

## Section 1: System setup with CHARMM software

### 1. Protonation scheme:

All Glu residues and Asp residues are deprotonated.

The  $\delta$ -N atom (HSD) protonated histidine residues correspond to residues numbered: 154, 249

The  $\epsilon$ -N atom (HSE) protonated histidine residues correspond to residues numbered: 3, 77, 119, 167

### 2. Active residues during geometry optimization:

The active region in QM/MM calculations:

LEU2 PHE4 ILE19 ILE22 ILE23 ARG26 ASP29 GLY30 MET31 ILE32 ILE33 LEU61  
ASN62 ASN64 PHE67 THR69 LYS70 VAL71 ALA72 GLN73 ILE74 TYR75 GLY76  
HSE77 ALA78 ILE79 VAL80 GLY81 GLN82 LEU86 TYR89 SER92 SER93 PHE96  
PHE110 VAL114 PHE118 PRO129 TYR137 THR138 PRO139 ALA140 THR141 ILE142  
ARG143 LEU144 LEU145 LEU146 ARG149 GLU150 ILE151 ALA152 VAL153 HSD154  
VAL155 GLY156 ASN157 ASP158 PHE159 LEU160 LEU161 MET162 ALA164 ALA165  
LEU168 LEU172 ASP173 LEU174 SER175 ASP176 GLN177 LEU178 SER179 TYR180  
PHE181 ILE182 PRO183 LEU184 THR185 VAL186 GLY191 GLU192 LEU193 VAL194  
VAL195 TYR196 SER197 LEU198 GLU199 TRP200 ASN201 PRO202 ALA205 MET211  
TYR214 MET215 VAL218 GLU219 ILE222 SER229 VAL230 ALA231 TYR232 ALA233  
PRO234 ASP238 MET239 LEU240 LEU241 PHE242 ASN243 GLY244 GLY245 ARG246  
TYR247 TYR248 HSD249 ARG250 VAL251 SER252 GLU253 VAL254 ARG260 ARG261  
THR262 ILE263 GLY264 GLY265 PHE266 LEU267 ALA268 PHE269 ILE276 TYR277  
TYR278 TRP279 SER280 FOC281 AKG282 6CU283 SOLV6 SOLV11 SOLV13 SOLV16  
SOLV28 SOLV29 SOLV40 SOLV48 SOLV56 SOLV57 SOLV266 SOLV379 SOLV525  
SOLV694 SOLV884 SOLV973 SOLV995 SOLV1724 SOLV1756 SOLV1913 SOLV1985  
SOLV2063 SOLV2432 SOLV2598 SOLV2621 SOLV2651 SOLV2665 SOLV2681  
SOLV2860 SOLV2884 SOLV2949 SOLV2999 SOLV3223 SOLV3277 SOLV3498  
SOLV3831 SOLV3967 SOLV4082 SOLV4295 SOLV4488 SOLV4514 SOLV4526  
SOLV4703 SOLV4707 SOLV4724 SOLV4920 SOLV5327 SOLV5557 SOLV5570  
SOLV5596 SOLV5744 SOLV5754 SOLV5812 SOLV6189 SOLV6421 SOLV6499  
SOLV6510 SOLV6755 SOLV6861 SOLV7251 SOLV7279 SOLV7427 SOLV7465  
SOLV7582 SOLV7601 SOLV7665 SOLV7767 SOLV7865 SOLV74 SOLV245 SOLV258  
SOLV459 SOLV479 SOLV484 SOLV589 SOLV616 SOLV1176 SOLV1240 SOLV1348  
SOLV1379 SOLV1444 SOLV1488 SOLV1565 SOLV1815 SOLV2256 SOLV2531  
SOLV2784 SOLV2893 SOLV3433 SOLV3499 SOLV3573

## Section 2: Yamaguchi's method to estimate the effect of spin contamination on the energies

During the calculation it was found that many species exhibited significant spin contamination, as judged by their  $\langle S^2 \rangle$  values. Large spin contaminations signify the inadequacy of the single-determinant Kohn-Sham framework, and may reduce the reliability of the results. To examine

whether spin contamination had an appreciable effect on the computed energetics, we performed spin projections using Yamaguchi's method on every species whose  $\langle S^2 \rangle$  was at least 0.1 larger than the theoretical value.<sup>1</sup> Specifically, we computed the single point energy,  $E_{LS}$ , of the desired spin state  $S$ , as well as the single point energy  $E_{HS}$  of the spin state  $S + 1$ . The  $\langle S^2 \rangle$  values of both spin states were also obtained from the calculations. Then, the spin-projected energy of the spin state  $S$  was calculated by

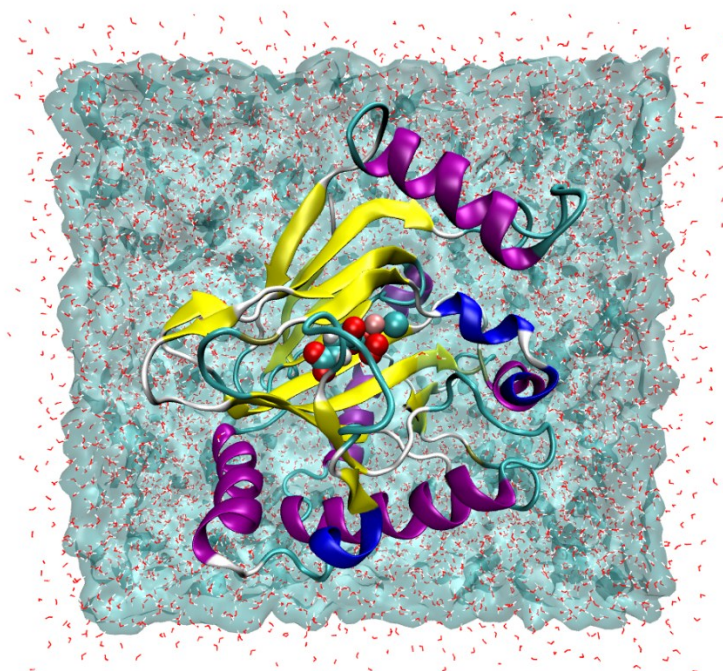
$$E_{LS,proj} = \frac{(\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS,theor})E_{LS} - (\langle S^2 \rangle_{LS} - \langle S^2 \rangle_{LS,theor})E_{HS}}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}}$$

