
H	-7.862814000000	-0.178171000000	-0.768008000000
C	-2.010318000000	-2.224264000000	0.083513000000
H	-1.961344000000	-3.198734000000	-0.402943000000
H	-1.710917000000	-2.227261000000	1.135829000000
H	-0.964173000000	-1.530678000000	-0.387015000000

Guanine: ***Part 1: Epoxidation (DFT calculations in UB3LYP/LANL2DZ)***

^{5}**RE**$_{E,\varepsilon G}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.070168043900
C	1.096700496300	0.000000000000	2.829400405600
N	0.726133445500	0.109208017800	4.137727552200
C	-0.663668416100	0.191127720500	4.203834766900
C	-1.108587414200	0.121536527700	2.906833158800
H	2.108697262100	-0.010159426300	2.457187569300
H	1.359841769800	0.176367390200	4.918647631900
H	-1.189898626600	0.301359285000	5.135687021800
H	-2.102776184500	0.170833478100	2.499438933400
N	-0.218717596900	-2.052445711600	0.053316495200
C	-1.281840338500	-2.734166772600	0.487020373500
N	-1.025441692900	-4.071283584000	0.400135553000
C	0.259094254800	-4.243057912500	-0.115567054300
C	0.751608575300	-2.980302418600	-0.327165511600
H	-2.199469081000	-2.295359306200	0.834502243100
H	-1.661026669600	-4.807427843800	0.662489763400
H	0.689142134600	-5.215351672600	-0.279849596500
H	1.699203005400	-2.646807133300	-0.706728013300
O	-1.124020599800	-0.015824236000	-1.761654000900
C	-2.293481647900	-0.000518644300	-1.181586944800
O	-2.332062811100	-0.060216279300	0.105856907400
C	-3.534308968200	0.105159206000	-2.016288977700
H	-4.422754442900	-0.058858222000	-1.405183266500
H	-3.500391059400	-0.615852495100	-2.838558881900
H	-3.576237203200	1.106967593600	-2.458282224900
C	-0.254505279900	2.351542188500	-3.019695606900
O	0.868697406700	1.999194453800	-3.166676624000
O	-1.368689762700	2.750651518900	-2.923888387200
C	2.950735756000	0.380672792200	-0.340616456200
O	1.859668371500	-0.378960805100	-0.408487446800
C	3.703177215000	0.543299017000	-1.637979684200
H	3.906104061400	-0.437521623200	-2.080629647900
H	4.638773854500	1.078763642300	-1.472172102200
H	3.071360201000	1.095059506400	-2.342687488900
O	0.130371835700	1.644569509200	-0.057522347000
O	3.341906950500	0.902253119000	0.734606888800
N	2.860839122100	2.813009740400	2.682178379700
C	3.347821326600	2.967687851800	3.948307127800
N	2.367155126300	3.668670330700	4.658697081900
C	4.621608784500	2.850651970500	5.761160928700
C	2.455260257100	4.006384654800	6.062915409300
O	1.508592699600	4.601659191700	6.612942677300
C	1.282461131800	3.936492171100	3.801064842400
H	0.422885627000	4.473454605500	4.157091623900
C	1.591702515500	3.399107020600	2.589462054000

H	1.022348348400	3.343081984200	1.676704118500
N	4.206452869100	3.641263129200	7.886089531900
N	4.501115415800	2.526293375900	4.447033462000
C	5.386717118700	3.051206752400	7.851147577200
H	6.062014351900	2.951330956400	8.684601001500
N	5.689247819300	2.549886936100	6.581791829400
H	6.527984345900	2.075121949000	6.289573034200
C	3.701450969100	3.535151669200	6.583562811800
H	3.290100011700	2.239082107300	1.953766915900

