## Spectroscopic and Computational Investigation of Second-Sphere Contributions to Redox Tuning in *Eschericia coli* Iron Superoxide Dismutase

Laurie E. Grove, Juan Xie, Emine Yikilmaz, Anne-Frances Miller, and Thomas C. Brunold<sup>\*</sup>

## **Supporting Information.**

Tables S1-18. Cartesian coordinates for the QM/MM geometry-optimized active-site models used in this study.

**Table S19.** Structural parameters of the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>SOD derived from PDB file 1ISB.

**Table S20.** INDO/S-CI computed electronic excitation energies and zero-field splitting parameters for the QM/MM geometry-optimized active-site model of  $Fe^{3+}SOD$  derived from PDB file 1ISB.

**Table S21.** Structural parameters of QM/MM geometry-optimized active-site models for the oxidized and reduced states of Fe(Mn)SOD derived from PDB file 1MMM.

**Tables S22-S23.** Structural parameters of QM/MM geometry-optimized active-site models for the oxidized and reduced states of Q69E FeSOD.

**Table S24.** INDO/S-CI computed electronic transition energies and zero-field splitting parameters for QM/MM geometry-optimized  $Fe^{2+}SOD$ ,  $Fe^{2+}(Mn)SOD$ , and Q69E  $Fe^{2+}SOD$  active-site models.

**Tables S25-S26.** Computed electronic transition energies and zero-field splitting parameters for QM/MM geometryoptimized active-site models of oxidized and reduced Fe(Mn)SOD derived from the PDB file 1MMM.

**Tables S27-S30.** Energies, occupations, and composition of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for Fe<sup>3+</sup>-bound SOD species, obtained from DFT/COSMO computations using ORCA 2.4 (B3LYP functional) and  $\varepsilon$  = 4.0.

**Tables S31-S34.** Energies, occupations, and composition of the  $Fe^{3+}$  3d-, Asp-, and Sol-based spin-down MOs for  $Fe^{3+}$ -bound SOD species, obtained from DFT computations using ADF 2006 (BP functional).

**Tables S35-S38.** Energies, occupations, and composition of the Fe<sup>2+</sup> 3d-based MOs for Fe<sup>2+</sup>-bound SOD species, obtained from DFT/COSMO computations using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

**Tables S39-S42.** Energies, occupations, and composition of the  $Fe^{2+}$  3d-based MOs for  $Fe^{2+}$ -bound SOD species, obtained from DFT computations using ADF 2006 (BP functional).

**Table S43.** DFT/COSMO ( $\varepsilon = 4.0$ ) computed total energies,  $\varepsilon_{PT}$ ,  $\varepsilon_{ET}$ , pK, and  $E^{\circ}$  values for Fe(Mn)SOD obtained with the QM/MM geometry-optimized active-site models derived from the PDB file 1MMM.

**Table S44.** DFT/COSMO ( $\varepsilon = 10.0$ ) computed total energies,  $\varepsilon_{PT}$ ,  $\varepsilon_{ET}$ , pK, and  $E^{\circ}$  values for the QM/MM geometryoptimized FeSOD, Fe(Mn)SOD, and Q69E FeSOD active-site models.

**Table S45.** DFT/COSMO computed solvation energies for the QM/MM geometry-optimized FeSOD, Fe(Mn)SOD, and Q69E FeSOD active-site models.

Figures S1-S2. Abs, CD, and MCD spectra of the Fe<sup>3+</sup>(Mn)SOD and Q69E Fe<sup>3+</sup>SOD species.

**Supplementary Calculations.** Effect of OH<sup>-</sup> binding to  $\text{Fe}^{3+}(\text{Mn})$ SOD and Q69E  $\text{Fe}^{3+}$ SOD on experimental  $E^{\circ}$  values.