where  $\langle S^2 \rangle_{LS,theor}$  is the theoretical  $\langle S^2 \rangle$  value of spin state  $S$ , namely  $\langle S^2 \rangle_{LS,theor} = S(S + 1)$ . In all cases, the correction introduced by the spin projection were less than 3 kcal/mol. Moreover, the conclusions in the article were not affected by the spin projection. Thus, it was deemed that spin contamination did not play a decisive role in the relative energetics of the species studied in this article.

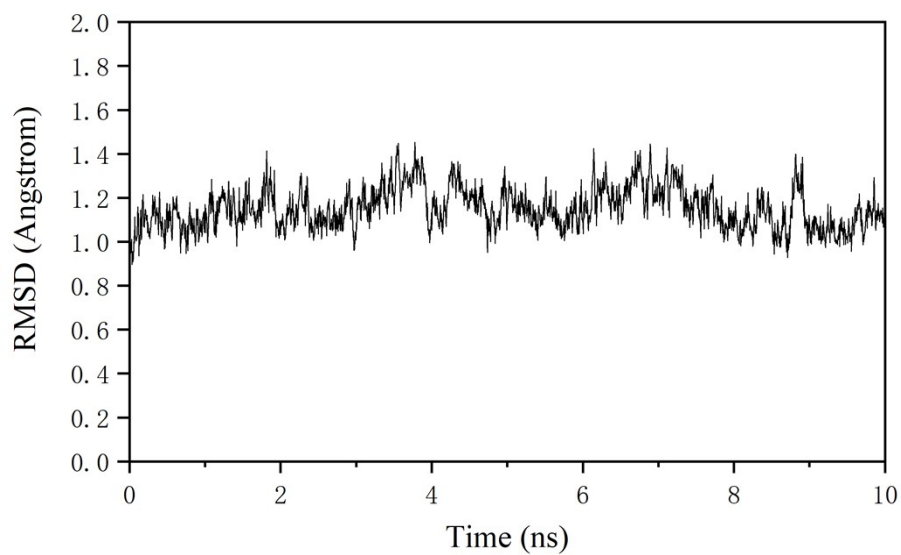
**Table S1.**  $\langle S^2 \rangle$  for all structures in QM/MM calculations.

	<b><sup>3</sup>RC1</b>	<b><sup>3</sup>TS1</b>	<b><sup>3</sup>Int1</b>	<b><sup>3</sup>TS2</b>	<b><sup>3</sup>Int2</b>	<b><sup>3</sup>TS3</b>	<b><sup>3</sup>Int3</b>
$\langle S^2 \rangle$	2.01	2.04	2.03	2.02	2.14	2.13	2.76
	<b><sup>3</sup>Int4</b>	<b><sup>3</sup>TS<sub>H</sub></b>	<b><sup>3</sup>Int5</b>	<b><sup>3</sup>TS<sub>OH</sub></b>	<b><sup>3</sup>TS<sub>Cl</sub></b>	<b><sup>3</sup>P<sub>OH</sub></b>	<b><sup>3</sup>P<sub>Cl</sub></b>
$\langle S^2 \rangle$	2.04	3.02	3.06	2.87	2.8	2.21	2.02
	<b><sup>5</sup>RC1</b>	/	/	<b><sup>5</sup>TS2</b>	<b><sup>5</sup>Int2</b>	<b><sup>5</sup>TS3</b>	<b><sup>5</sup>Int3</b>
$\langle S^2 \rangle$	6.9	/	/	6.06	6.01	6.63	6.05
	<b><sup>5</sup>Int4</b>	<b><sup>5</sup>TS<sub>H</sub></b>	<b><sup>5</sup>Int5</b>	<b><sup>5</sup>TS<sub>OH</sub></b>	<b><sup>5</sup>TS<sub>Cl</sub></b>	<b><sup>5</sup>P<sub>OH</sub></b>	<b><sup>5</sup>P<sub>Cl</sub></b>
$\langle S^2 \rangle$	6.05	6.94	6.08	6.98	6.98	6.01	6.01