$^{5}TS_{E,\varepsilon G}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.122770766000
C	1.096350981900	0.000000000000	2.880587268300
N	0.746526126700	0.258189960200	4.175744152000
C	-0.634930929700	0.433224211100	4.235005930500
C	-1.090238529700	0.267826321600	2.949602782200
H	2.104551000000	-0.128875926200	2.527854728200
H	1.393261129900	0.380862266700	4.938161964400
H	-1.146676641800	0.669592308500	5.151392401800
H	-2.082122410400	0.351628656100	2.541409259600
N	-0.616757995100	-2.106572606200	0.121841754500
C	-1.817700322900	-2.575754318000	0.463385748500
N	-1.786449774300	-3.942488819200	0.496126825600
C	-0.499687943200	-4.357860663300	0.156021073000
C	0.216379826100	-3.209144761600	-0.072833961300
H	-2.679648439800	-1.968609596000	0.674247458500
H	-2.561882071900	-4.543275989300	0.722896818100
H	-0.224227916000	-5.396332194300	0.107829338200
H	1.241906108500	-3.064340004000	-0.357284521200
O	-1.096372335100	0.086844367600	-1.830565834500
C	-2.245435602200	0.294376413300	-1.254859687200
O	-2.295875517500	0.282977039200	0.036923617700
C	-3.471417133900	0.526086989700	-2.091560609100
H	-4.324828948800	0.775758756900	-1.458481822200
H	-3.696262155200	-0.370045971400	-2.680951086400
H	-3.283611744700	1.335941339300	-2.803576557600
C	-0.216316671900	-0.033771128500	-4.373691327400
O	0.846526324300	-0.435026576300	-4.030687924400
O	-1.251174472400	0.357513803500	-4.806171457300
C	3.002164479000	-0.336025785900	-0.661851637900
O	1.778991045800	-0.757169565500	-0.381981625500
C	3.654415682100	-1.020209939100	-1.843850634300
H	3.697756076200	-2.102003580100	-1.675544235400
H	4.662301001300	-0.632232418100	-2.000944107400
H	3.040093355400	-0.855057637900	-2.735679480300
O	0.395853703400	1.674964163500	-0.062597932900
O	3.623602303400	0.544991015200	-0.004537908500
N	2.531255764300	2.752820756800	1.104594872900
C	2.378258392900	3.115917436000	2.407090188200
N	1.286093875000	4.004815213000	2.450075516100
C	2.660831183700	3.331899403600	4.602068934700
C	0.798503825300	4.649264866400	3.654412133700
O	-0.176002896100	5.416824850400	3.589032955500
C	0.774093733700	4.153834437500	1.165696565300
H	-0.060347785000	4.800517400000	0.969190216800
C	1.509435096700	3.315223850500	0.328300477100
H	1.590709293700	3.376231149300	-0.741041251400
N	1.509162332100	4.634229988500	6.109127500800
N	3.085026003300	2.722417503600	3.461477818900
C	2.476576626600	3.986018372000	6.730419842700
H	2.706423287300	4.057080225600	7.780301519300
N	3.203695691800	3.166846844900	5.860272280100
H	4.032882878400	2.633970783400	6.067071360700
C	1.601116573700	4.242391869100	4.768492153800
H	3.090449352200	1.945125396800	0.775756327000

Guanine: ***Part 2: Hydroxylation***

^{5}**RE**$_{\mathbf{H,1-}meG}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.072578643000
C	1.097720252500	0.000000000000	2.832027125000
N	0.726946949900	0.143390459000	4.137802959200
C	-0.661543730600	0.245547892200	4.201466892200
C	-1.106273407300	0.155815334100	2.905871354100
H	2.109680650800	-0.035016991300	2.453747850800
H	1.360311076200	0.214230905200	4.918244638200
H	-1.186987107100	0.385195312100	5.129759458400
H	-2.098913961400	0.220793986100	2.497305398400
N	-0.366390937300	-2.030789336300	0.016042441100
C	-1.484708853700	-2.639973397500	0.417245365100
N	-1.332983677400	-3.989889717600	0.290740084400
C	-0.059437401300	-4.246088177200	-0.217186649100
C	0.533131904400	-3.020108746100	-0.383127637900
H	-2.370063496100	-2.140790591300	0.767035074900
H	-2.027957419800	-4.681312027200	0.522139979800
H	0.295006936500	-5.243575638900	-0.408474255900
H	1.508292957600	-2.750706874200	-0.743271344900
O	-1.115165385400	0.114773884800	-1.775258449800
C	-2.273572796600	0.225885982200	-1.185355284800
O	-2.309404157300	0.130456870100	0.101273378000
C	-3.503589696700	0.489568221200	-1.999758602600
H	-4.401471844300	0.329400096900	-1.401272110400
H	-3.517237507100	-0.148896713900	-2.887479221000
H	-3.478608232900	1.530897365900	-2.340986257700
C	-0.045504286000	2.536834174000	-2.892282738200
O	1.052871893100	2.120577322400	-3.059745377700
O	-1.132202860600	3.000915696900	-2.777697754900
C	2.977911186900	0.157631924900	-0.294239151700
O	1.835624466800	-0.505479844900	-0.416795174400
C	3.746758258700	0.370077446100	-1.574754931000
H	3.891651490100	-0.586507256800	-2.087668728000
H	4.713604562200	0.833391293000	-1.372643841000
H	3.155568518400	1.008019265400	-2.240761850700
O	0.265329190000	1.627028018000	-0.032861806600
O	3.406272653200	0.558885838100	0.822430406700
N	5.087896512300	2.153764458300	2.455538607500
C	4.791703408700	3.020459090200	3.457288673700
N	3.584011601900	3.705956634500	3.411534569200
C	5.322650660300	4.047851127300	5.397604646100
C	3.144991480500	4.624608416400	4.452338168100
O	2.031409166300	5.179643654500	4.359015354700
N	4.110209091300	5.556925989200	6.636011941100
N	5.693490292400	3.165951643000	4.437935401000
C	5.268784386700	5.324471649000	7.227012061900
H	5.604598478000	5.771572453900	8.147785288600
N	6.049032893700	4.407420361300	6.513448537600
H	6.969210122500	4.068969989500	6.743140281600
C	4.125412674700	4.763622832500	5.481827660200
H	5.984735065300	1.701527652900	2.536609864300
H	4.431004857000	1.782454024200	1.772736405300
C	2.703037841300	3.571675507600	2.235820699000
H	3.246730452300	3.845778390400	1.326731055000
H	2.325735373500	2.552845098000	2.126365397400
H	1.866456566500	4.251128473900	2.389539318000