Atom	х	У	Z	С	3.429016	2.808319	6.163834
С	-1.968597	-0.456619	-5.893906	С	2.227432	2.513336	5.562836
С	-0.434052	-0.331833	-5.839310	Ν	1.191971	2.535141	6.210678
C	0.073029	-0.201645	-4.444107	С	1,682373	2.863449	5.318375
N	1 414871	-0 312622	-4 107727	Ċ.	1.008102	3.039276	4.067917
C	1 5/2755	-0 177109	-2 763229	Ċ	1 762878	3 448242	2 862808
N	0 352150	0.177105	-2 210205	C	3 147476	3 672531	1 7598/2
N C	0.552150	0.000377	2 242607	Ċ	3 000505	3 177075	1 060637
C III	-0.004423	0.007120	-3.243007	C	2 006022	2 050007	2 072100
H	-2.314/43	-0.9/9446	-4.994080	C II	5.000025	0.009097	3.072109
H	-2.299/59	-1.080933	-6./49/41	H	5.670441	0.967133	4.194900
H	-2.446884	0.545868	-5.888855	H	4.840/14	0.809830	5.419556
Н	0.045212	-1.229431	-6.255859	H	6.464539	1.642441	6.996414
Н	-0.085388	0.510208	-6.455994	Н	4.725281	3.348022	6.895981
Н	2.218536	-0.527237	-4.715576	Н	5.445160	3.477982	7.133804
Н	2.482437	-0.210602	-2.228134	Н	2.050858	2.298065	5.536407
Н	-1.612732	0.201080	-3.058609	Н	0.189346	2.387802	7.262756
С	-9.049591	4.085724	0.871033	Н	-0.065750	2.876678	5.502594
С	-7.550095	4.171616	1.188934	Н	1.276642	3.608139	2.791138
С	-6.875168	2.823883	1.361450	Н	3.702026	3.994965	0.796280
С	-7.460892	1.774292	2.088531	Н	4.900681	3.647049	0.989777
С	-6.768250	0.587524	2.336487	С	5.172592	0.580093	3.136429
С	-5.477905	0.419403	1.824722	С	4.118851	0.630814	1.708939
0	-4.708557	-0.716415	2.063600	С	2.773804	0.043945	0.602753
С	-4.912308	1.407974	1.021484	0	2.514893	-0.346069	1.016724
C	-5.605728	2,599945	0.816986	0	1.908875	0.00000	2.152542
H	-9.594696	3,642136	1.717743	Fe	0.00000	0.00000	-0.000061
н	-9.223541	3,414169	-0.002731	0	-0.547562	0.000015	0.00000
н	-9 489578	5 094696	0 744843	н	4.743088	0.971405	1.820877
н	-7 016357	4 723923	0 400574	н	6 070100	1 185272	2 638992
и и	-7 103366	4 760121	2 110900	н	5 458466	-0 473328	1 447540
n u	- 7.405500	4.702131	2.110009	н	3 901047	1 667160	1 876114
п	7 222016	106225	2.4//009	11 U	1 116157	0 117523	1.070114
п	-7.222910	-0.196333	2.94/900	п 11	4.440457	0.11/020	0.299409
H	-5.084366	-1.185242	2.854630	п	0.303647	-0.140091 E 00100C	-0.310374
H	-3.916611	1.261246	0.607162	C	0.283013	- 5.991226	2.300903
н	-5.116882	3.40/288	0.26812/	C	-1.1458/4	-5.410233	-1./0104/
C	-3./14249	4.955048	4.015640	C	-1.209702	-4.054/03	-1.600494
С	-4.569885	3.690872	4.204483	N	-1.840942	-3.808624	-0.9518/4
С	-3.965317	2.670090	5.201019	C	-1.66/8//	-2.504654	0.261993
С	-2.617400	2.097778	4.770996	N	-0.967636	-1.886673	0.599808
0	-1.560196	2.481186	5.301376	С	-0.684814	-2.834595	-0.347946
N	-2.623657	1.162170	3.783844	Н	0.206223	-6.929596	-1.315704
Н	-2.654100	4.652328	3.942505	Н	0.709991	-6.261169	-2.331741
Н	-3.741028	5.643478	4.898224	Н	0.933853	-5.291855	-0.768539
Н	-3.966217	5.460144	3.035736	Н	-1.602631	-5.343826	-2.375946
Н	-5.579285	3.957870	4.547775	Н	-1.770279	-6.116409	-2.598526
Н	-4.721848	3.174561	3.245514	Н	-2.327744	-4.489716	-1.031800
Н	-3.785034	3.137527	6.175690	Н	-2.007645	-2.043060	0.837311
Н	-4.676453	1.840103	5.341248	Н	-0.096954	-2.573349	1.519867
Н	-1.753159	0.746063	3.428711				-2.189178
Н	-3.492889	0.825424	3.380554				
С	0.262772	6.143784	-0.882065				
С	-0.994980	5.453308	-1.455429				
С	-1.146942	4.054962	-0.950729				
Ν	-1.775070	3.777557	0.250046				
С	-1.601669	2.479355	0.563248				
N	-0.893524	1.876648	-0.389175				
C	-0.603622	2.851105	-1.338257				
H	1.1072.08	5.446121	-0.976257				
н	0 214523	6 445328	0 204086				
H	0 500427	6 991971	-1 534424				
H	-1 896530	6 029495	-1 210632				
H	-0 936569	5 417023	1.210032				
н	-2 3/7077	A A22101	-2 550116				
и П	-1 QE/200	J UJJJUU 4.400TQT	2.JJU440 0 7000£1				
и П	1.734200	2.023300	1 /70501				
С	5 106610	2.0410/1 1 /71570	1,4/0074 -2 210000				
C	J.400049 / 001361	7 0//00C	-2.210092 6 376343				
C	4.001301	2.044080	0.3/0343				