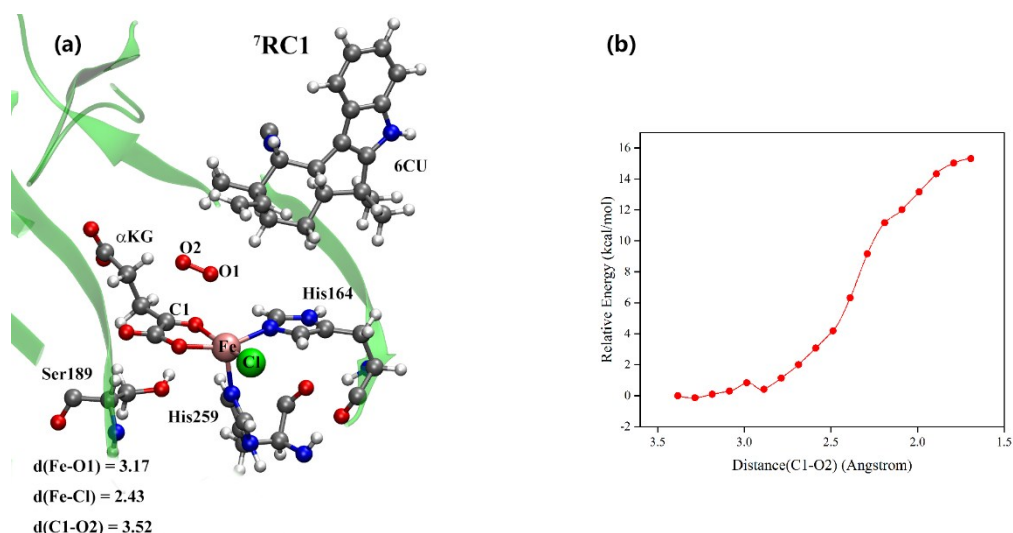
### Section 3: QM/MM results with the ChemShell program.



**Figure S1.** Wild-type WelO5 with a water layer of 12 Å thickness from solvation setup. Atoms of QM region are shown in the VMD model. Water molecules are shown in lines. Others are shown in the “New Cartoon” model.

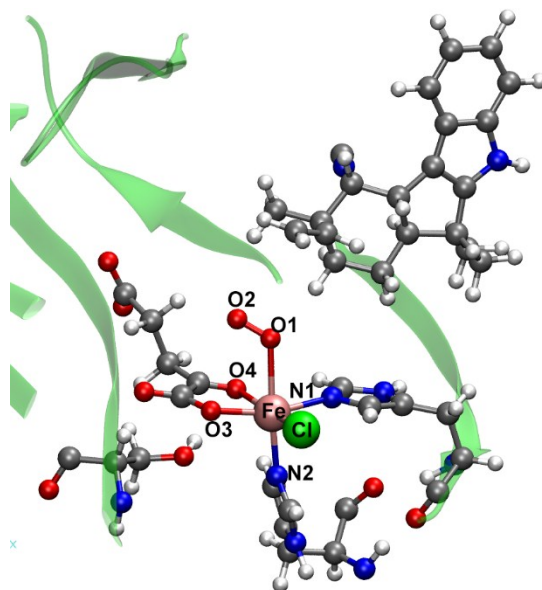


**Figure S2.** RMSD in the MD simulation for 10 ns. (Benchmark is protein backbone.)



**Figure S3.**  $\text{O}_2$  activation on the septet surface. (a) The QM/MM-optimized geometry (in Å) of  ${}^7\text{RC1}$ , along with the key structural parameters at UB3LYP/B1. (b) UB3LYP/B2 relative QM/MM energies (kcal/mol) for  $\text{O}_2$  binding to Fe(II) species on the septet pathway. As we can see from (b), the approach of  $\text{O}_2$  to C1 is accompanied by an almost monotonic increase in energy. Therefore, no stable adduct of the enzyme with  $\text{O}_2$  is present on the septet PES.

**Table S2.** The Mulliken spin populations of key atoms of the enlarged QM region (total 277 atoms) versus those of the chosen QM region (total 89 atoms). Geometry is from  ${}^5\text{RC1}$ .



Spin populations	Fe	Cl	O1	O2	O3	O4	N1	N2
Large QM region	3.77919	0.05640	0.02245	-0.01298	0.03601	0.02304	0.02149	0.01276
Chosen QM region	3.77672	0.06226	0.02728	-0.01157	0.03837	0.02227	0.02174	0.01201

The large QM region contains ARG143, ILE151, HSD154, VAL155, GLY156, GLN177, SER179, LEU193, PHE 242, GLY244, HSD249, PHE266, FOC281, AKG282, 6CU283 and five water molecules. As seen from the table, the large QM region shares similar spin populations with the

chosen QM region for the first coordination shell of Fe.

**Table S3.** Spin populations for species in the S=1 and S=2 pathways.

	<sup>3</sup> RC1	<sup>3</sup> TS1	<sup>3</sup> Int1	<sup>3</sup> TS2		<sup>3</sup> Int2	<sup>3</sup> TS3	<sup>3</sup> Int3
<b>Fe</b>	3.77133	1.07617	1.10570	0.98423	<b>Fe</b>	1.97854	2.14566	2.77313
<b>Cl</b>	0.06007	0.00237	0.00874	-0.02381	<b>Cl</b>	-0.00600	-0.01960	-0.04474
<b>O1</b>	-0.97198	0.52362	0.53116	0.10923	<b>O1</b>	0.01940	-0.01153	-0.51671
<b>O2</b>	-0.99512	0.46884	0.37651	0.06367	<b>CO<sub>2</sub></b>	0.00117	0.00186	0.00463
<b>α-KG</b>	0.06361	-0.02339	0.02626	0.86775	<b>SUC</b>	-0.02126	-0.15627	-0.26996
<b>His164</b>	0.03014	-0.02170	-0.02271	-0.01316	<b>His164</b>	0.04050	0.04831	0.06084
<b>His259</b>	0.04262	-0.02692	-0.02748	-0.00852	<b>His259</b>	-0.01269	-0.00914	-0.00927
<b>6CU</b>	-0.00169	-0.00102	-0.00069	0.00122	<b>6CU</b>	0.00018	0.00027	0.00145
<b>Ser189</b>	0.00102	0.00204	0.00252	0.01935	<b>Ser189</b>	0.00016	0.00042	0.00062

