Electronic Supplementary Information (ESI)

MD Simulations and QM/MM Calculations Show that Single-Site Mutations of Cytochrome $P450_{BM3}$ Alter the Active Site's Complexity and the Chemoselectivity of Oxidation Without Having Changed the Active Species

Kshatresh Dutta Dubey[†], Binju Wang[†], Manu Vajpai[‡] and Sason Shaik[†]*

[†]Institute of Chemistry and The Lise Meitner-Minerva Center for Computational Quantum Chemistry, The Hebrew University of Jerusalem, 91904, Jerusalem, Israel.
[‡]Department of Biological Sciences and Bioengineering, Indian Institute of Technology-Kanpur, Kanpur-208016, (UP), India.

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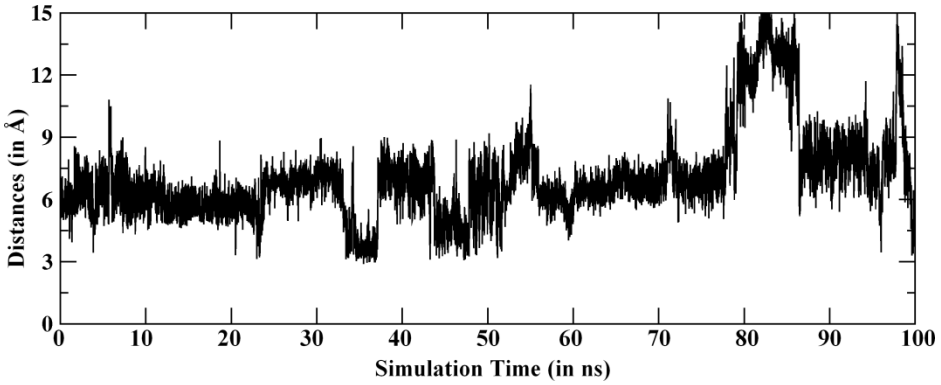

Figure S1. The distance of O_d—S (**Sub1**) during MD simulations of Cpd 0. The MD simulations show a very dynamic nature of **Sub1** in Cpd 0 state of $P450_{BM3}$.

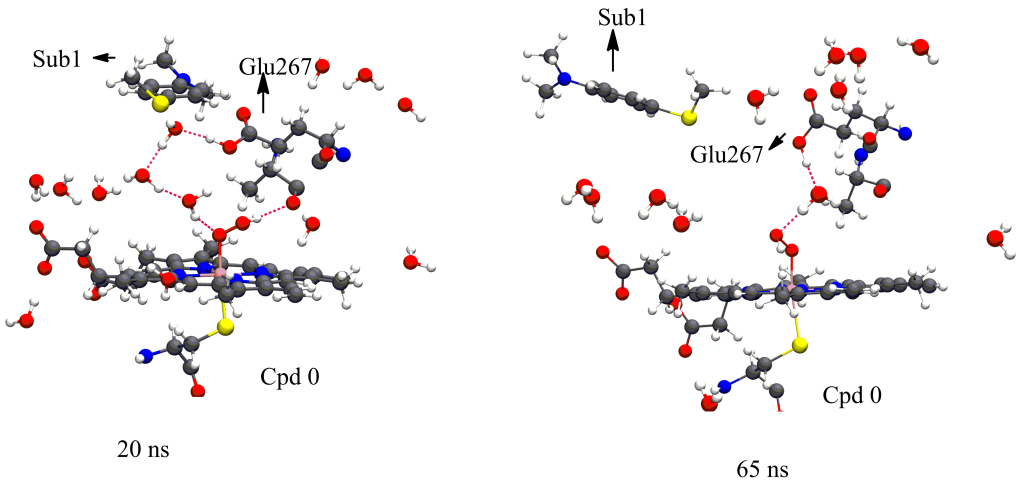

Figure S2. Two typical snapshots taken from MD simulation of **Sub1** with Cpd 0 at two entirely different time scales. We can see that organized water channels are connecting Cpd 0 to the protonated Glu267. These water channels were persistent during entire simulation.

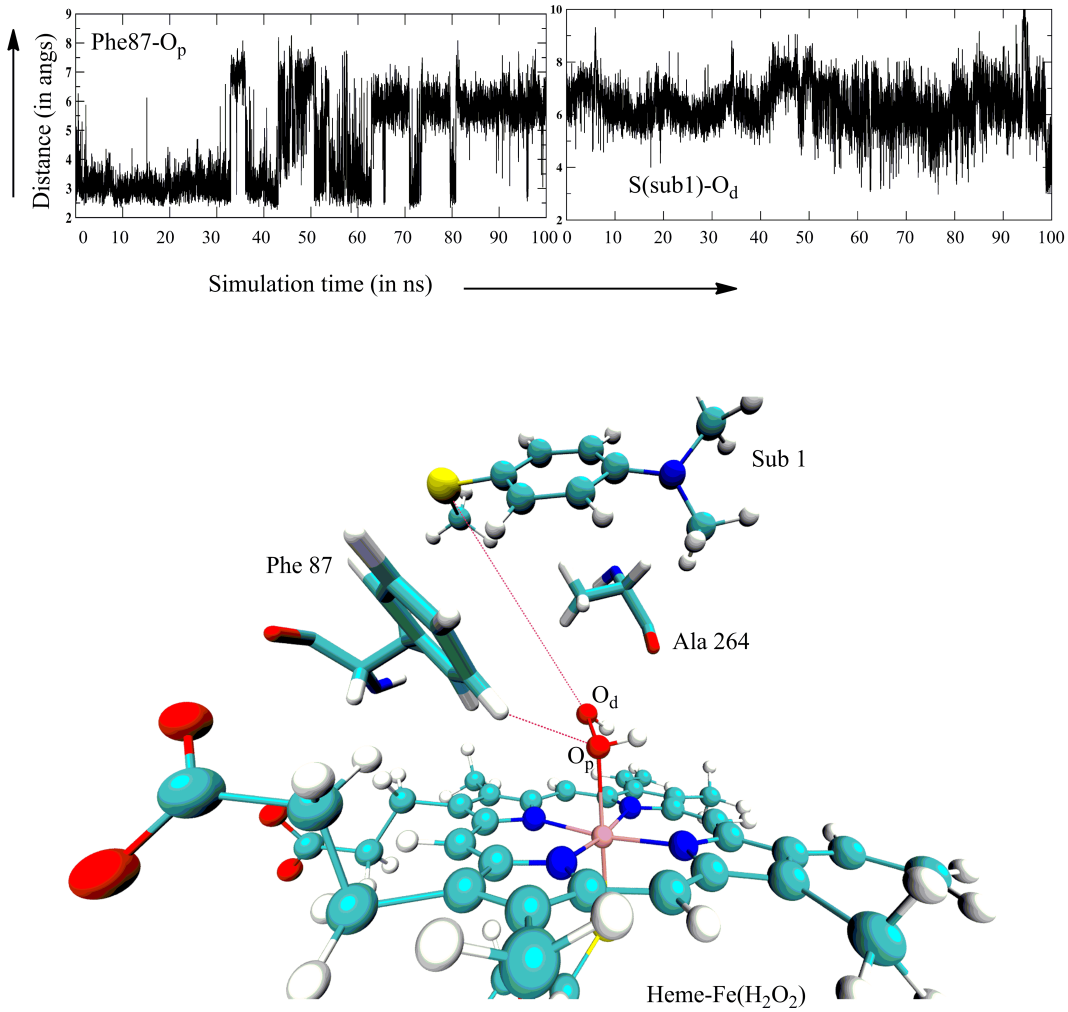

Figure S3. The dynamics of **Sub1** in Fe(H_2O_2). Note that **Sub1** lies away from Fe(H_2O_2) at most of the time of simulation. The bulky residue Phe87 which may restrict the dynamics of H_2O_2 also lies distant.

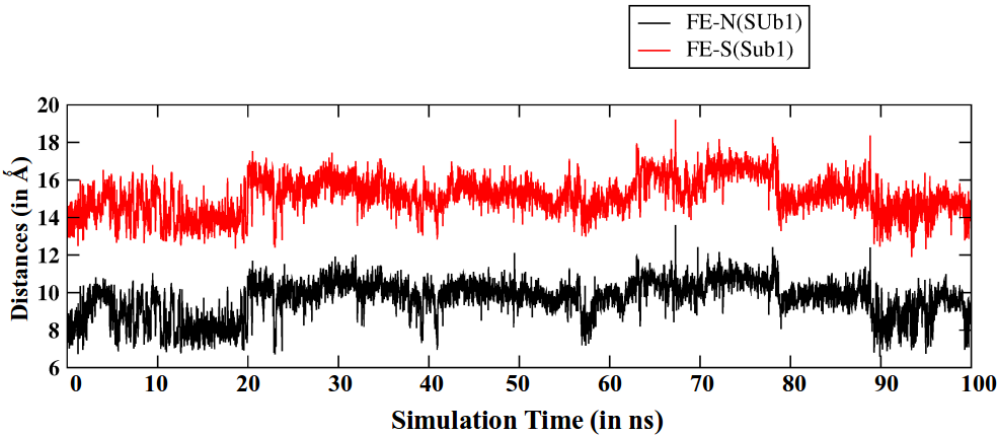

Figure S4. Distance fluctuation of Fe---N(**Sub1**) and Fe---S(**Sub1**) in the flipped orientation of substrate (starting from N(CH_3) pointing towards Cpd I)**.** Note the distances of both ends are too long to show any activity, therefore this model does not constitute a good starting model to mimic the experimental observations

Table S1. Spin and charge density for the QM system.