^{5}**TS**$_{\mathbf{H,1-}meG}$

Fe	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	2.143383170200
C	1.117466093600	0.000000000000	2.872512562200

N	0.806420844500	0.314232372900	4.165673843300
C	-0.569665711100	0.524756492900	4.252804455100
C	-1.060780469500	0.325633409300	2.986573105700
H	2.111788077500	-0.150238242300	2.481469656400
H	1.470445735400	0.424030685400	4.915302796700
H	-1.051106923200	0.818668529300	5.167803389300
H	-2.059471241000	0.431329066400	2.601399896600
N	-0.802133583000	-2.045898156400	0.094969609200
C	-2.054913735100	-2.402329718600	0.387890007100
N	-2.156220502000	-3.765714190900	0.392567924500
C	-0.902239975100	-4.298535025700	0.087445919800
C	-0.070320124500	-3.220594507900	-0.094492211300
H	-2.860517213200	-1.715689833700	0.583060426800
H	-2.992194736200	-4.292888941500	0.582852909600
H	-0.727353328500	-5.358900929300	0.029233397200
H	0.975786619300	-3.172036760300	-0.343289816400
O	-1.053285342800	0.274718989800	-1.827417498100
C	-2.182892891600	0.579150963200	-1.256592494500
O	-2.256959406400	0.478374673200	0.031151237500
C	-3.342109446400	1.046568582800	-2.087884417400
H	-4.237376679100	1.160195711400	-1.472457591400
H	-3.530591973500	0.342163518500	-2.904445837100
H	-3.087615717200	2.008339887200	-2.545559708600
C	0.117581004000	1.271687960700	-4.029981979300
O	1.134814331300	0.684973386800	-3.855238201400
O	-0.859033325900	1.901132941900	-4.289273763300
C	2.936487809200	-0.400441294600	-0.430284061100
O	1.697977231300	-0.879671129000	-0.415812085400
C	3.735263421200	-0.739768169100	-1.672688896400
H	3.723070329500	-1.825474698700	-1.840793080900
H	4.764980332900	-0.390516516900	-1.572640413900
H	3.259402050500	-0.270295978000	-2.545449372800
O	0.611662550700	1.645843924000	0.006126984900
O	3.432320483900	0.270205991900	0.516814428800
N	3.679685104400	2.647748584200	2.015832417700
C	2.883632268500	3.194156321500	2.973315116600
N	1.617833441700	3.656276640300	2.588766135200
C	2.471899451200	3.813876305400	5.108045840900
C	0.602711780800	4.097715051600	3.558067613000
O	-0.540578952400	4.378472922100	3.161333992000
N	0.545271737200	4.619137176100	6.063926760900
N	3.348877142800	3.278897643400	4.221409440700
C	1.496670989400	4.539505720200	6.979830708600
H	1.398406234300	4.817955764800	8.009777070000
N	2.692130824600	4.044969452200	6.452507246900
H	3.572346513300	3.918503481600	6.923567938000
C	1.139963927200	4.171081520900	4.879336713000
H	4.599343620000	2.386876527800	2.340505346900
H	3.320753971500	2.058659558600	1.261759048400
C	1.288275619700	3.780037290400	1.199735326100
H	2.148683647600	4.094110649100	0.605729041600
H	0.946978785000	2.661263155900	0.653897498400
H	0.389705972200	4.389561199200	1.078518984000