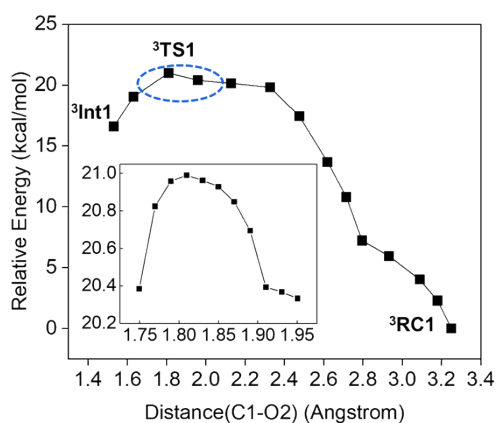
  

	<sup>5</sup> RC1	/	/	<sup>5</sup> TS2		<sup>5</sup> Int2	<sup>5</sup> TS3	<sup>5</sup> Int3
<b>Fe</b>	3.77672			4.21949	<b>Fe</b>	3.75382	3.09597	3.08648
<b>Cl</b>	0.06226			0.15244	<b>Cl</b>	0.05570	0.00375	0.10137
<b>O1</b>	0.02728			-0.39838	<b>O1</b>	0.07602	0.52324	0.66056
<b>O2</b>	-0.01157			-0.32834	<b>CO<sub>2</sub></b>	0.00000	0.00000	0.00022
<b>α-KG</b>	0.06984			0.18426	<b>SUC</b>	0.03904	0.30031	0.10229
<b>His164</b>	0.03444			0.07799	<b>His164</b>	0.03115	-0.00384	-0.02629
<b>His259</b>	0.04146			0.09189	<b>His259</b>	0.04297	0.07211	0.07424
<b>6CU</b>	-0.00139			0.00115	<b>6CU</b>	0.00027	0.00000	0.00000
<b>Ser189</b>	0.00100			-0.00053	<b>Ser189</b>	0.00104	0.00843	0.00118

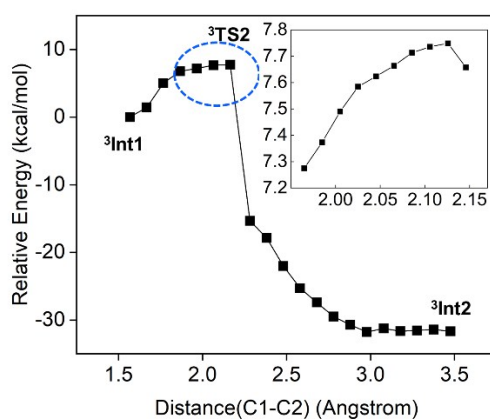
  

	<sup>5</sup> Int4	<sup>5</sup> TS <sub>H</sub>	<sup>5</sup> Int5	<sup>5</sup> TS <sub>Cl</sub>	<sup>5</sup> P <sub>Cl</sub>	<sup>5</sup> TS <sub>OH</sub>	<sup>5</sup> P <sub>OH</sub>
<b>Fe</b>	3.05635	4.16192	4.19003	4.17004	3.7578	4.18492	3.77875
<b>Cl</b>	0.07890	0.15389	0.17051	0.18010	0.01932	0.14507	0.05975
<b>O1</b>	0.69052	0.11493	0.27875	0.26923	0.09438	0.27927	0.01045
<b>SUC</b>	0.09596	0.16017	0.18381	0.18371	0.07265	0.19049	0.07924
<b>His164</b>	-0.02181	0.06027	0.04906	0.04911	0.01731	0.05810	0.03569
<b>His259</b>	0.09440	0.09115	0.10366	0.09425	0.03070	0.09288	0.03129
<b>Ser189</b>	-0.00130	0.00193	0.00458	0.00478	0.00516	0.00411	0.00052
<b>6CU</b>	0.00702	-0.74432	-0.98026	-0.95101	0.00286	-0.95503	0.00415

	<sup>3</sup> Int4	<sup>3</sup> TS <sub>H</sub>	<sup>3</sup> Int5	<sup>3</sup> TS <sub>Cl</sub>	<sup>3</sup> P <sub>Cl</sub>	<sup>3</sup> TS <sub>OH</sub>	<sup>3</sup> P <sub>OH</sub>
<b>Fe</b>	3.05635	4.16192	4.19003	4.17004	3.7578	4.18492	3.77875
<b>Cl</b>	0.07890	0.15389	0.17051	0.18010	0.01932	0.14507	0.05975
<b>O1</b>	0.69052	0.11493	0.27875	0.26923	0.09438	0.27927	0.01045
<b>SUC</b>	0.09596	0.16017	0.18381	0.18371	0.07265	0.19049	0.07924
<b>His164</b>	-0.02181	0.06027	0.04906	0.04911	0.01731	0.05810	0.03569
<b>His259</b>	0.09440	0.09115	0.10366	0.09425	0.03070	0.09288	0.03129
<b>Ser189</b>	-0.00130	0.00193	0.00458	0.00478	0.00516	0.00411	0.00052
<b>6CU</b>	0.00702	-0.74432	-0.98026	-0.95101	0.00286	-0.95503	0.00415



**Figure S4.** Energy scans for C1-O2 bonding process from <sup>3</sup>RC1 to <sup>3</sup>Int1.



**Figure S5.** Energy scans for decarboxylation process from <sup>3</sup>Int1 to <sup>3</sup>Int2.

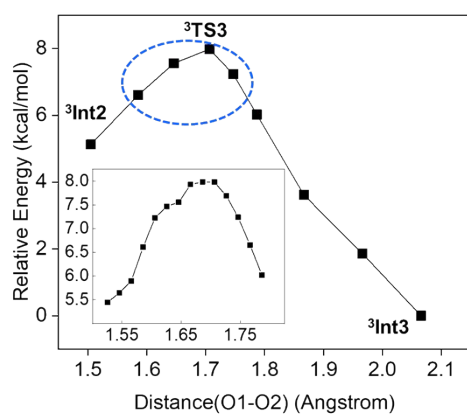


Figure S6. Energy scans for O1-O2 cleavage process from  $^3\text{Int2}$  to  $^3\text{Int3}$ .