**Table S1.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{3+}SOD$  (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	х	У	Z	С	3.824142	2.349442	5.486374
С	-1.927597	-0.584091	-5.886459	С	2.622528	2.165771	6.169312
С	-0.394424	-0.463196	-5.826584	N	1.565536	2.358292	5.323456
C	0.103668	-0.188522	-4,449432	С	2.042740	2.702057	4.071716
N	1 448059	-0 264374	-4 107941	C	1.353180	3.006744	2,900360
C	1 567917	-0 118073	-2 765289	C	2.113266	3.379639	1.789139
N	0 374405	0.019515	-2 215317	C	3 516571	3 446548	1 856094
C	-0 530353	0.040040	-3 253201	C	1 201153	3 110092	3 019775
	-0.559552	1 067022	4 067200	C	3 163000	2 7200/7	1 150009
п	-2.200209	1 226252	-4.907209	U U	5.405909	2.720947	4.1J0009 E 220210
H	-2.2/9251	-1.236252	-6./15912	п	5.900373	0.295792	C 001122
H	-2.3/18/2	0.424866	-5.929184	н	5.053818	0.144257	0.8U113Z
H	0.101364	-1.396240	-6.119888	н	6./5544/	0.855300	6./18323
Н	-0.037460	0.291229	-6.544083	Н	5.215973	2.698471	7.022385
Н	2.239349	-0.522202	-4.713837	Н	5.896332	2.793671	5.409119
Н	2.506700	-0.134323	-2.227158	Н	2.458069	1.935074	7.218277
Н	-1.598785	0.146912	-3.076218	Н	0.567490	2.339400	5.549194
С	-8.499268	4.451263	0.693985	Н	0.266754	2.968369	2.864975
С	-7.014130	4.532257	1.091385	Н	1.615982	3.624649	0.849167
С	-6.424835	3.204636	1.525986	Н	4.076340	3.742096	0.971741
С	-6.930313	2.511230	2.637329	Н	5.295990	3.135208	3.046021
С	-6.402222	1.284119	3.038025	С	5.301758	0.190048	1.505554
С	-5.336411	0.721069	2.328873	С	4.190842	0.389862	0.479675
0	-4.766571	-0.500519	2.671890	С	2.837570	-0.151459	0.938660
С	-4.807693	1.390472	1.225052	0	2.630783	-0.677582	2.029297
C	-5.349960	2,620500	0.848175	0	1.903488	0.000000	0.000015
н	-9.054810	3.996552	1.529266	Fe	0.000000	0.000000	0.000000
н	-8.741806	3.814926	-0.199249	0	-0.472397	0.000000	1.856766
н	-8 921600	5 469498	0 591293	н	4.955048	0.533340	2.488266
н	-6 402176	4 954269	0 282013	н	6 236618	0 736633	1 251190
и П	-6 932693	5 226020	1 0/10/0	н	5 523834	-0.884460	1 574081
п 11	7 744005	2 022746	2 224210	и и	1 023666	1 /56131	0 263687
п 11	- 7.744095	2.955740	2 000720	и и	4.025000	-0 077957	-0 199911
п	-0.010010	0.700990	3.909729	п	4.429409	0.000000	- 0.409944 0.20100E
H	-5.102585	-0.767441	3.552/34	п	0.301207	-0.200100	2.301093
H	-3.959183	0.968872	0.684906	C	-0.201000	- 3.932203	-2.00/813
Н	-4.895981	3.155014	0.015533	C	-1.60/330	-5.1/3050	-1.896/13
C	-2.920593	5.467178	4.050537	C	-1.533844	-3.883804	-1.129410
С	-3.897293	4.280685	4.014755	N	-2.066269	-3.698486	0.142//6
С	-3.525269	3.121811	4.975266	С	-1.756424	-2.450226	0.575775
С	-2.201019	2.472214	4.599503	N	-1.033432	-1.821335	-0.348419
0	-1.121277	2.924988	5.024597	С	-0.900757	-2.697495	-1.412582
N	-2.261063	1.428055	3.731200	Н	-0.428436	-6.841217	-2.606781
Н	-1.894089	5.073593	4.147629	Н	0.111115	-6.272690	-1.006073
Н	-3.039215	6.139221	4.933151	Н	0.491531	-5.308365	-2.575623
Н	-2.958710	6.020782	3.078903	Н	-1.973251	-4.954041	-2.911667
Н	-4.927368	4.598587	4.238617	Н	-2.370010	-5.824921	-1.445007
Η	-3.953476	3.855255	2.999176	Н	-2.682297	-4.350357	0.615646
Н	-3.403580	3.488571	5.999954	Н	-2.018036	-2.033325	1.541229
Н	-4.335205	2.376282	4.965302	H	-0.361465	-2.419586	-2.310944
Н	-1.424866	0.941177	3.373000				
Н	-3.154755	1.017853	3.477005				
С	0.735336	6.040680	-0.945938				
С	-0.560074	5.426254	-1.515625				
С	-0.855103	4.069626	-0.965530				
Ν	-1.479355	3.883926	0.255890				
C	-1.445709	2.578979	0.588120				
N	-0.862869	1.883728	-0.385620				
C.	-0.491409	2.805511	-1.360031				
н	1 525787	5 275558	-0 994736				
и П	0 700531	6 387665	0 126190				
н	1 057800	6 836823	-1 631073				
н	-1 /10701	6 001/61	-1 207011				
ц 11	-0 163150	5 301/70	-2 6027/E				
л ц	-U.40313U -1 703076	J.JZI4/2 1 6/3060	-2.003/43 0 069505				
л u	-1.017C00	4.04380U 3 100500	U.002335 1 E00700				
п	-T.OT/000	2,10UD00 0 F0CF1C	1.343/88 2.057767				
п	0.035339	2.5U0510	-2.25//6/				
C	5./59430	0.1/3529	6.205200				
C	5.207260	2.213379	6.040802				

**Table S2.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{3+}SOD$  (starting coordinates based on PDB file 1ISB).<sup>1</sup>