Spin	Fe	O	Por	SH	Substrate	Sub-H	H(sub)
^{2}RC(minor)	1.4722	0.6584	-0.1542	-0.0395	-0.9371	-0.939	0.0019
^{2}TS$_H$(minor)	1.6274	0.3816	-0.1371	-0.0621	-0.8092	-0.7736	-0.0363
^{2}TS$_S$(minor)	1.8134	0.0345	-0.1859	-0.1295	-0.5323	-0.5312	-0.0011
^{2}RC(major)	1.3341	0.8077	-0.8979	-0.199	-0.0445	-0.0444	-0.0001
^{2}TS$_S$(major)	1.7034	0.2589	-0.2923	-0.2061	-0.4627	-0.4628	-0.0005
^{2}TS$_H$(major)	1.6709	0.2731	-0.1386	-0.0702	-0.735	-0.6976	-0.0374

Charge	Fe	O	Por	SH	Substrate	Sub-H	H(sub)
^{2}RC(minor)	0.1202	-0.6478	0.3772	-0.7611	0.9118	0.7238	0.1879
^{2}TS$_H$(minor)	0.0572	-0.6394	0.4627	-0.6657	0.7851	0.471	0.3141
^{2}TS$_S$(minor)	0.0262	-0.5575	0.6543	-0.6011	0.4785	0.3496	0.1289
^{2}RC(major)	0.0715	-0.5063	0.9545	-0.5726	0.0535	-0.0536	0.1071
^{2}TS$_S$(major)	0.0494	-0.5695	0.5995	-0.5305	0.4509	0.342	0.1089
^{2}TS$_H$(major)	0.0231	-0.6493	0.3772	-0.5734	0.726	0.3618	0.3608

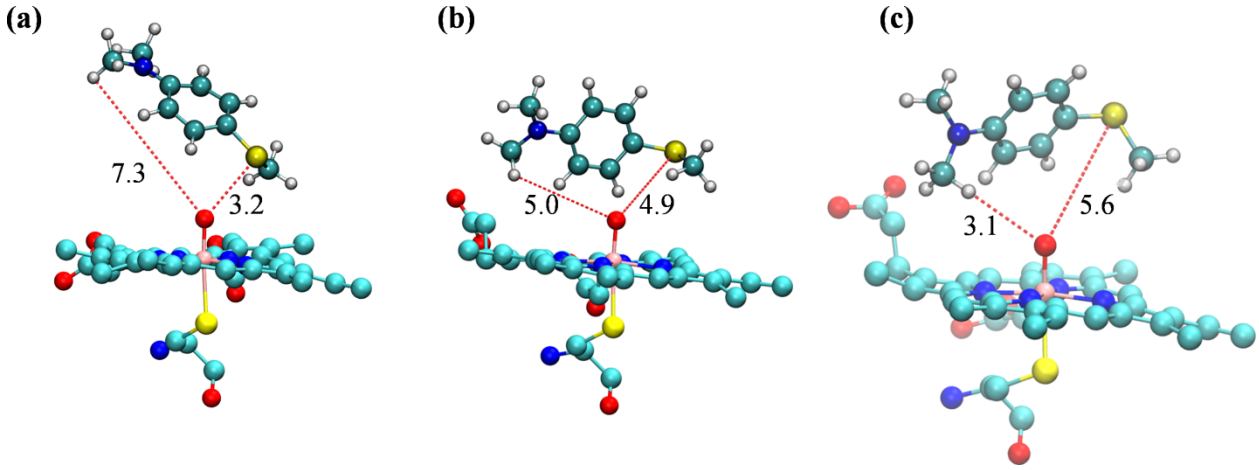

Figure S5. Representative snapshots of three most populated clusters out of ten clusters of MD trajectories of WT. The most populated cluster is shown in (a), while (b) and (c) show two lesser populated clusters, in respective order.

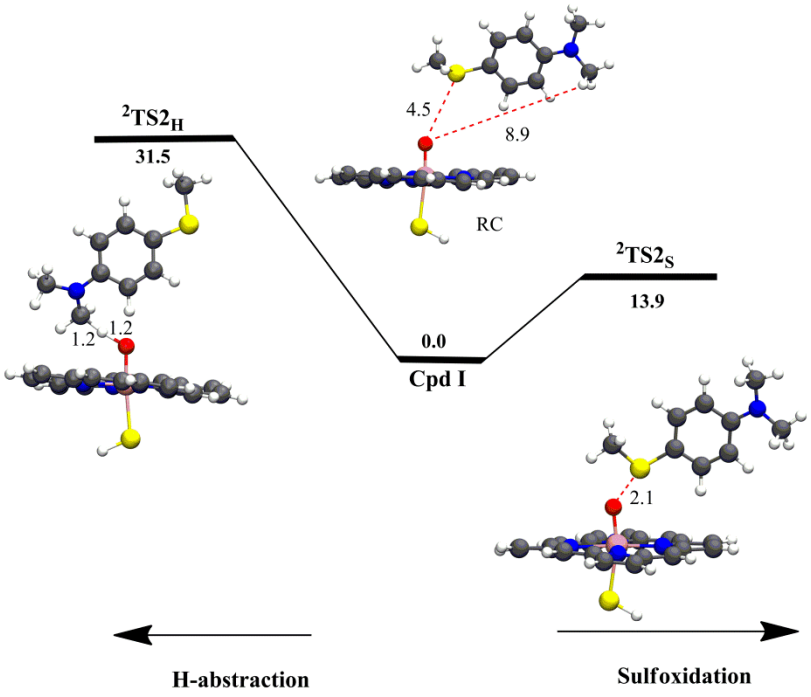

Figure S6. QM(B2)/MM calculated energy profile (in kcal/mol) for the sulfoxidation and hydroxylation in another snapshot from the major basin in WT enzyme.

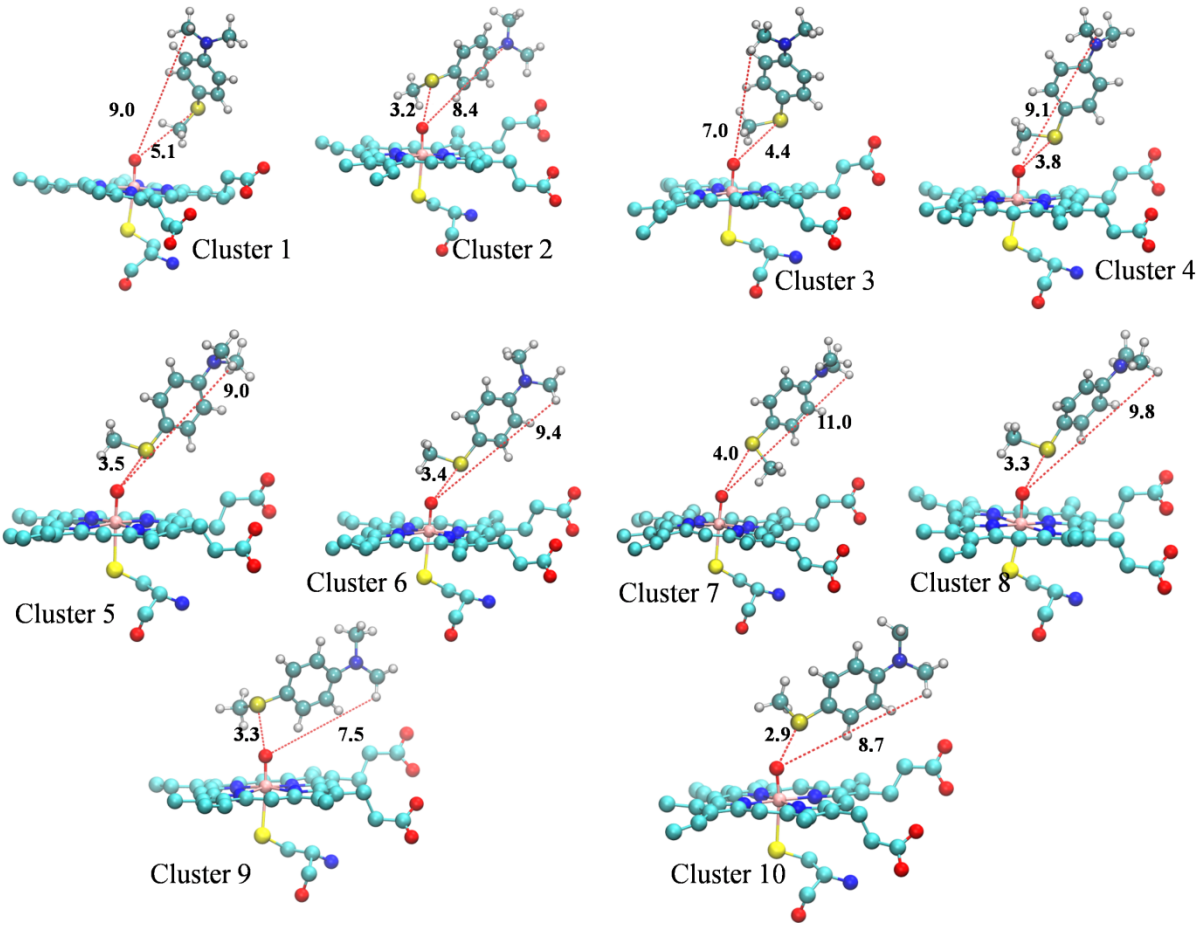

Figure S7. The structure of representative snapshots of all ten clusters in T268A mutants.