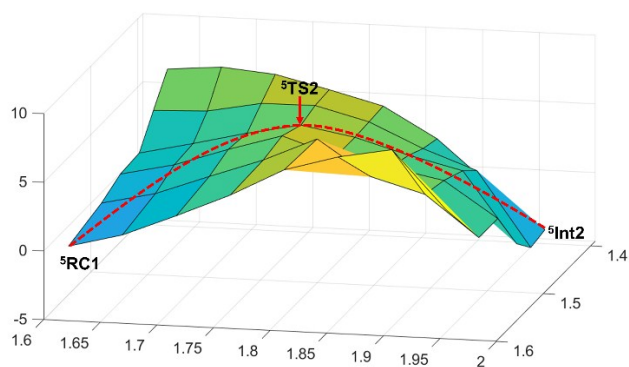


Figure S7. 2D energy scan for decarboxylation process from  $^5\text{RC1}$  to  $^5\text{Int2}$ .

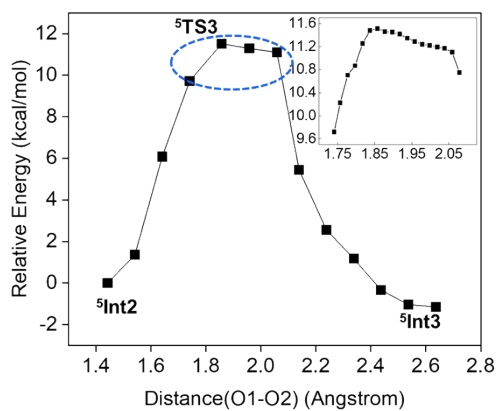


Figure S8. Energy scans for O1-O2 cleavage process from  $^5\text{Int2}$  to  $^5\text{Int3}$ .

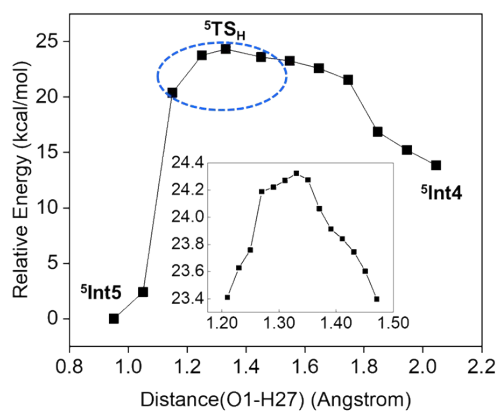


Figure S9. Energy scans for H-abstraction process from  $^5\text{Int4}$  to  $^5\text{Int5}$ .

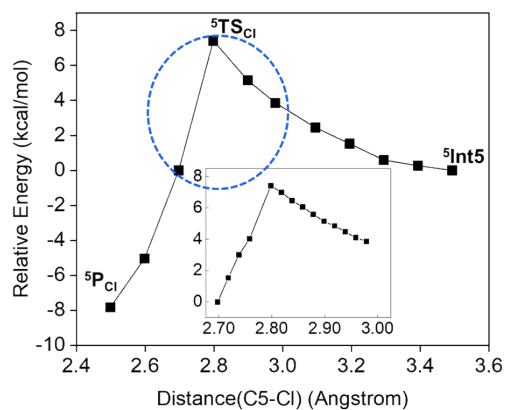


Figure S10. Energy scans for chlorination process from  $^5\text{Int5}$  to  $^5\text{P}_{\text{Cl}}$ .

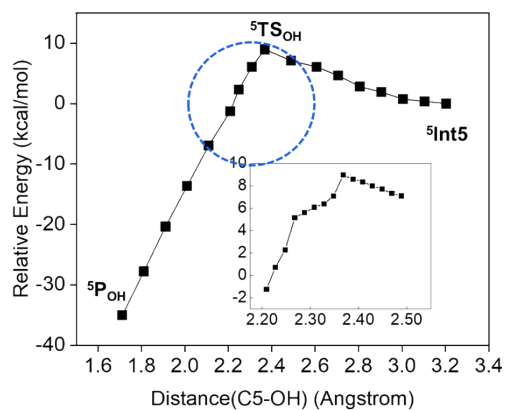


Figure S11. Energy scans for hydroxylation process from  $^5\text{Int5}$  to  $^5\text{P}_{\text{OH}}$ .



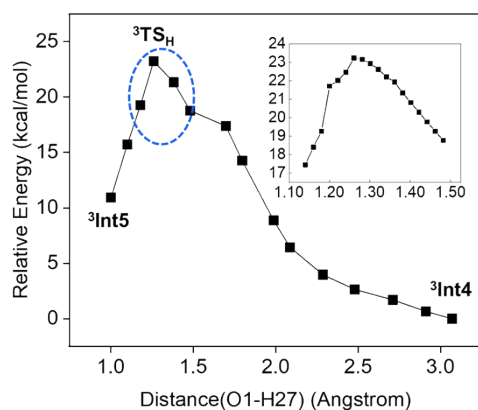


Figure S12. Energy scans for H-abstraction process from  $^3\text{Int4}$  to  $^3\text{Int5}$ .