Atom	x	Y	7.	C	2.585632	6.649963	-1.742096
				-	1.000002	5.015100	1 1 2 4 9 9
С	-1.722977	-5.977570	-0.285675	C	1.461639	7.217422	-1.174408
C	-0 225143	-5 756119	-0 544800	N	0 389450	6 350784	-1 254486
~	0.229119	3.730113	0.511000		0.000100	5.004102	1 001010
C	0.168182	-4.318573	-0.628036	C	0./930/6	5.204193	-1.891312
N	1 487152	-3 915421	-0 762848	С	0.065048	4.061417	-2.255859
	1 544660	0,010101	0.00000	G	0 700726	2 077104	2 002661
C	1.544662	-2.5605//	-0.69/006	L	0.729736	3.077194	-2.992001
N	0.330795	-2.063416	-0.501572	С	2.081680	3.236938	-3.364944
0	0 522210	2 144700	0 471756	C	2 000272	1 262110	2 007502
C	-0.533218	-3.144/00	-0.4/1/56	C	2.000275	4.303449	-2.90/303
H	-2.036514	-5.281982	0.503922	С	2.173843	5.363251	-2.228668
U	-1 011530	- 6 995122	0 122071	ч	5 173935	6 053986	-0 157031
п	-1.911330	-0.995422	0.1229/1	11	5.1/5555	0.055500	0.437031
H	-2.340302	-5.759430	-1.183868	Н	4.381409	7.472610	0.287598
ч	0 355118	-6 156570	0 300964	н	5 811340	7 727142	-0 803986
11	0.333110	0.130370	0.300304		5.011510		0.000000
H	0.100266	-6.306473	-1.438614	Н	3.818039	8.335556	-2.031113
н	2 334763	-1 193123	-0 848984	н	4 456940	6 866241	-2 742065
	2.351,03	1.155125	0.010901		1 220222	0 107076	0 710070
н	2.451019	-1.9//386	-0./91168	H	1.338333	8.19/8/6	-0./180/9
H	-1.599106	-3.002960	-0.365555	Н	-0.569855	6.521133	-0.937622
0	0 040217	1 467056	2 264022	ч	-1 006729	3 000710	-2 056152
C	-9.840317	1.40/030	-2.204023	11	1.000725	5.555710	2.050152
С	-8.426193	2.005219	-2.529419	H	0.193359	2.190414	-3.329880
C	-7 527161	2 032288	-1 312088	н	2 552628	2 473038	-3 986771
C	7.527101	2.052200	1.512000	11	2.552020	2.175050	5.500771
С	-7.903625	2.687637	-0.130157	Н	3.851349	4.473526	-3.294968
С	-7.015350	2.818802	0.938416	С	4,910034	2.328323	-0.949417
°	5 620000	0 0 1 1 5 0	0.011866		2 000142	1 100075	1 1 6 6 0 2 1
C	-5./39502	2.261459	0.841/66	C	3.906143	1.1989/5	-1.100931
0	-4.779205	2.428604	1.844254	С	2.691574	1.255432	-0.254318
- -	E 274466	1 516632	0 077020	0	2 102600	2 100240	0 540296
C	-5.3/4466	1.516632	-0.277939	0	2.492000	2.109240	0.549200
С	-6.265656	1.426071	-1.347778	0	1.872498	0.241653	-0.416977
U	-10 375900	2 120002	-1 567474	Fo	0 00000	0 00000	0 000000
п	-10.375900	2.129003	-1.30/4/4	re	0.000000	0.000000	0.000000
Н	-9.801620	0.459824	-1.784622	H	4.394608	3.294296	-0.984253
н	-10 437012	1 489212	-3 191895	н	5 703873	2 315292	-1 725723
11	10.457012	1.405212	5.151055		5.705075	2.313232	1.725725
Н	-7.927551	1.416779	-3.313187	Н	5.367783	2.207825	0.049103
н	-8 501770	3 032745	-2 923279	Н	3,490219	1,224426	-2.187744
	0.001000	3.100056	2.925279		4 3 6 9 2 6 9	0 202576	1 057405
Н	-8.903839	3.108276	-0.026093	H	4.360260	0.202576	-1.05/495
Н	-7.310135	3.367554	1.835526	С	1.225220	-2.782288	5.403290
TT	E 117/77	2 110010	2 170010	C	-0 272593	-2 5/1/00	5 073909
п	-3.11/4//	3.119919	2.4/9019	C	-0.272383	-2.541409	5.075898
Н	-4.389465	1.055649	-0.333038	C	-0.549820	-1.588257	3.943298
н	-5 959518	0 916321	-2 262054	N	-1 262466	-0 402618	4 076660
11	5.555510	0.910321	2.202034	14	1.202400	0.402010	4.070000
С	-4.490143	5.166092	-3.440826	C	-1.305573	0.232986	2.876144
C	-5 176102	4 811615	-2 114639	N	-0.661453	-0.486160	1,960846
ő	5.10102	1.011013	2.111035		0 100500	1 (10220	2 (12250
C	-4./10526	5.640991	-0.889923	C	-0.199509	-1.018332	2.012259
С	-3.246613	5.440796	-0.539368	Н	1.276291	-3.552490	6.187180
0	2 274406	6 106109	0 002042	ч	1 695165	-1 965//9	E 033033
0	-2.574490	0.190190	-0.993042	11	1.005105	1.000440	5.055052
N	-2.921707	4.380295	0.263550	Н	1.779861	-3.198730	4.505707
ч	-3 101297	5 260971	-3 26/709	н	-0 722168	-3 514297	4 819870
11	5.404257	5.200571	5.204705		0.722100	0 101100	1.019070
Н	-4.787231	6.150757	-3.869049	Н	-0./93091	-2.191193	5.9/9095
Н	-4.629227	4.327759	-4.177307	Н	-1.740463	-0.060043	4.920944
	6 260002	4 002046	2 102000		1 774204	1 100200	0 710245
н	-0.269882	4.903046	-2.193909	H	-1.//4384	1.190390	2./19345
H	-5.002762	3.751709	-1.870926	Н	0.368469	-2.367950	2.070114
U	-1 000330	6 710077	-1 070541	0	-0 117950	2 182892	0 380753
11	4.000555	0.710277	1.070341	0	0.117950	2.102052	0.500755
Н	-5.343658	5.378662	-0.027573	Н	0.868454	2.201201	0.666763
н	-1.953979	4,295212	0.571533	Н	-0.071747	2.644379	-0.495956
11	2.004605	2 020755	0 740005				
н	-3.624695	3.820/55	0.742935				
С	-0.870392	0.823868	-5.923752				
C	-1 995270	0 066010	-5 187927				
C	-1.995270	0.000010	- 3.10/92/				
С	-1.946167	0.216064	-3.701370				
N	-2 482468	1,312653	-3 053482				
	2.102100	1.0512033	1 848806				
C	-2.122298	1.2/4/04	-1./4//26				
N	-1,448090	0.173630	-1.491669				
C	_1 210/ =1	-0 /0//21	-2 705020				
C	-1.318451	-U.494431	-2./00032				
Н	0.074112	0.658798	-5.383789				
ч	-1 000365	1 027100	-6 01040F				
п	- T . UUZ 303	1.22/100	-0.010400				
Н	-0.737228	0.342636	-6.903000				
н	-2 973251	0.403519	-5 553833				
**	1 001000	1 000000	5.555055				
н	-1.921906	-1.006836	-5.405975				
Н	-2.963730	2.077652	-3.531662				
ц	-0 /1/01E	2 056505	-1 016040				
п	-7.477273	2.000090	-1.040249				
Н	-0.747574	-1.412140	-2.789978				
C	4 892853	7,098083	-0 623749				
C			0.020/49				
C	3.952454	1.265442	-1.845000				