Calculation of population of the Minor and Major Basin: The S—O and H—O distances were calculated by in-built Cpptraj module of Amber 14. The population of major and minor basin was calculated by in-house python script where a cutoff of 2.7 for S—O and H—O distances were taken.

Water permeability calculations: Number of waters permeated

WT: 5

MUTANT: 5

Calculation protocol: The pore forming the water channel traverses the protein in a twisted manner and a permeation event occurs when a water molecule enters the channel from one end of the pore and exits from the other, at a later time. To measure this permeation, a virtual cylinder is constructed across the channel, as has been shown previously for water channels[1] and numbers of water molecules exiting and entering this channel are monitored in the simulation, in

this case using our in-house program. The axis of this cylinder has been chosen to be the line joining the C-alpha atoms of residue 72 and 267, with a total cylinder length of 20Å, based on the observations on the water file behavior. This axis rotates along with the protein, which can change its orientation in the simulation box, ensuring the correct enveloping of the water file.
The radius of the cylinder has been chosen to be 10Å to ensure that it is large enough to encapsulate the twisted pore, without extending to bulk waters. The waters present in this cylinder, and hence the channel, are updated in every frame of the simulation and entering and exiting waters are monitored to register permeation events. A total of 5 permeation events have been observed for the wild-type protein and 5 for the mutant protein, indicating that there is no difference in the outright permeation behavior of the two channels.

1. Zhu, F.; Tajkhorshid, E.; Schulten, K. *Biophys J*, **2004,***86*, 50-57.

Kinetic Isotope Effects (KIEs) in WT and T268A MT Enzymes

As we mentioned before, Voltz et al [Ref. 6, text] showed experimentally that even though the T268A mutation affected the S/Me oxidative ratio, the mutation did not affect the intrinsic kinetic isotope effect for H-abstractions ($KIE_{H/D}$ ~2 for both WT and T268A MT enzymes). This has been taken as an indication that Cpd I coexists with Cpd 0, and while Cpd I performs H-abstraction under all conditions, Cpd 0 performs sulfoxidation in the WT and the MTs. However as we showed in the text, sulfoxidation is performed by Cpd I with a tiny barrier, while variations in the yield of the sulfoxide product in the MTs arise from changes in the active site and the water pathways. To verify the experimental observation of constant KIE, we performed the KIE calculations for the H-abstraction process in both WT and T268A MT enzymes using the QM/MM method. Specifically, the KIE of the H-abstraction process was determined using the QM/MM frequency data based on the semi-classical Eyring equation. To the semiclassical KIE we added a Wigner correction due to tunneling. The resulting KIE of the C-H abstraction are indeed, virtually identical for the WT and MT enzymes; 1.69 (1.74) for the minor basin of WT and 1.62 (1.68) in the T268A MT where values in parenthesis are Wigner corrected ones (see below for details, page S9). These results are in a reasonably good agreement with the experimental data in Scheme 2 (text). Furthermore, since the S/Me oxidation ratio in T268A mutant is 60, it means that the maximum experimental yield of C-H hydroxylation for the

MT is 1.6%. As this yield is very tiny and as the KIE is rather small, the deuteration of the methyl groups of **Sub 1** does not affect the experimental S/Me ratio[6] within the accuracy of yield determination. Thus, the KIE calculations further support the conclusion that Cpd I is the sole oxidant in both WT and T268A mutant enzymes. The KIE is determined by the structure of the transition state, which is common to the WT and the MTs, and hence insensitive to the modifications in the active site.

KIE Calculations Details:

KIE of the H-abstraction process wasdetermined using the QM/MM frequency data based on the semi-classical Eyring equation, where the KIE is given as**:**

$$\left(\frac{k_H}{k_D}\right) = exp\left[\frac{-\left(G_H^{\#} - G_H^R\right) - \left(G_D^{\#} - G_D^R\right)}{RT}\right]$$

To the semiclassical KIE we added a Wigner correction due to tunneling using:

$$\left(\frac{K_H}{K_D}\right)_W = Q_w^{corr}\left(\frac{k_H}{k_D}\right)$$

here $Q_w^{corr} = (1 + u_t^2/24)/(1 + u_t'^2/24)$

Where $u_t = h\nu_H/k_BT$ and $u_t' = h\nu_D/k_BT$ where ν is imaginary frequency of transition state.

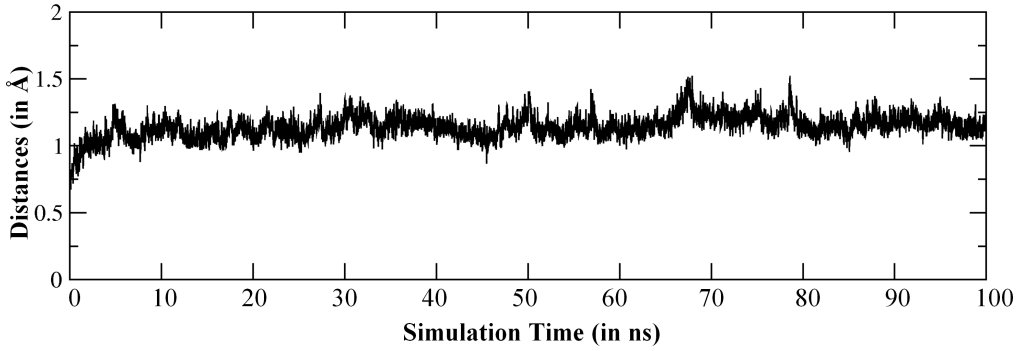

Figure S8. The root mean square deviations for protein during 100 ns. Note that MD trajectory is virtually constant with simulation time which shows a well converged MD simulation.

Table S2: The calculations of enthalpy changes upon binding for pose 1 and pose 2 using MMPBSA. All energy values are in kcal/mol.

Energetics for Pose 1		
Parameters	**Values**	**Standard Deviations**
ΔE_{int}	0.00	0.00
ΔE_{vdw}	-22.59	1.88
ΔE_{ele}	-1.42	1.41
ΔG_{polar}	5.35	2.03
$\Delta G_{non\text{-}polar}$	-3.15	0.26
$\mathbf{\Delta H_{total}}$	**-21.82**	2.58

Energetics for Pose 2		
Parameters	**Values**	**Standard Deviations**
ΔE_{int}	0.00	0.00
ΔE_{vdw}	-26.64	1.73
ΔE_{ele}	0.21	1.82
ΔG_{polar}	4.35	1.67
$\Delta G_{non\text{-}polar}$	-3.24	0.15
$\mathbf{\Delta H_{total}}$	**-25.31**	2.17

We can notice that the enthalpy change upon binding of **Sub1** is more favorable in Pose 2. Here, ΔE_{vdw} = Change in van der Waals interaction on ligand associations, ΔE_{ele} = Change in electrostatic interaction on ligand associations, ΔG_{polar} = Change in polar interaction on ligand associations, $\Delta G_{non\text{-}polar}$ = Change in nonpolar interaction on ligand associations and $\Delta H_{total} = \Delta E_{vdw} + \Delta E_{ele} + \Delta G_{polar} + \Delta G_{non\text{-}polar}$.

Coordinates for QM region from different QM/MM calculations:

^{2}RC(minor)

Total QM/MM energy at B2=-3491.205522 (a.u).

ZPE(B1)= 0.417902 (a.u)

S 1.341690 -4.333669 -4.817635
O -0.139108 -3.945675 -0.898488
Fe 0.514226 -4.182590 -2.386849
N 2.352984 -4.649651 -1.580238
N 1.084777 -2.234817 -2.555276
N -1.239743 -3.771995 -3.338767
N 0.052239 -6.161886 -2.400344
C 2.775302 -5.875006 -1.119753
C 4.068426 -5.762648 -0.450566
C 4.414135 -4.432261 -0.526311
C 3.337346 -3.758976 -1.243345
C 2.292633 -1.696719 -2.196065
C 2.329158 -0.272877 -2.513879
C 1.094232 0.056755 -3.027972
C 0.342825 -1.207431 -3.068005
C -1.688310 -2.533532 -3.706657
C -3.024435 -2.612546 -4.295753
C -3.370162 -3.945224 -4.306876
C -2.238626 -4.647298 -3.674231
C -1.119300 -6.721652 -2.841966
C -1.132223 -8.155585 -2.584044
C 0.059651 -8.441562 -1.965307
C 0.787540 -7.186498 -1.860181
C 2.046716 -7.049905 -1.275179
H 2.498440 -7.958702 -0.893044
C 3.318475 -2.400703 -1.566964
H 4.191023 -1.833590 -1.258469
C -0.945456 -1.365663 -3.584501
H -1.419242 -0.471148 -3.972498
C -2.158421 -6.019127 -3.441996
H -3.017917 -6.614296 -3.732315
h 0.657017 1.007781 -3.332044
C -2.549940 -6.567844 2.104567
C -2.380454 -6.046184 3.415183
C -1.448720 -6.532163 1.214799
C -1.195333 -5.460972 3.794485
H -3.216572 -6.047276 4.106928
C -0.270373 -5.930337 1.578400
H -1.519629 -6.947978 0.218813
C -0.112546 -5.353533 2.870892
H -1.130754 -4.994098 4.770335
H 0.544086 -5.918864 0.867021
N 1.045136 -4.713400 3.199937
C 1.432022 -4.486973 4.586803
H 1.066724 -3.528060 4.973331
H 1.056199 -5.289768 5.222411
C 1.912412 -4.113202 2.186701
H 2.886666 -4.610488 2.146708
H 1.447979 -4.142628 1.202962
H 2.061195 -3.056315 2.437868
H 2.524038 -4.492116 4.645067
S -4.119991 -7.161717 1.663366
C -3.960224 -7.402540 -0.130167
H -4.942241 -7.716278 -0.475143
H -3.680673 -6.462756 -0.607067
H -3.221705 -8.175146 -0.346068
h 2.629231 -4.828300 -4.861491
h 4.614566 -6.574672 0.029449
h 5.284842 -3.918947 -0.118334
h 3.231618 0.327521 -2.399193
h -1.923598 -8.854669 -2.854367
h 0.439233 -9.407825 -1.633163
h -4.243110 -4.467808 -4.697944