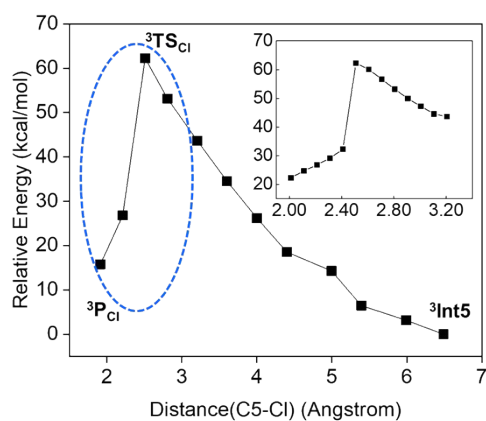


Figure S13. Energy scans for chlorination process from  $^3\text{Int5}$  to  $^3\text{P}_{\text{Cl}}$ .

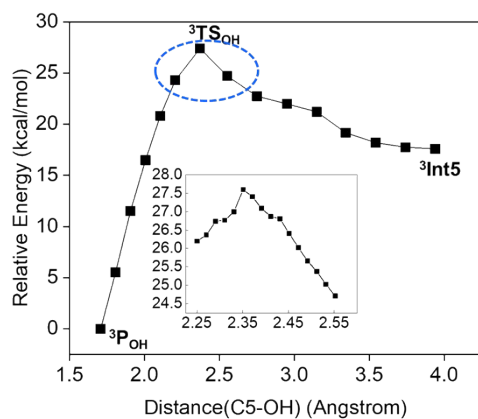


Figure S14. Energy scans for hydroxylation process from  $^3\text{Int5}$  to  $^3\text{P}_{\text{OH}}$ .

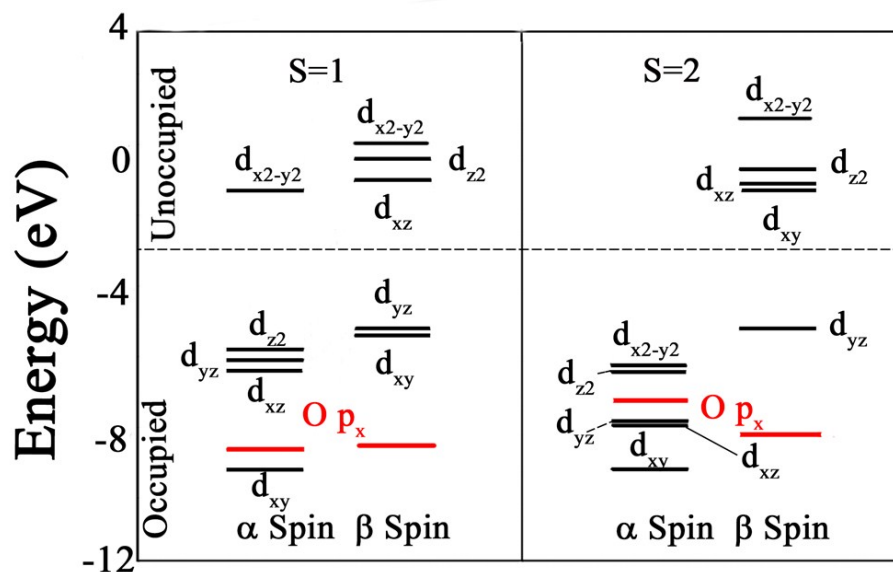


Figure S15. Molecular orbital diagrams of  $^3\text{Int2}$  and  $^5\text{on}^3\text{Int2}$ .

#### Section 4: Cartesian coordinates

The Cartesian coordinates of the QM regions in QM/MM calculations

<b><math>^3\text{RC1}</math>:</b>	C	41.041318	30.876903	43.196567			
C	43.196973	25.308853	42.803678	H	41.995478	31.318347	42.944431
H	44.156732	25.582019	42.356048	N	40.215200	30.282124	42.345575
H	43.091843	24.224818	42.690709	C	39.139697	29.841365	43.084827
N	40.773210	25.672191	42.010170	H	38.318271	29.310748	42.626268
H	40.358540	24.828093	42.409644	Fe	40.543088	29.652446	40.358849
C	42.106288	26.056445	42.096258	Cl	42.874198	30.341679	40.258163
C	40.101653	26.633551	41.332425	O	39.945669	28.920339	36.953440
H	39.043217	26.597596	41.124478	O	40.765721	28.601668	37.792200
N	40.923689	27.612553	40.968308	C	36.363667	29.781880	38.715217
C	42.174439	27.254015	41.436255	C	37.765911	29.938011	39.219752
H	43.028554	27.893043	41.277014	H	35.792982	30.678759	38.986596
C	40.071280	34.617223	39.021856	H	35.896301	28.911551	39.178570
H	39.577445	35.070319	39.896200	O	38.331229	29.118237	39.950519
H	39.305740	34.096576	38.431956	C	38.604384	31.176713	38.781515
O	41.084774	33.716166	39.417641	O	39.819842	31.152097	39.210185
H	40.748138	32.810994	39.286975	O	38.083249	32.056526	38.093138
C	38.438701	29.851748	45.563675	C	36.359100	29.651514	37.176421
H	37.401110	29.742870	45.238883	C	35.002674	29.256892	36.533075
H	38.462496	30.664940	46.293795	H	37.092018	28.899024	36.856239
N	40.529477	30.841523	44.448650	H	36.673170	30.605923	36.751169
H	41.001825	31.226265	45.271890	O	34.076004	28.887928	37.295092
C	39.314489	30.164300	44.400683	O	34.994205	29.328337	35.270705