**Table S3.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}SOD^{HOH}$  (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	x	V	7	C	3 600891	5 667023	-1 733063
		1		ő	5.000091	6.001023	1.755005
C	-2.698685	-5.871689	-0.808838	C	2.639816	6.291/02	-0.95/6/2
С	-1.225983	-5.846893	-1.250305	N	1.453537	5.590134	-1.011215
C	-0 622147	-4 480652	-1 253876	С	1.611511	4.514389	-1.853348
	0.022117	1.100032	1.405010	ő	0,000057	2 520122	2 251541
IN	0./32635	-4.2/0844	-1.485916	C	0.092057	3.330132	-2.231341
С	0.996109	-2.940933	-1.333115	С	1.121613	2.592346	-3.178619
N	-0.099472	-2.287415	-0.992600	С	2,435150	2,618225	-3.691162
 C	1 100704	2 220226	0 0 5 1 2 4 9	Ċ	2 257122	3 573373	-3 273026
C	-1.108/04	-3.220220	-0.951248	C	3.337132	3.372372	-3.273920
Н	-2.805588	-5.199921	0.053192	С	2.952835	4.539169	-2.336273
Н	-2.994232	-6.884628	-0.443298	Н	6.156891	4.653351	-0.685776
U	-3 375024	- 5 197350	-1 600342	н	5 686630	6 170059	0 137421
п	-3.373824	- 3.487330	-1.000342	11	3.000030	6.202122	1 007762
Н	-0.625153	-6.430800	-0.534637	н	/.035/82	6.202133	-1.097763
Н	-1.112930	-6.336639	-2.227844	Н	5.035950	7.174179	-2.067017
н	1 457458	-4 965805	-1 713730	н	5.382828	5.666473	-2.891968
11	1 0 0 1 0 0	2,402500	1 4 6 5 0 1 0	 TT	2 711210	7 212900	0 204502
п	1.969100	-2.402590	-1.405912	п	2.711319	7.212000	-0.304303
Н	-2.126587	-2.933548	-0.732849	Н	0.560211	5.831055	-0.573715
С	-9.488495	2.720291	-0.980591	Н	-0.320618	3.527802	-1.855133
Ċ	- 9 036545	3 002300	-1 303290	н	0 437622	1 811600	-3 516815
c	0.030343	5.002500	1.333200	11	0.13/022	1.051000	4 414020
C	-/.024551	2./36938	-0.298248	Н	2./383/3	1.802808	-4.414932
С	-7.183792	3.264877	0.992325	Н	4.380402	3.558990	-3.658463
С	-6.205139	3,093246	1,970963	С	5.136475	1.178543	-1.462280
Ċ	-5 056564	2 355209	1 673601	C	3 917877	0 260193	-1 593033
0	1 001004		1.0/JUJ1	~	2 020005	0 100100	1 500051
U	-4.034714	∠.163513	2.596664	C	2.828995	0.405195	-0.529251
С	-4.900833	1.764862	0.418839	0	2.926880	1.296707	0.380463
С	-5.875534	1.981125	-0.555222	0	1.807663	-0.351273	-0.702515
- u	-9 70/100	3 300/07	-0 160700	Fo	0 00000	0 000000	0 000000
п	-9.784180	3.392407	-0.100782	re	0.000000	1 812886	0.000000
Н	-9.597153	1.686752	-0.581207	0	-0.4/6456	1./13//6	0.842422
H	-10.196411	2.945053	-1.801620	Н	4.803223	2.221893	-1.396133
н	-7.757172	2.411331	-2.277924	Н	5.809784	1.076645	-2.352127
11	7 040406	4 057061	1 700050	п.	5 679611	0 02700/	-0 533030
п	-7.940400	4.057861	-1.700938	11	2 41 40 50	0.027004	0.555025
H	-8.089005	3.810410	1.257263	Н	3.4149/8	0.412415	-2.560394
Н	-6.335510	3.536026	2.961578	Н	4.206909	-0.804749	-1.574387
н	-4.084641	2.899078	3,270432	Н	0.420486	2.083710	0.990509
11	1 000626	1 105077	0 102041	C	1 395294	- / 113/10	1 600342
н	-4.000626	1.1958//	0.192841	C	1.395294	-4.113419	4.000342
Н	-5.712570	1.601471	-1.564163	C	-0.08/38/	-3.66813/	4.488068
С	-3.914047	5.713364	-2.544922	С	-0.362091	-2.518829	3.554565
C	-4 454727	5 315125	-1 162903	N	-0.894012	-1.302139	3.967758
0	2 (20122)	5.515125	0 022722	 C	0 071176	0 160600	2 000701
C	-3.620132	5.838425	0.033722	C	-0.9/11/6	-0.400020	2.000/94
С	-2.224991	5.216049	0.107361	N	-0.518097	-1.083527	1.802567
0	-1.258377	5.772995	-0.445679	С	-0.148880	-2.354889	2.204437
N	-2 120621	4 046783	0 786560	н	1 435043	-4 960129	5 303940
10	2.120021	4.040703	0.700500	11	2 004202	2 200220	5.505510 E 0E2C42
н	-2.81/000	5.588669	-2.53/338	п	2.004303	-3.300390	5.052645
Н	-4.067078	6.787384	-2.815292	Н	1.798645	-4.478439	3.598831
Н	-4.309464	5.015762	-3.333145	Н	-0.665161	-4.543427	4.155777
ч	-5 500595	5 636581	-1 031967	н	-0 463348	-3 416031	5 491898
11	1 100075	4.017202	1 074707	11	1 244005	1 007017	4 002564
н	-4.4899/5	4.21/392	-1.0/4/0/	н	-1.244995	-1.06/91/	4.903564
Н	-3.455719	6.920288	-0.033081	Н	-1.286102	0.568436	2.913162
Н	-4.168594	5.630264	0.967010	Н	0.265579	-3.056885	1.486862
н	-1 291763	3 412354	0 766205				
11 TT	2 055607	2 627060	1 102045				
н	-2.955627	3.62/869	1.183945				
С	-1.448090	1.132965	-5.929916				
С	-2.557953	0.467148	-5.092758				
C	-2 293381	0 487259	-3 619934				
	2.295501	1 507000	0.0101004				
IN	-2.606674	1.58/800	-2.846130				
С	-2.099197	1.417877	-1.603638				
N	-1.504500	0.233139	-1.507004				
C	-1 620911	-0 354202	-2 763092				
	1.020JII	0.334202					
н	-0.4/5952	0./59277	-5.5/5104				
Η	-1.393143	2.255402	-5.867889				
Н	-1.543182	0.773331	-6.965652				
 U	-3 515266	0 965020	-5 201722				
п	- 3 . J I J J D D D	0.505020	- 2.231/33				
Н	-2.672363	-0.581604	-5.396988				
Η	-3.020447	2.447540	-3.211761				
Н	-2.124344	2.168427	-0.826630				
н	-1 173706	-1 3160/0	-2 980728				
	L.L.J.UU	1.J10J40	0.010720				
C	6.044159	5.135977	-0.819763				
С	5.027786	6.086166	-1.937607				