h -3.602746 -1.738959 -4.596534

^{2}TS$_H$(minor)

Total QM/MM energy at B2=-3491.187486 (a.u).

ZPE(B1)= 0.411456 (a.u.)

S 1.408994 -4.292154 -4.622137
O 0.142172 -3.972650 -0.620528
Fe 0.754999 -4.199906 -2.184313
N 2.612635 -4.642699 -1.447275
N 1.288883 -2.240003 -2.358247
N -1.052083 -3.787673 -3.060378
N 0.318970 -6.171222 -2.213695
C 3.065700 -5.866289 -1.007413
C 4.338529 -5.729135 -0.312320
C 4.647085 -4.388219 -0.347974
C 3.575523 -3.730429 -1.081321
C 2.503161 -1.692446 -2.039083
C 2.531486 -0.278779 -2.388839
C 1.283779 0.041636 -2.877911
C 0.532312 -1.220697 -2.879038
C -1.506723 -2.558888 -3.451844
C -2.837977 -2.656820 -4.048830
C -3.171451 -3.993318 -4.046424
C -2.034822 -4.678341 -3.407338
C -0.859293 -6.739978 -2.629703
C -0.845089 -8.174415 -2.388533
C 0.368849 -8.451300 -1.810151
C 1.088780 -7.196061 -1.716274
C 2.363205 -7.054398 -1.170742
H 2.849215 -7.957065 -0.816937
C 3.540011 -2.377423 -1.407173
H 4.407434 -1.797032 -1.113273
C -0.764242 -1.387054 -3.363246
H -1.240390 -0.501066 -3.766195
C -1.922669 -6.049533 -3.200141
H -2.763569 -6.659143 -3.511235
C -2.795600 -7.003392 1.982451
C -2.653755 -6.334002 3.218978
C -1.669700 -7.091005 1.137692
C -1.524966 -5.588232 3.487509
H -3.474475 -6.323827 3.927155
C -0.533140 -6.361641 1.398949
H -1.700931 -7.673694 0.225945
C -0.482744 -5.496072 2.522546
H -1.490199 -5.016856 4.406666
H 0.278161 -6.394440 0.686782
N 0.503746 -4.544954 2.601028
C 0.467761 -3.551478 3.672577
H -0.552561 -3.202969 3.843546
H 0.861852 -3.971110 4.605384
C 1.453408 -4.387295 1.543815
H 2.014696 -5.305104 1.350856
H 0.862110 -4.169484 0.473226
H 2.133004 -3.567167 1.761036
H 1.084498 -2.701664 3.383803
S -4.379290 -7.562172 1.482136
C -4.215259 -7.389825 -0.331665
H -5.228318 -7.373516 -0.728002
H -3.715825 -6.447511 -0.561136
H -3.672300 -8.232280 -0.762512
h 2.682450 -4.813348 -4.727080
h 4.895341 -6.528745 0.176199
h 5.484092 -3.874587 0.124962
h 3.441831 0.315694 -2.311763
h 0.836889 0.989174 -3.178789
h -3.414906 -1.796970 -4.389238
h -4.038720 -4.528059 -4.433672
h -1.637815 -8.887617 -2.614356
h 0.756357 -9.419958 -1.494546

^{2}TS$_S$(minor)

Total QM/MM energy at B2=-3491.180049 (a.u)

ZPE(B1)= 0.411355 (a.u)

S 1.178041 -4.294251 -4.790063
O -0.250211 -4.131619 -0.771643
Fe 0.316787 -4.313622 -2.371758
N 2.178330 -4.742554 -1.609322
N 0.850436 -2.329888 -2.460024
N -1.446066 -3.895398 -3.266580
N -0.086869 -6.275970 -2.502192
C 2.641257 -5.972698 -1.210912
C 3.947568 -5.862790 -0.573019
C 4.261191 -4.523947 -0.596395
C 3.157697 -3.851468 -1.265089
C 2.075838 -1.782822 -2.175808
C 2.101775 -0.363438 -2.507006
C 0.834146 -0.033673 -2.938237
C 0.076755 -1.295364 -2.899448
C -1.958305 -2.648460 -3.497315
C -3.275416 -2.720133 -4.123084
C -3.523761 -4.054847 -4.356360
C -2.390598 -4.768545 -3.750245
C -1.259109 -6.845714 -2.926613
C -1.289378 -8.265822 -2.626622
C -0.081128 -8.553712 -2.042992
C 0.654047 -7.302385 -1.970520
C 1.923727 -7.152403 -1.400713
H 2.404080 -8.061158 -1.050724
C 3.118180 -2.488206 -1.577299
H 3.995526 -1.914938 -1.290254
C -1.258736 -1.460709 -3.291488
H -1.806691 -0.555997 -3.531174
C -2.283023 -6.147250 -3.568893
H -3.117095 -6.754501 -3.909023
C -0.821283 -5.336310 1.607269
C -1.133009 -4.366299 2.571908
C 0.313142 -6.130377 1.813538
C -0.317006 -4.177613 3.681755
H -2.012558 -3.740806 2.463837
C 1.139616 -5.939429 2.917232
H 0.570249 -6.890866 1.083641
C 0.860309 -4.940462 3.875222
H -0.615786 -3.440041 4.412724
H 2.016561 -6.563353 3.025000
N 1.696370 -4.713184 4.965353
C 1.646091 -3.406021 5.611890
H 1.892986 -2.581557 4.924066
H 0.659640 -3.197597 6.029789
C 2.978518 -5.400948 5.018765
H 3.466299 -5.163064 5.966813
H 2.847711 -6.485925 4.978102
H 3.662836 -5.120827 4.200991
H 2.351488 -3.388175 6.443694
S -1.734971 -5.506163 0.079888
C -3.444430 -5.753130 0.762948
H -4.095532 -5.950901 -0.090164
H -3.452955 -6.618178 1.430826
H -3.803986 -4.868307 1.289966
h 2.469532 -4.777794 -4.840878
h 4.525671 -6.674944 -0.132260
h 5.111706 -4.002494 -0.157331
h 3.021264 0.219736 -2.456871
h 0.386938 0.910056 -3.250404
h -3.904736 -1.840769 -4.259987
h -4.326971 -4.566185 -4.886882
h -2.165350 -8.901895 -2.753700
h 0.305609 -9.512706 -1.698275

^{2}RC(major)

Total QM/MM energy at B2=-3646.494394 (a.u)

ZPE(B1)= 0.416630 (a.u)

S 1.411933 -4.334035 -5.373704

O -0.020915 -4.042422 -1.466737
Fe 0.587059 -4.266909 -2.965289
N 2.459187 -4.585561 -2.215641
N 1.003718 -2.281069 -3.172150
N -1.235436 -3.983136 -3.849101
N 0.265039 -6.269303 -2.958458
C 2.970147 -5.765315 -1.755728
C 4.266911 -5.565057 -1.133633
C 4.538039 -4.222852 -1.220687
C 3.397308 -3.625905 -1.898830
C 2.147600 -1.640988 -2.787272
C 2.056273 -0.212848 -3.042485
C 0.809655 0.013585 -3.590443
C 0.185568 -1.309304 -3.684613
C -1.786609 -2.787494 -4.218705
C -3.171191 -2.948865 -4.653165
C -3.455164 -4.295565 -4.560051
C -2.220767 -4.912862 -4.048860
C -0.891271 -6.914789 -3.305021
C -0.796611 -8.345489 -3.046828
C 0.445571 -8.554234 -2.507220
C 1.081355 -7.247396 -2.436965
C 2.323410 -7.003408 -1.866874
H 2.824522 -7.857549 -1.425008
C 3.241673 -2.276682 -2.184153
H 4.065258 -1.633281 -1.896671
C -1.096135 -1.578047 -4.178318
H -1.637493 -0.725268 -4.572568
C -2.027414 -6.273713 -3.797167
H -2.875099 -6.922052 -3.986900
C -0.995889 -5.995378 1.923806
C -1.425454 -5.285484 3.059062
C 0.278980 -6.575988 1.956820
C -0.632617 -5.205930 4.200939
H -2.392459 -4.792424 3.065877
C 1.074198 -6.503003 3.102871
H 0.650853 -7.134365 1.102830
C 0.625865 -5.837097 4.258019
H -1.011267 -4.639542 5.044458
H 2.025530 -7.019720 3.078068
N 1.402274 -5.775299 5.458333
C 0.645873 -6.070445 6.688822
H 0.281229 -7.108522 6.720711
H -0.212894 -5.406863 6.788353
C 2.656578 -6.530842 5.429351
H 3.188289 -6.366169 6.370947
H 3.291419 -6.181621 4.609965
H 2.505338 -7.614037 5.302068
H 1.297193 -5.906580 7.553048
S -1.990646 -6.154968 0.445079
C -3.655449 -6.483062 1.128132
H -4.075636 -5.599144 1.609793
H -4.291785 -6.734010 0.276975
H -3.635635 -7.325075 1.821600
h 2.655359 -4.929196 -5.437116
h 4.838092 -6.348882 -0.636203
h 5.400891 -3.704865 -0.802069
h 2.899697 0.453487 -2.861652
h 0.284796 0.930629 -3.858061
h -3.819026 -2.118435 -4.933811
h -4.348709 -4.873100 -4.796899
h -1.580322 -9.086936 -3.202137
h 0.882262 -9.488577 -2.154558