C 42.040982 26.808131 35.044581  
C 41.889767 25.768981 35.867884  
H 42.988425 27.338140 34.993123  
H 41.251486 27.176387 34.396944  
H 42.743802 25.491296 36.482306  
C 39.429917 25.553957 35.331928  
H 39.601595 25.579856 34.250305  
H 38.524201 24.969471 35.510438  
H 39.246050 26.579110 35.667489  
C 41.319648 20.812453 39.667244  
H 40.397350 20.401023 39.243205  
H 41.864196 19.989601 40.143946  
H 41.050040 21.526023 40.455832  
C 42.181052 21.499419 38.592974  
C 43.525305 21.954463 39.204927  
H 44.148854 22.475057 38.471270  
H 44.095259 21.093316 39.568884  
H 43.360339 22.628613 40.053457  
C 38.746952 22.012738 35.599849  
N 39.683695 22.715141 35.497738  
C 40.897371 23.481440 35.539667  
H 41.263114 23.562026 34.509626  
C 40.628225 24.943957 36.080881  
C 40.305420 24.889877 37.608834  
H 39.306060 24.448550 37.703750  
H 40.233250 25.917475 37.981805  
C 41.279743 24.067635 38.488878  
H 40.880056 24.033757 39.510196  
H 42.260136 24.555319 38.556690  
C 41.395479 22.667664 37.888837  
C 41.928654 22.751227 36.430978  
H 40.373384 22.277419 37.799634  
H 42.834400 23.372741 36.394985  
C 42.407882 20.647352 37.359599  
N 42.804407 19.346926 37.139552  
C 42.895786 19.166636 35.761030  
C 43.195786 18.012696 35.030248  
C 43.219039 18.104050 33.641397  
C 42.952437 19.324630 32.987583  
C 42.644723 20.471431 33.708824  
C 42.598496 20.408345 35.113770  
C 42.277681 21.318246 36.171221  
H 42.783315 18.582179 37.818271  
H 43.387348 17.076049 35.538408

H 43.448039 17.220648 33.053960  
H 42.990978 19.372714 31.903247  
H 42.440284 21.405109 33.190970  
H 43.218747 25.474460 43.880788  
H 38.747629 28.966424 46.119401  
H 40.496667 35.447039 38.457482

**<sup>3</sup>TS1:**

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### <sup>3</sup>Int1

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C	42.179821	27.105392	41.522692	H	39.319865	26.660718	35.906708
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C	40.181435	34.543519	38.907627	H	40.482514	20.421864	39.362576
H	39.478684	34.869212	39.689930	H	41.973419	19.993413	40.216606
H	39.630659	33.939810	38.171840	H	41.181609	21.533929	40.561597
O	41.270849	33.833244	39.446605	C	42.254404	21.509343	38.664782
H	41.025792	32.904615	39.569512	C	43.622839	21.944331	39.237361
C	38.438687	29.805108	45.489082	H	44.228222	22.464753	38.488545
H	37.397590	29.683499	45.179547	H	44.194483	21.073892	39.575599
H	38.469128	30.649307	46.184150	H	43.492357	22.613260	40.095837
N	40.514895	30.755480	44.325909	C	38.739506	22.083367	35.750651
H	40.982606	31.160996	45.136952	N	39.679155	22.782604	35.652011
C	39.304942	30.067378	44.304064	C	40.903979	23.534741	35.670218
C	41.027249	30.746873	43.072697	H	41.239397	23.621370	34.630238
H	41.971202	31.198042	42.802839	C	40.679389	24.996722	36.233355
N	40.207529	30.110000	42.243738	C	40.414247	24.945331	37.772144
C	39.132720	29.692755	43.000523	H	39.406462	24.532556	37.904410
H	38.319276	29.140288	42.555011	H	40.391128	25.974381	38.147167
FE	40.479527	29.483849	40.323753	C	41.395139	24.088891	38.610114
CL	42.591742	30.575416	40.243056	H	41.028983	24.053966	39.643307
O	39.209586	28.760621	37.976894	H	42.387995	24.553411	38.651028
O	40.459661	29.374037	38.487655	C	41.462694	22.692616	37.994446
C	36.934792	28.206071	38.371694	C	41.951310	22.779012	36.520884
C	38.286600	28.637880	38.899274	H	40.431683	22.319928	37.935405
H	36.181500	28.530716	39.092687	H	42.863360	23.389420	36.463755
H	36.901711	27.108574	38.360502	C	42.436662	20.664117	37.419907
O	38.512352	28.902394	40.098051	N	42.835508	19.366948	37.183851
C	37.905508	32.088976	38.737326	C	42.904292	19.196487	35.803278
O	38.637535	31.944056	39.639083	C	43.207621	18.050979	35.060629
O	37.170830	32.256331	37.844766	C	43.215806	18.153229	33.672233
C	36.629534	28.771343	36.980201	C	42.930572	19.376187	33.031229
C	35.159326	28.697353	36.507367	C	42.618798	20.514490	33.764791
H	37.259158	28.287417	36.226064	C	42.588621	20.441973	35.169897
H	36.902135	29.833375	36.959159	C	42.279952	21.343453	36.239570
O	34.297888	28.301738	37.333838	H	42.817891	18.596073	37.855036
O	34.975515	29.075402	35.314402	H	43.417060	17.111864	35.558397
C	42.084705	26.842455	35.154176	H	43.448897	17.276727	33.075813
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H	41.277199	27.226815	34.539120	H	43.279935	25.392601	44.007315
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C	39.465247	25.639688	35.540250	H	40.555059	35.431286	38.397389
H	39.594762	25.681449	34.453127				
H	38.556972	25.066000	35.742501				