**Table S4.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}SOD^{OH-}$  (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	х	У	Z	Н	0.389572	2.276550	4.602875
С	-2.005539	-0.606537	-5.903351	Н	0.823212	2.950043	1.889771
С	-0.474884	-0.577515	-5.765244	Н	2.566513	3.970673	0.416702
C	-0.005936	-0.255142	-4.392990	Н	4.846298	4.448685	1.284729
N	1 343170	-0 178253	-4 087875	н	5.468887	3.847382	3.610138
C	1 / 88510	-0 005508	-2 753265	C	-1 828232	2 697311	7 522720
N	0 201070	0.005355	-2 175000	C	-3 102371	2 977/32	6 716888
N C	0.291070	0.000000	2 105264	Ċ	-3 355/30	1 006450	5 57/112
U U	-0.042/01	1 100200	-3.103304 E 002ECE	C	- 3.333430	1 025700	J.J/4112 / E26601
H	-2.444977	-1.190200	-5.082565	C	-2.233047	1.933700	4.330021
H	-2.2/5024	-1.123184	-6.844528	U	-1.360062	2.82/454	4.449921
H	-2.433///	0.4148/1	-5.868668	IN	-2.269/00	0.885345	3.083075
H	-0.067871	-1.579636	-5.977127	H	-0.987045	2.698318	6.816162
Н	-0.023407	0.108994	-6.499725	Н	-1.854691	1.704529	8.041092
Н	2.120895	-0.258255	-4.762466	Н	-1.611664	3.542694	8.215683
Н	2.436111	0.077606	-2.236053	Н	-3.976364	2.970749	7.381210
Н	-1.703995	-0.092117	-2.979630	Н	-3.035492	3.975784	6.267258
С	-8.816391	4.337265	0.809021	Н	-3.519775	0.967560	5.962173
С	-7.299423	4.458755	1.049286	Н	-4.276215	2.254517	5.029114
С	-6.624115	3.160965	1.433945	Н	-1.460648	0.619171	3.073746
С	-7.154694	2.364822	2.457611	Н	-2.983673	0.170334	3.805603
С	-6.564758	1.159332	2.828842	С	5.101624	0.430222	1.903824
С	-5.429413	0.708664	2.153503	С	4.132767	0.443222	0.718155
0	-4.848663	-0.530396	2.416245	С	2.753510	-0.119080	1.030090
С	-4.854050	1.498932	1.156357	0	2.430038	-0.611282	2.113373
С	-5.446518	2.718689	0.818268	0	1.915375	0.00000	0.000015
Н	-9.294708	3,868256	1,682007	Fe	0.000000	0.000000	0.000000
н	-9.058502	3.682663	-0.058167	0	-0.386719	0.000015	1.860016
н	-9.245895	5.364182	0.725113	Н	4.581650	0.774750	2.805969
н	-6 799988	4 881805	0 165298	н	5.952500	1.120010	1.707306
и и	-7 1/7339	5 1879/3	1 862991	н	5 448471	-0 605377	2 067734
и П	-0 010300	2 601162	2 002071	н	3 945389	1 471954	0 368454
и П	-6 992422	0 560779	3 650772	и Ц	1 523849	-0.098312	-0 160278
п 11	-0.902422 E 440104	1 02509778	2 047694	11 U	4.525645	-0.301041	2 220/71
п	2 051600	-1.033060 1.157012	0 6E1442	п С	-0 002773	-6 159615	-1 760992
п	-3.951000	2 241050	0.051445	C	1 420250	- 0.130013	1 570100
H G	-4.9/18/8	3.341858	0.058670	C	-1.430339 1.250760	- 3.403243	-1.570190
C	0.230530	6.2191//	-0.853348	L	-1.350/69	-4.053140	-0.913925
C	-1.00/141	5.480637	-1.414368	N	-2.024368	-3./43118	0.263397
C	-1.146713	4.092606	-0.864944	C	-1./59613	-2.45//33	0.605011
N	-1.742981	3.838516	0.363388	N	-0.977982	-1.89/003	-0.315277
С	-1.576965	2.536758	0.683960	C	-0.718094	-2.878189	-1.261078
N	-0.903885	1.916946	-0.284058	Н	-0.304474	-7.068771	-2.353317
С	-0.630417	2.877533	-1.252075	Н	0.342361	-6.501251	-0.803802
Н	1.112442	5.575104	-0.979813	Н	0.635132	-5.571182	-2.398682
Н	0.139206	6.430176	0.246140	H	-1.887238	-5.276047	-2.564194
Н	0.422989	7.131592	-1.454865	Н	-2.118668	-6.045364	-0.999313
Н	-1.913071	6.051025	-1.169373	Н	-2.513107	-4.398087	0.867279
Н	-0.960648	5.420456	-2.507690	Н	-2.109314	-1.976547	1.510544
Н	-2.323853	4.504807	0.880890	H	-0.079666	-2.670853	-2.114349
Н	-1.926834	2.093231	1.607727				
Н	-0.065414	2.639587	-2.146576				
С	5.294540	1.080139	6.490829				
С	4.728424	2.512405	6.304291				
С	3.513504	2.612946	5.436951				
С	2.205429	2.218979	5.728867				
N	1.414902	2.349838	4.623215				
С	2.173462	2.868637	3.584167				
С	1.818329	3.166382	2.269897				
С	2.801498	3.745529	1.456924				
С	4.096054	4.012604	1.944595				
c	4,452011	3,670990	3.247772				
c	3.490005	3,074600	4.081253				
н	5.495453	0,601318	5.525406				
H	4.570847	0.431870	7.046219				
н	6 256256	1 20068/	7 047043				
н	4 507706	2 925858	7 206021				
н	5 50160/	3 161250	5 868881				
ц ц	1 70/067	1 840030	5.00000L				
11	1.194001	T.040900	0.000910	_			