$^{2}TS_{S}$ (major)

Total QM/MM energy at B2=-3646.494394 (a.u)

ZPE(B1)= 0.416630 (a.u)

S 1.282094 -4.413540 -5.193382
O -0.078815 -4.383627 -1.166196
Fe 0.432230 -4.473867 -2.772576
N 2.326647 -4.773713 -2.060475
N 0.845479 -2.459776 -2.913446
N -1.388651 -4.166506 -3.635281
N 0.148802 -6.455103 -2.900226

C 2.856638 -5.967105 -1.662761
C 4.180492 -5.783704 -1.091294
C 4.448294 -4.440772 -1.151208
C 3.276386 -3.823270 -1.754207
C 2.007220 -1.826750 -2.566475
C 1.938911 -0.404470 -2.868542
C 0.693499 -0.176670 -3.422762
C 0.042566 -1.490607 -3.455657
C -1.930137 -2.962699 -4.000092
C -3.290714 -3.121090 -4.507825
C -3.563433 -4.472460 -4.482984
C -2.347822 -5.098656 -3.939068
C -0.985310 -7.108228 -3.307364
C -0.857365 -8.546003 -3.122011
C 0.375547 -8.748707 -2.559893
C 0.979709 -7.434612 -2.409333
C 2.214223 -7.199903 -1.814002
H 2.724605 -8.064583 -1.405399
C 3.115224 -2.468424 -1.999867
H 3.951212 -1.833633 -1.726010
C -1.240277 -1.754441 -3.946485
H -1.771685 -0.903986 -4.359399
C -2.130781 -6.468011 -3.775935
H -2.956187 -7.121093 -4.035396
C -0.696218 -5.649236 1.447991
C -1.181262 -4.881085 2.523262
C 0.483827 -6.381790 1.635923
C -0.531145 -4.877835 3.750964
H -2.073374 -4.273824 2.405124
C 1.135764 -6.386828 2.871693
H 0.885673 -6.991827 0.833375
C 0.629822 -5.653303 3.961974
H -0.939682 -4.268567 4.547457
H 2.015053 -7.012253 2.965882
N 1.244313 -5.660396 5.244667
C 0.312947 -5.844507 6.376076
H -0.148440 -6.843707 6.372981
H -0.484651 -5.100983 6.358589
C 2.424035 -6.517071 5.378410
H 2.845861 -6.382020 6.378339
H 3.184489 -6.232858 4.645458
H 2.202496 -7.586085 5.237501
H 0.866713 -5.723593 7.311785
S -1.552214 -5.721694 -0.117900
C -3.244027 -6.157773 0.505924
H -3.712403 -5.342958 1.060303
H -3.854983 -6.379427 -0.371644
H -3.187158 -7.049053 1.135834
h 2.532651 -4.990110 -5.282943
h 4.784824 -6.574257 -0.646463
h 5.332132 -3.931706 -0.766829
h 2.792714 0.257466 -2.723877
h 0.199135 0.736928 -3.752926
h -3.926075 -2.283510 -4.795646
h -4.437912 -5.048753 -4.785041
h -1.612899 -9.300262 -3.341851
h 0.828084 -9.686127 -2.236595

^2TS_H (major)

Total QM/MM energy at B2=-3646.446695(a.u.)

ZPE(B1)=0.411237 (a.u.)

S 1.490535 -4.309282 -5.256896
O 0.538263 -3.913852 -1.188284
Fe 0.968241 -4.197034 -2.820337
N 2.856459 -4.592449 -2.256103
N 1.397215 -2.216513 -3.009195
N -0.935101 -3.835578 -3.550736
N 0.541695 -6.178987 -2.796406
C 3.377450 -5.824020 -1.927056
C 4.681322 -5.667773 -1.316193
C 4.940035 -4.315377 -1.275857
C 3.794318 -3.654756 -1.878357
C 2.540525 -1.605555 -2.572881
C 2.443489 -0.161664 -2.756537
C 1.212543 0.090054 -3.325225

C 0.581342 -1.227217 -3.488065
C -1.421472 -2.640068 -4.007752
C -2.807558 -2.773098 -4.458247
C -3.164503 -4.088324 -4.251650
C -1.962875 -4.733188 -3.695228
C -0.683716 -6.758246 -3.007032
C -0.626471 -8.194273 -2.765772
C 0.667915 -8.471681 -2.406556
C 1.381517 -7.203653 -2.426835
C 2.707827 -7.038756 -2.054234
H 3.236263 -7.929918 -1.739602
C 3.633412 -2.277857 -2.026824
H 4.450981 -1.660118 -1.679527
C -0.698829 -1.454287 -3.997756
H -1.213129 -0.587419 -4.395367
C -1.833649 -6.087627 -3.403784
H -2.716234 -6.706858 -3.515623
C -1.997291 -6.583877 1.231909
C -1.958733 -5.720708 2.344586
C -0.791328 -6.908860 0.582310
C -0.782558 -5.065342 2.681394
H -2.850701 -5.504920 2.919204
C 0.382064 -6.281425 0.918098
H -0.784782 -7.629637 -0.226202
C 0.376449 -5.261425 1.896809
H -0.815524 -4.344156 3.490647
H 1.284668 -6.550680 0.386778
N 1.426961 -4.351781 1.918763
C 1.377754 -3.241632 2.862700
H 2.341231 -2.732662 2.852660
H 1.182460 -3.609843 3.871400
C 2.233832 -4.217515 0.783484
H 2.969408 -3.429382 0.894993
H 1.422780 -3.999989 -0.293568
H 2.681104 -5.146954 0.439238
H 0.587032 -2.540316 2.582373
S -3.455753 -7.240405 0.535001
C -4.637074 -6.971442 1.869402
H -4.902223 -5.916459 1.933995
H -5.526569 -7.541986 1.620170
H -4.238780 -7.334876 2.814563
h 2.739541 -4.869143 -5.432641
h 5.263435 -6.478711 -0.878482
h 5.788419 -3.833690 -0.789764
h 3.279058 0.495717 -2.516244
h 0.688428 1.011574 -3.578545
h -3.405840 -1.957393 -4.864142
h -4.088560 -4.634425 -4.441278
h -1.478682 -8.872028 -2.815289
h 1.088874 -9.421651 -2.077289

Cpd I-MT

Total QM/MM energy at B2=-3644.995102(a.u.)

ZPE(B1)=0.415563 (a.u.)

S 4.110172 -4.043377 2.991796
O 1.656550 -3.737506 -0.401099
Fe 2.596432 -3.897253 0.929358
N 1.234905 -5.082588 1.820557
N 1.830919 -2.249775 1.902401
N 4.099394 -2.710472 0.169514
N 3.504812 -5.539472 0.163556
C 1.097651 -6.442119 1.694763
C -0.072675 -6.913911 2.422997
C -0.642348 -5.805606 2.998146
C 0.200442 -4.673963 2.625667
C 0.766257 -2.235870 2.751638
C 0.531532 -0.893668 3.280267
C 1.482420 -0.074927 2.709912
C 2.298578 -0.960978 1.864544
C 4.280495 -1.372414 0.376098
C 5.412760 -0.873295 -0.392201
C 5.868306 -1.935397 -1.151436
C 5.050214 -3.082533 -0.743979
C 4.575275 -5.547089 -0.690441
C 4.889895 -6.906313 -1.111189