**<sup>3</sup>TS3:**

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C	40.179870	26.406539	41.470766	C	39.472088	25.637199	35.546669
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H	43.054751	27.755567	41.347551	C	41.422769	20.816476	39.759912
C	40.184932	34.528250	38.925565	H	40.483704	20.418374	39.360421
H	39.495983	34.851864	39.719919	H	41.972356	19.985269	40.216282
H	39.622823	33.930734	38.193729	H	41.184717	21.528155	40.560146
O	41.281516	33.811399	39.443192	C	42.259322	21.501333	38.664866
H	41.030773	32.885983	39.578585	C	43.628382	21.931299	39.239319
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H	37.399714	29.682856	45.157787	H	44.196998	21.058458	39.576625
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C	39.310503	30.061169	44.289458	C	40.910533	23.531498	35.672860
C	41.043500	30.727174	43.066449	H	41.245001	23.617840	34.632598
H	41.994404	31.167330	42.803541	C	40.687423	24.993582	36.237165
N	40.224548	30.091759	42.234359	C	40.424931	24.942153	37.776229
C	39.141787	29.684405	42.984933	H	39.416374	24.531701	37.909963
H	38.326986	29.139280	42.534711	H	40.403916	25.971395	38.150382
FE	40.514442	29.458177	40.304818	C	41.405078	24.083183	38.612532
CL	42.624197	30.572175	40.283964	H	41.039149	24.047783	39.645794
O	39.191476	28.667927	37.957476	H	42.398959	24.545728	38.653842
O	40.592215	29.353695	38.582825	C	41.470324	22.687314	37.995783
C	36.898657	28.267961	38.409121	C	41.958007	22.774583	36.522277
C	38.298773	28.628104	38.888643	H	40.438531	22.316557	37.937007
H	36.178778	28.640508	39.141747	H	42.870356	23.384614	36.465088
H	36.806618	27.174489	38.409357	C	42.440240	20.657554	37.418729
O	38.557025	28.904685	40.089118	N	42.837026	19.360054	37.180366
C	37.919582	32.084614	38.711660	C	42.904917	19.191644	35.799419
O	38.645081	31.923814	39.616106	C	43.204997	18.046544	35.054575
O	37.192018	32.267995	37.816726	C	43.212361	18.151249	33.666359
C	36.605136	28.825909	37.010031	C	42.929495	19.376020	33.027489
C	35.140687	28.753486	36.519993	C	42.620643	20.513796	33.763345
H	37.230898	28.317235	36.269109	C	42.591339	20.438807	35.168355
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**<sup>3</sup>Int3:**

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**<sup>5</sup>RC1:**

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**<sup>5</sup>TS1:**

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C	38.751144	22.033215	35.657380	H	43.240751	27.788035	41.378724
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C	40.897362	23.509597	35.598265	H	39.519766	34.758533	39.822437
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C	40.632946	24.969941	36.149733	O	41.136146	33.525390	39.369279
C	40.318540	24.908514	37.678510	H	40.810189	32.611308	39.277340
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H	40.913818	24.042532	39.570357	N	40.589298	30.807099	44.456828
H	42.283185	24.572006	38.604811	H	41.048755	31.204570	45.280488
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C	41.935730	22.772065	36.476034	C	41.120497	30.818015	43.211066
H	40.394687	22.291757	37.858162	H	42.081668	31.249885	42.968750
H	42.842193	23.392230	36.434595	N	40.303578	30.218939	42.355340
C	42.423504	20.665727	37.395619	C	39.210815	29.803562	43.083223
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C	43.195926	18.031359	35.060949	CL	42.953556	30.338088	40.294955
C	43.208489	18.122216	33.671858	O	38.626638	30.424669	38.522914
C	42.934901	19.342187	33.019993	O	39.942386	30.741917	39.038196
C	42.630665	20.488961	33.743184	C	36.704245	29.005422	38.525445
C	42.594693	20.427601	35.148665	C	38.066866	29.360625	39.087182
C	42.281939	21.337806	36.209150	H	35.942292	29.514795	39.125652
H	42.795463	18.599069	37.848997	H	36.568232	27.936896	38.711251
H	43.393965	17.094495	35.567091	O	38.624271	28.728098	39.991487
H	43.434457	17.238898	33.082939	C	36.814809	32.584561	38.687456
H	42.965994	19.389128	31.935217	O	36.356279	32.066182	39.629381
H	42.420472	21.421746	33.226093	O	37.248718	33.137531	37.752868
H	43.261325	25.429219	43.963091	C	36.508935	29.333445	37.043306
H	38.756634	28.959986	46.120657	C	35.098158	29.041108	36.469623
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**<sup>5</sup>Int2:**

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C	42.313661	25.951432	42.202056	H	41.279292	27.192187	34.488799
C	40.324878	26.504972	41.384368	H	42.772587	25.526193	36.589002
H	39.271970	26.464395	41.151713	C	39.448690	25.605837	35.478021
				H	39.598002	25.639977	34.393305

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**<sup>5</sup>TS3:**

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H	38.934741	28.373337	38.782358	H	37.457746	28.882153	35.717644
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C	35.539171	28.138127	32.109209	H	36.133465	26.692555	42.693878
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**<sup>5</sup>P<sub>Cl</sub>**

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### <sup>3</sup>Int4

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**<sup>3</sup>Int5**

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<sup>3</sup>P<sub>Cl</sub>

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H	38.834936	25.166029	36.880326	N	42.847681	19.474200	37.245694
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C	40.947389	25.229483	36.357698	H	38.739953	29.033334	46.046054
C	41.395187	25.409056	37.884530				

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