**Table S5.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{3+}(Mn)SOD$  (starting coordinates based on PDB file 1VEW).<sup>2</sup>

Atom	x	v	7.	Н	4,972244	-1.865555	0.188446
	E 01 B 0 0 0		0 106640		2 220254	2 002205	0 504620
C	-5.81/032	0.236893	-2.126648	н	2.328354	-2.902206	0.504639
С	-5,700333	0.218369	-0.595261	Н	0.890106	-3.972427	2.228760
0	1 210672	0.000000	0.004574		1 700010	4 224402	4 547012
C	-4.319672	0.003922	-0.0945/4	н	1./28012	-4.324402	4.54/913
N	-4.047012	-0.049988	1,260208	Н	3.966141	-3.525253	5.223053
0	2 700010	0 142272	1 441770	C	7 000170	-2 001002	-2 062759
C	-2./06818	-0.1433/2	1.441//2	C	1.902110	-2.001002	-2.062/39
N	-2.098587	-0.146530	0.259537	С	7.124847	-2.398911	-3.293381
0	2 000271	0 0 0 0 4 0 0	0 701240	C	E 061000	1 126096	2 527460
C	-3.0902/1	-0.068420	-0.701340	C	3.901000	-1.420000	-3.337400
Н	-5.043747	0.890686	-2.551529	С	4.929825	-1.415848	-2.415222
TT	6 700006	0 (70000	2 200205	0	1 921000	2 240102	1 506156
н	-0./98996	0.6/2089	-2.398285	0	4.034900	-2.340103	-1.300430
Н	-5.688538	-0.772766	-2.559555	N	4.054138	-0.368042	-2.406906
	E 000010	1 202057	0 100100	TT	7 220404	2 120560	1 105070
н	-5.992310	1.203857	-0.198120	п	7.520404	-2.130309	-1.1032/2
Н	-6.388870	-0.519958	-0.153152	Н	8.434555	-1.057266	-2.084473
TT	1 717000	0 027612	0 017007	TT	0 742001	0 0010E1	1 062000
п	-4./4/900	-0.03/013	2.01/00/	п	0.742001	-2.001031	-1.003000
H	-2.211243	-0.193527	2.403046	Н	7.730911	-2.451797	-4.206619
U	-2 95/97/	-0 079651	-1 756714	ч	6 677521	-3 387268	-3 1/3951
п	-2.054074	-0.079051	-1./30/14	11	0.077521	5.507200	3.143331
С	1.365768	-3.833847	-8.965332	Н	6.316193	-0.397873	-3.717514
C	1 563300	-3 057003	-7 /30010	н	5 406250	-1 722549	-4 443481
C	1.303309	-3.93/993	-7.430919	11	5.400250	1.722549	1.115101
С	1.887726	-2.645279	-6.754410	Н	3.524261	-0.163254	-1.550385
C	2 898422	-1 813751	-7 252853	н	4 200394	0 412247	-3 045029
0	2.090422	1.013/31	7.252055		1.200391	0.112217	5.015025
С	3.197952	-0.584305	-6.671188	C	2.049744	-0.324402	5.077225
C	2 457855	-0 140518	-5 573730	C	0.856995	-0.413452	4.124100
	2.15,055	0.110510	3.373730	e e	1 054500	0.005485	1,121100
0	2.650162	1.113785	-4.994812	C	1.0/4/22	0.2054/5	2./59338
C	1 470993	-0 963776	-5 028458	0	2.124481	0.807678	2.438858
-	1.900505	0.905770	5.020450	°	0 000000	0.00015	1 00 00 10
C	1.209686	-2.207993	-5.609300	0	0.080627	0.000015	1.926819
н	2 240952	-3 335434	-9 407486	Fe	0.00000	0.00000	0.00000
	2.210992	3.333131	9.10,100	10	0.000000	0.500000	4 546006
Н	0.490128	-3.193588	-9.209015	н	2.9/004/	-0.598923	4.546906
Н	1.318893	-4.850113	-9.434464	Н	1.903320	-1.045181	5.906921
	2.520033	1 1000110	6 064255		0 140417	0 711000	E 4440EE
н	0.6/9123	-4.403381	-6.964355	н	2.143417	0./11288	5.444855
Н	2.383636	-4.664108	-7.252853	Н	0.612946	-1.466202	3.901047