C 3.970193 -7.725035 -0.505644
C 3.096437 -6.846326 0.263704
C 1.970579 -7.257890 0.974813
H 1.743090 -8.317624 0.956033
C 0.009165 -3.369575 3.067325
H -0.821907 -3.234735 3.748717
C 3.435505 -0.580676 1.156192
H 3.686341 0.475116 1.190379
C 5.251499 -4.412532 -1.127651
H 6.046929 -4.601208 -1.844028
C -2.597747 -3.746939 -1.184447
C -3.340050 -3.899358 -2.373708
C -2.715599 -4.740569 -0.192618
C -4.177215 -4.982935 -2.560816
H -3.280023 -3.139610 -3.147865
C -3.555535 -5.828085 -0.360423
H -2.132560 -4.658663 0.719699
C -4.332038 -5.972690 -1.543547
H -4.736315 -5.059229 -3.484836
H -3.647615 -6.548808 0.439422
N -5.203272 -7.010218 -1.688698
C -6.091108 -7.067586 -2.846504
H -6.569506 -6.102347 -3.017462
H -5.543474 -7.349464 -3.755805
C -5.286987 -8.074595 -0.684581
H -5.597223 -7.668118 0.283791
H -6.035091 -8.796459 -1.006409
H -4.328863 -8.593417 -0.562268
H -6.871424 -7.805498 -2.668898
S -1.649137 -2.288245 -0.838280
C -0.460642 -2.222178 -2.228349
H -0.906828 -2.672999 -3.116250
H -0.246310 -1.170218 -2.434050
H 0.452271 -2.748053 -1.936949
h 3.720572 -5.096651 3.793776
h -0.414983 -7.948530 2.444375
h -1.561625 -5.729110 3.578788
h -0.241599 -0.656565 4.011100
h 1.669698 0.995865 2.789894
h 5.811828 0.137304 -0.305584
h 6.622320 -1.999376 -1.935933
h 5.674561 -7.158624 -1.824424
h 3.843298 -8.800579 -0.628801

$^{2}TS_{S}$-MT

Total QM/MM energy at B2=-3644.990316

ZPE(B1)=0.415567(a.u.)

S 4.040362 -4.051498 2.878868
O 1.455715 -3.631674 -0.422506
Fe 2.404912 -3.850400 0.958924
N 1.061954 -5.017521 1.872761
N 1.676056 -2.205050 1.953874
N 3.905256 -2.669984 0.148524
N 3.281303 -5.487725 0.139482
C 0.932892 -6.383957 1.756057
C -0.209776 -6.854863 2.524877
C -0.753545 -5.749940 3.134536
C 0.071514 -4.614999 2.739491
C 0.637778 -2.186183 2.846195
C 0.422563 -0.838110 3.361669
C 1.369399 -0.029847 2.766149
C 2.156299 -0.921119 1.899166
C 4.106955 -1.337103 0.372709
C 5.260183 -0.853892 -0.380697
C 5.706395 -1.917624 -1.141445
C 4.860435 -3.054619 -0.755800
C 4.354514 -5.503964 -0.710605
C 4.677123 -6.870610 -1.102434
C 3.767058 -7.683175 -0.475349
C 2.890071 -6.796226 0.282194
C 1.793867 -7.206455 1.032707
H 1.586831 -8.270512 1.049873
C -0.098941 -3.314754 3.204872
H -0.888036 -3.187079 3.935194
C 3.281309 -0.542215 1.165159

H 3.547269 0.509408 1.210157
C 5.048499 -4.381224 -1.147525
H 5.847497 -4.579706 -1.856990
C -2.041799 -4.066569 -0.939743
C -2.591114 -4.113970 -2.245548
C -2.539958 -4.990731 0.019814
C -3.617999 -4.986036 -2.554006
H -2.225400 -3.451460 -3.022722
C -3.535043 -5.884237 -0.289593
H -2.106022 -5.017314 1.014727
C -4.127042 -5.910471 -1.587736
H -4.027503 -4.973363 -3.556426
H -3.875394 -6.565744 0.475493
N -5.120387 -6.785595 -1.874843
C -5.788264 -6.760274 -3.177109
H -6.141848 -5.754769 -3.418735
H -5.118854 -7.106069 -3.974153
C -5.516663 -7.812342 -0.898785
H -5.868344 -7.352232 0.030371
H -6.334211 -8.395238 -1.319442
H -4.681673 -8.485713 -0.668838
H -6.660266 -7.411709 -3.146072
S -0.711624 -3.078578 -0.384377
C -0.283944 -2.082339 -1.834178
H 0.127817 -2.725672 -2.613092
H -1.151054 -1.524377 -2.192551
H 0.497500 -1.405535 -1.492712
h 3.669532 -5.088726 3.710125
h -0.554591 -7.888798 2.536943
h -1.657047 -5.675063 3.739635
h -0.349294 -0.583102 4.087805
h 1.576209 1.037108 2.849234
h 5.683869 0.145035 -0.277250
h 6.475625 -1.993083 -1.909988
h 5.467003 -7.137002 -1.804710
h 3.645548 -8.761042 -0.582614

$^{2}TS_{H}$-MT

Total QM/MM energy at B2=-3644.955823

ZPE(B1)=0.406435(a.u.)

S 4.388344 -4.063762 2.389244
O 1.671738 -3.743439 -0.954403
Fe 2.657822 -3.904243 0.420481
N 1.336457 -5.079900 1.421135
N 1.963374 -2.268789 1.421541
N 4.233050 -2.787513 -0.292146
N 3.480020 -5.573459 -0.384733
C 1.201937 -6.449017 1.336401
C 0.048677 -6.901855 2.102410
C -0.516559 -5.773334 2.646811
C 0.314593 -4.650281 2.232354
C 0.858270 -2.219471 2.227096
C 0.639622 -0.864249 2.721879
C 1.675500 -0.093193 2.239790
C 2.500556 -1.007072 1.431539
C 4.548839 -1.506777 0.070931
C 5.839951 -1.121909 -0.483101
C 6.276491 -2.189077 -1.250633
C 5.248753 -3.225319 -1.100852
C 4.483753 -5.598257 -1.315138
C 4.632159 -6.939550 -1.869490
C 3.711978 -7.733489 -1.236040
C 3.004813 -6.858154 -0.307713
C 1.985023 -7.273706 0.539145
H 1.750664 -8.332199 0.547687
C 0.099095 -3.328204 2.599835
H -0.723495 -3.161369 3.285495
C 3.716717 -0.683869 0.830880
H 4.068411 0.330615 0.994769
C 5.299027 -4.519159 -1.633222
H 6.088245 -4.735023 -2.349219
C -3.632192 -5.729334 -4.911154
C -3.162481 -5.773796 -3.580838
C -3.112100 -4.722745 -5.763697
C -2.224702 -4.872265 -3.120839

H -3.515976 -6.538029 -2.898416
C -2.181689 -3.808951 -5.311965
H -3.466648 -4.656416 -6.788746
C -1.707187 -3.856866 -3.966630
H -1.859166 -4.992139 -2.105816
H -1.838040 -3.046203 -6.000501
N -0.777181 -2.945885 -3.502987
C -0.180580 -2.017870 -4.459297
H 0.304093 -2.560679 -5.277518
H -0.931242 -1.350164 -4.896276
C -0.392466 -2.801527 -2.119896
H -1.143311 -3.202551 -1.465011
H 0.723577 -3.320793 -1.647104
H -0.227452 -1.732835 -1.923191
H 0.562692 -1.415694 -3.937997
S -4.793634 -6.845815 -5.581572
C -5.393869 -7.790582 -4.141918
H -5.762950 -7.111119 -3.373593
H -6.227577 -8.392956 -4.506557
H -4.628364 -8.454341 -3.736160
h 3.950267 -5.017369 3.285385
h -0.303339 -7.933159 2.126131
h -1.465958 -5.667053 3.171609
h -0.220382 -0.604741 3.339226
h 1.927249 0.958625 2.375319
h 6.339428 -0.187654 -0.226672
h 7.177514 -2.348903 -1.842816
h 5.340995 -7.188762 -2.659117
h 3.470283 -8.784002 -1.397514

^{2}RC1-Cpd0$_{major}$

Total QM/MM energy at B2= -3601.437609

ZPE(B1)= 0.447766

N 1.452115 2.545677 -6.954306
H 0.843671 2.810191 -7.721213
C 0.931513 1.582526 -5.978204
H 0.726819 2.032365 -4.994480
C -0.422015 1.065400 -6.518986
H -1.084895 1.917595 -6.694803
H -0.287063 0.534899 -7.467205
H -0.906877 0.394748 -5.807503
C 1.840576 0.362453 -5.702851
O 1.630170 -0.267590 -4.665216
C 2.812099 2.701947 -2.153908
H 2.870558 2.081417 -3.056632
H 2.205795 2.148756 -1.430802
C 2.034205 3.955412 -2.552880
O 2.498360 5.065373 -2.754750
O 0.724911 3.732185 -2.728711
H -0.660382 4.876901 -2.423783
S -3.207791 -4.775069 -4.095518
O -2.040556 -0.636357 -3.647018
O -0.714638 -0.505277 -3.063024
H -0.118471 -0.520643 -3.835919
Fe -2.596241 -2.382872 -3.795436
N -4.313424 -1.865917 -2.808891
N -1.713349 -2.952314 -2.052436
N -0.913011 -2.931270 -4.823124
N -3.532040 -1.845277 -5.548608
C -5.494645 -1.397257 -3.331930
C -6.466579 -1.150111 -2.271907
C -5.844869 -1.480702 -1.095058
C -4.505619 -1.940520 -1.455895
C -2.284642 -2.911640 -0.812951
C -1.368185 -3.435951 0.201878
C -0.208972 -3.782252 -0.454915
C -0.462626 -3.474341 -1.878251
C 0.215014 -3.501857 -4.300942
C 1.147046 -3.872781 -5.362999
C 0.549725 -3.509909 -6.556498
C -0.738887 -2.895184 -6.184261
C -2.947099 -1.828115 -6.785354

C -3.863490 -1.261827 -7.777089
C -5.044840 -1.007946 -7.120072
C -4.802491 -1.357880 -5.721863
C -5.718785 -1.178367 -4.688345
H -6.698154 -0.814054 -4.977790
C -3.569345 -2.436961 -0.550937
H -3.895025 -2.454591 0.482087
C 0.424935 -3.709458 -2.932608
H 1.373990 -4.165037 -2.661873
C -1.678401 -2.342282 -7.066633
H -1.399302 -2.315513 -8.117839
O -1.440136 5.282133 -1.985718
H -1.052289 5.924734 -1.378316
H -2.122356 3.889305 -1.091625
O -0.208501 1.700135 -1.659210
H -0.417726 0.908326 -2.225283
H 0.374650 2.820359 -2.326842
O -2.362624 3.032458 -0.665607
H -1.040625 2.019474 -1.236146
H -3.138104 2.716525 -1.146781
h -4.512094 -4.969174 -3.688749
h -7.487253 -0.793913 -2.411239
h -6.239100 -1.389051 -0.083007
h -1.632342 -3.521156 1.255931
h 0.737856 -4.183688 -0.093760
h 2.104347 -4.358222 -5.173297
h 0.843596 -3.658377 -7.595567
h -3.602080 -1.010864 -8.805072
h -5.964907 -0.567313 -7.503980
h 3.813852 2.859565 -1.754267
h 2.085870 3.254725 -6.645151
h 2.613744 0.047203 -6.403490

^{2}TS1$_{major}$

Total QM/MM energy at B2= -3601.413991

ZPE(B1)= 0.442253

N 1.356353 2.562205 -6.905238
H 0.757039 2.823555 -7.680563
C 0.831050 1.583367 -5.949216
H 0.590111 2.018994 -4.967974
C -0.494499 1.039512 -6.532502
H -1.161327 1.881077 -6.737701
H -0.316643 0.503744 -7.470783
H -0.989567 0.366940 -5.829619
C 1.746339 0.371619 -5.673588
O 1.535489 -0.271145 -4.642017
C 2.406473 2.681232 -2.093171
H 2.355333 1.999767 -2.951102
H 1.934827 2.161156 -1.252833
C 1.533594 3.907718 -2.416741
O 1.956171 5.019024 -2.688127
O 0.224132 3.647027 -2.393625
H -1.143682 4.720332 -1.684142
S -3.208656 -4.761298 -4.114403
O -2.074928 -0.628419 -3.709495
O -0.699156 -0.432726 -2.961301
H -0.075679 -0.354727 -3.717491
Fe -2.600101 -2.385899 -3.820154
N -4.316155 -1.871083 -2.835801
N -1.713903 -2.947126 -2.079594
N -0.927406 -2.947761 -4.848668
N -3.536355 -1.841631 -5.571868
C -5.498320 -1.400506 -3.358079
C -6.471948 -1.163535 -2.298779
C -5.853506 -1.505598 -1.123505
C -4.513167 -1.959577 -1.483701
C -2.286751 -2.913768 -0.840412
C -1.363816 -3.423897 0.175562

C -0.201814 -3.761138 -0.480649
C -0.460675 -3.464223 -1.904863
C 0.202874 -3.515347 -4.328449
C 1.127603 -3.897379 -5.390693
C 0.526611 -3.540051 -6.584570
C -0.759573 -2.917179 -6.211421
C -2.955102 -1.835420 -6.810873
C -3.871851 -1.268597 -7.802648
C -5.050261 -1.006477 -7.143989
C -4.806465 -1.351717 -5.745549
C -5.722627 -1.173123 -4.712354
H -6.701636 -0.807343 -5.000772
C -3.578837 -2.460668 -0.580443
H -3.912616 -2.497700 0.448602
C 0.421138 -3.710625 -2.960039
H 1.371387 -4.163071 -2.690316
C -1.692349 -2.361233 -7.093015
H -1.415806 -2.339937 -8.144857
O -2.003990 4.997106 -1.298462
H -1.844266 5.145106 -0.354488
H -2.852075 3.458344 -1.099124
O -0.627102 1.503673 -1.618941
H -0.726618 0.623214 -2.278519
H -0.098527 2.632299 -2.082952
O -3.131099 2.544940 -0.859581
H -1.508677 1.734221 -1.255662
H -3.685860 2.233229 -1.585662
h -4.510524 -4.962332 -3.703221
h -7.492489 -0.806448 -2.436812
h -6.251147 -1.416668 -0.112545
h -1.621017 -3.502978 1.231810
h 0.750659 -4.148636 -0.119117
h 2.086184 -4.381075 -5.203003
h 0.817018 -3.693968 -7.623820
h -3.613921 -1.027817 -8.833940
h -5.971823 -0.569269 -7.528229
h 3.451187 2.892487 -1.865115
h 1.967061 3.282723 -6.576813
h 2.523523 0.062770 -6.372633

^{2}IC1-CpdI$_{major}$

Total QM/MM energy at B2= -3601.429242

ZPE(B1)= 0.443823

N 1.514307 2.555365 -6.892445
H 0.851747 2.842416 -7.602617
C 1.014795 1.642690 -5.848100
H 0.919675 2.131816 -4.864458
C -0.404383 1.199461 -6.270886
H -1.048975 2.080368 -6.337479
H -0.386267 0.709792 -7.251421
H -0.834654 0.510907 -5.541422
C 1.872164 0.382009 -5.623246
O 1.636942 -0.292284 -4.616563
C 2.896611 2.664425 -2.208522
H 2.999253 2.020917 -3.090598
H 2.248799 2.127118 -1.505889
C 2.085386 3.900393 -2.657669
O 2.498191 5.068487 -2.526204
O 0.937725 3.586684 -3.163350
H -0.029635 4.953149 -3.021778
S -3.211955 -4.774362 -4.120931
O -2.127777 -0.796160 -3.733380
O -0.384962 -0.406736 -2.628245
H 0.155137 -0.235289 -3.427131
Fe -2.610719 -2.383263 -3.781894
N -4.345707 -1.928523 -2.799266
N -1.760738 -2.967573 -2.059161
N -0.974580 -2.990688 -4.828512
N -3.570580 -1.913932 -5.553548

C -5.531579 -1.472995 -3.333309
C -6.495932 -1.205782 -2.275269
C -5.867282 -1.498886 -1.091605
C -4.532405 -1.960338 -1.442174
C -2.316795 -2.901974 -0.807924
C -1.391179 -3.414407 0.196139
C -0.240187 -3.773557 -0.468790
C -0.504034 -3.489499 -1.890184
C 0.162343 -3.538408 -4.302608
C 1.104453 -3.885859 -5.359615
C 0.510848 -3.523729 -6.553141
C -0.786752 -2.929883 -6.189119
C -2.977667 -1.861213 -6.787004
C -3.893720 -1.284714 -7.765903
C -5.081110 -1.057109 -7.109331
C -4.844968 -1.429411 -5.718666
C -5.763504 -1.267476 -4.687793
H -6.745644 -0.913131 -4.976835
C -3.591213 -2.423144 -0.531170
H -3.899102 -2.405810 0.506374
C 0.375743 -3.740812 -2.939619
H 1.334781 -4.167365 -2.666990
C -1.710198 -2.363535 -7.072562
H -1.418018 -2.305938 -8.117442
O -0.477564 5.752522 -2.621891
H 0.308250 6.207430 -2.280779
H -1.311340 4.877659 -1.404248
O -0.486411 1.959211 -1.605431
H -0.615597 0.503107 -2.245679
H 0.063758 2.500681 -2.230260
O -1.845825 4.277669 -0.814406
H -1.118673 2.615416 -1.244223
H -2.748084 4.378616 -1.140330
h -4.506731 -4.995551 -3.697874
h -7.516255 -0.848954 -2.415564
h -6.250945 -1.380629 -0.078252
h -1.645887 -3.489367 1.253291
h 0.709013 -4.170510 -0.108909
h 2.071271 -4.349743 -5.164314
h 0.818433 -3.653934 -7.590688
h -3.626610 -1.013964 -8.787379
h -6.001280 -0.613357 -7.489381
h 3.871971 2.827161 -1.749985
h 2.163376 3.267688 -6.625466
h 2.639843 0.074792 -6.333425

^{2}RC2-Cpd0$_{minor}$

Total QM/MM energy at B2= -3601.430236

ZPE(B1)= 0.447766

N 1.405645 2.523495 -6.995065
H 0.792571 2.793151 -7.757610
C 0.888338 1.537072 -6.040848
H 0.664714 1.967539 -5.054010
C -0.452601 1.011680 -6.603104
H -1.124253 1.858556 -6.768476
H -0.302567 0.499040 -7.559146
H -0.930648 0.323199 -5.904681
C 1.806552 0.321584 -5.779876
O 1.594753 -0.332856 -4.759235
C 2.225976 2.299751 -2.393000
H 2.469210 2.113853 -3.440983
H 1.877252 1.375030 -1.935617
C 1.080822 3.311775 -2.351621
O 1.002817 4.290418 -3.069479
O 0.160497 2.984278 -1.427572
H -0.571589 3.668621 -1.359080
S -3.209913 -4.804524 -4.106654
O -2.016678 -0.671206 -3.655276
O -0.693951 -0.518232 -3.070515

H -0.115328 -0.476150 -3.853701
Fe -2.594451 -2.423955 -3.813121
N -4.308835 -1.892349 -2.824929
N -1.713725 -2.988442 -2.071572
N -0.917207 -2.970586 -4.844598
N -3.531926 -1.879116 -5.566467
C -5.491010 -1.423147 -3.348242
C -6.462443 -1.177450 -2.288634
C -5.842143 -1.511297 -1.111906
C -4.504144 -1.973030 -1.471955
C -2.285465 -2.950106 -0.831992
C -1.365874 -3.470496 0.182021
C -0.206404 -3.814359 -0.476133
C -0.461895 -3.507314 -1.899012
C 0.214653 -3.530559 -4.321979
C 1.149615 -3.897106 -5.383114
C 0.548247 -3.544877 -6.577394
C -0.743548 -2.935601 -6.205328
C -2.948703 -1.864026 -6.804266
C -3.862820 -1.291410 -7.793847
C -5.041964 -1.030829 -7.135187
C -4.800176 -1.384159 -5.738253
C -5.715281 -1.202657 -4.704075
H -6.694173 -0.836698 -4.993299
C -3.571295 -2.479214 -0.569362
H -3.899700 -2.503171 0.462201
C 0.424870 -3.740296 -2.954316
H 1.378664 -4.184817 -2.684374
C -1.683081 -2.383952 -7.087937
H -1.404243 -2.356860 -8.139156
O -1.892600 4.627635 -0.836203
H -1.879114 4.873462 0.103403
H -2.734309 4.105545 -0.896459
O -2.547183 1.241052 -1.842894
H -2.617544 0.494793 -2.482485
H -1.592815 1.361290 -1.747424
O -4.063013 3.035075 -0.682225
H -3.586710 2.255236 -1.083825
H -4.829913 3.177626 -1.250629
h -4.514863 -4.995660 -3.700552
h -7.481809 -0.817460 -2.427795
h -6.233580 -1.409560 -0.099734
h -1.624626 -3.551364 1.237755
h 0.743081 -4.210662 -0.116288
h 2.113402 -4.368154 -5.189995
h 0.841096 -3.696415 -7.616307
h -3.601680 -1.041387 -8.822128
h -5.961017 -0.587233 -7.518110
h 3.132482 2.659747 -1.906465
h 2.016783 3.244374 -6.668239
h 2.590693 0.022641 -6.475449

^{2}TS2$_{minor}$

Total QM/MM energy at B2= -3601.408401

ZPE(B1)= 0.441955

N 1.399333 2.544282 -6.996899
H 0.787300 2.825525 -7.755845
C 0.868670 1.558798 -6.046531
H 0.648858 1.993938 -5.061205
C -0.474971 1.049526 -6.614786
H -1.136582 1.904168 -6.778487
H -0.328752 0.538636 -7.572621
H -0.960620 0.362642 -5.920186
C 1.776525 0.333402 -5.801873
O 1.562642 -0.340579 -4.794245
C 1.839682 2.273866 -2.275042
H 2.010043 1.899804 -3.287357
H 1.529584 1.443157 -1.642174
C 0.676917 3.288940 -2.305495

O 0.606596 4.170777 -3.158383
O -0.203975 3.092075 -1.344633
H -1.158247 3.994350 -1.185873
S -3.220425 -4.774956 -4.098293
O -2.010858 -0.645537 -3.583529
O -0.661320 -0.524748 -3.058173
H -0.117418 -0.458191 -3.864592
Fe -2.600288 -2.394972 -3.783593
N -4.312977 -1.865955 -2.791539
N -1.721887 -2.976970 -2.050176
N -0.928753 -2.941560 -4.824800
N -3.540273 -1.841664 -5.535014
C -5.496380 -1.397847 -3.311914
C -6.466412 -1.156183 -2.250212
C -5.843206 -1.490004 -1.074934
C -4.505424 -1.949910 -1.438276
C -2.289321 -2.939001 -0.808724
C -1.368477 -3.465955 0.200364
C -0.210580 -3.807747 -0.461861
C -0.469979 -3.497150 -1.883126
C 0.203361 -3.505186 -4.306848
C 1.137009 -3.866998 -5.371191
C 0.532367 -3.513691 -6.562751
C -0.758088 -2.904086 -6.185577
C -2.963328 -1.830818 -6.775848
C -3.883617 -1.266628 -7.764061
C -5.061868 -1.009888 -7.101941
C -4.812508 -1.355034 -5.704308
C -5.724908 -1.176884 -4.667426
H -6.706807 -0.816706 -4.954273
C -3.571047 -2.460340 -0.539482
H -3.892630 -2.480743 0.494588
C 0.414098 -3.726539 -2.941520
H 1.369750 -4.168713 -2.675624
C -1.699199 -2.351161 -7.064669
H -1.424663 -2.324470 -8.116969
O -2.081369 4.655899 -0.903471
H -2.030372 4.925433 0.034209
H -2.935385 4.049152 -0.957001
O -2.449753 1.237874 -1.696391
H -2.470232 0.520434 -2.375522
H -1.535022 1.570401 -1.672937
O -4.006812 3.054455 -0.900664
H -3.487358 2.235437 -1.239522
H -4.739054 3.191710 -1.514657
h -4.524700 -4.967026 -3.690468
h -7.486921 -0.798743 -2.387560
h -6.234321 -1.391916 -0.062276
h -1.628805 -3.554503 1.255094
h 0.742034 -4.199705 -0.105543
h 2.104633 -4.330769 -5.179653
h 0.821078 -3.665657 -7.602760
h -3.626219 -1.018720 -8.793796
h -5.983665 -0.572147 -7.485006
h 2.779699 2.697795 -1.921888
h 2.009417 3.261365 -6.659909
h 2.563266 0.045344 -6.499102

^{2}IC2-Fe(H_2O_2)$_{minor}$

Total QM/MM energy at B2= -3601.416174

ZPE(B1)= 0.446275

N 1.480167 2.533938 -7.018807
H 0.851681 2.822976 -7.761102
C 0.938283 1.573076 -6.041884
H 0.776673 2.034804 -5.053441
C -0.452860 1.136640 -6.553904
H -1.090187 2.021120 -6.628938
H -0.382597 0.673659 -7.545004
H -0.922391 0.430056 -5.868365

C 1.800645 0.315371 -5.836488
O 1.537727 -0.417127 -4.878197
C 1.818958 2.008893 -2.292565
H 2.061003 1.544061 -3.252092
H 1.520867 1.229871 -1.591209
C 0.580898 2.929215 -2.463181
O 0.452249 3.581491 -3.511515
O -0.245200 2.911609 -1.467151
H -1.370874 4.083932 -1.224788
S -3.195723 -4.703278 -4.072677
O -1.832280 -0.571828 -3.513903
O -0.461815 -0.582256 -3.040766
H 0.046250 -0.389589 -3.858666
Fe -2.599591 -2.433104 -3.757897
N -4.272368 -1.828273 -2.754567
N -1.704899 -2.981993 -2.031307
N -0.927363 -2.962890 -4.804067
N -3.513512 -1.820278 -5.491834
C -5.463904 -1.366211 -3.271939
C -6.434373 -1.139581 -2.211084
C -5.810039 -1.475570 -1.037151
C -4.471518 -1.927357 -1.400185
C -2.270188 -2.946552 -0.785462
C -1.351697 -3.484930 0.215122
C -0.196718 -3.831891 -0.451889
C -0.455401 -3.517593 -1.868648
C 0.207606 -3.528359 -4.290080
C 1.141568 -3.881619 -5.355550
C 0.535807 -3.527158 -6.544767
C -0.755148 -2.922567 -6.165637
C -2.945057 -1.823653 -6.740337
C -3.865551 -1.257451 -7.722649
C -5.040651 -0.991399 -7.056920
C -4.788063 -1.327511 -5.661092
C -5.697373 -1.144411 -4.624852
H -6.679295 -0.784320 -4.910039
C -3.544389 -2.456155 -0.507501
H -3.863397 -2.483819 0.526531
C 0.422539 -3.753907 -2.928689
H 1.380725 -4.190263 -2.666169
C -1.691731 -2.359844 -7.040010
H -1.423204 -2.333159 -8.093255
O -2.139908 4.669902 -0.928243
H -2.012894 4.799959 0.023769
H -3.464520 3.658128 -0.957457
O -2.329049 1.102262 -1.779145
H -2.211278 0.122917 -2.796279
H -1.525988 1.673825 -1.685574
O -4.175905 2.955329 -0.969148
H -3.106876 1.669673 -1.569534
H -4.820916 3.256573 -1.620278
h -4.502456 -4.892817 -3.671591
h -7.458940 -0.794393 -2.349552
h -6.203813 -1.376949 -0.025577
h -1.607652 -3.573069 1.270956
h 0.755871 -4.226239 -0.098151
h 2.115818 -4.331363 -5.164152
h 0.827912 -3.667749 -7.585428
h -3.609635 -1.010132 -8.752894
h -5.961622 -0.552293 -7.440410
h 2.716824 2.514750 -1.937582
h 2.082157 3.259644 -6.685745
h 2.611502 0.044472 -6.512646