	2.000000	2 1 2 2 2 7	0 104000	TT	0 066222	0 017471	1 517601
н	3.46/9/2	-2.12333/	-8.124283	п	-0.000223	0.01/4/1	4.54/004
Н	4.017715	0.021591	-7.072784	С	-1.969391	6.003647	-0.052567
	2 200820	1 (2240)	E EC0102	Ċ	1 651001	E 206241	1 202067
н	3.299820	1.022400	-2.209183	C	-1.031291	5.290341	-1.393907
H	0.910934	-0.628448	-4.156937	С	-0.893616	3.996765	-1.318893
TT	0 460257	2 952669	E 140006	NT	0 319665	3 70/303	-1 06/523
п	0.402337	-2.033000	-3.140920	TN	0.310003	5.704595	-1.904525
С	-0.115631	-6.166595	-0.120941	С	0.734512	2.513062	-1.728653
C	-0 766291	- 5 444702	-1 201522	N	-0 162613	1 870987	-0 985275
C	-0.700201	- 5.444702	-1.321333	T.	0.102015	1.070507	0.909275
С	-0.345062	-4.010620	-1.419998	C	-1.176819	2.783371	-0.728165
M	0 801346	-3 610931	-2 088318	н	-2 616653	6 865509	-0 276886
TN	0.001340	5.010551	2.000510		2.010033	6.005505	0.2/0000
С	1.017319	-2.294464	-1.867844	Н	-1.049408	6.419540	0.415466
N	0 051376	-1 802826	-1 090637	Н	-2.571808	5.355896	0.650543
10	0.051570	1.002020	1.090037		2.571000	5.555050	1 00 00 10
С	-0.802400	-2.865356	-0.809845	Н	-2.611526	5.094/42	-1.896286
н	-0 285370	-5 561340	0 781723	Н	-1.106857	5,994781	-2.045822
	1 001000	6 001560	0.016400		0 000145	4 400740	2 426066
Н	1.001282	-6.291/63	-0.216492	н	0.889145	4.480/43	-2.436966
Н	-0.643784	-7.122345	0.049667	Н	1.670685	2.109619	-2.096176
	0 500700	E 0 C 4 0 0 0	2 250221	TT	2 022020	2 500412	0 102077
н	-0.520/82	-5.964890	-2.238331	п	-2.032920	2.300412	-0.1230//
Н	-1.858261	-5.472733	-1.229584	0	2.248291	0.000000	0.000015
TT	1 266021	1 221602	2 695242	ч	2 305954	0 518295	0 905090
п	1.300021	-4.221005	-2.005242	11	2.303334	0.510255	0.909090
Н	1.865646	-1.752258	-2.268707	Н	2.440384	-0.901443	0.331543
н	-1 667175	-2 7/1165	-0 167664				
	1.00/1/3	2.171103	5.10,004				
С	6.699280	-0.660568	5.200455				
С	6.592926	-2.063904	4.558151				
~		2.000501	1.000101				
C	5.747574	-2.152542	3.319580				
С	6.036789	-1.725296	2.040344				
	4 047760	1 004500	1 200527				
IN	4.94//69	-1.924500	1.20852/				
С	3.944046	-2.533508	1.929703				
C	2 672002	- 2 0700CE	1 520201				
L	2.0/2002	-2.9/9005	T.23A7AT				
С	1.886566	-3.620590	2.497437				
C	2 250000	-3 032000	2 011074				
C	2.339009	-2.023090	J.0⊥⊥0/4				
С	3.614563	-3.368668	4.199982				
C	4 420303	-2 700301	3 263535				
	4.420303	2.100394	J.20JJJJ				
Н	5.708557	-0.237930	5.408585				
н	7,237259	0.035919	4.513306				
		0.701000	1.01000				
н	1.254395	-0./91290	6.162567				
н	7,607803	-2.422119	4.334518				
 TT	C 10112	0 770140	E 0000774				
н	p.18113/	-2.1/3148	5.2923/4				
Н	6.947830	-1.285507	1.643127				

**Table S6.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}(Mn)SOD^{HOH}$  (starting coordinates based on PDB file 1VEW).<sup>2</sup>

Atom	х	У	Z	Н	1.205154	4.709641	-0.357697
С	-2.595734	-5.336212	-2.208145	Н	1.629227	2.377441	-1.926422
С	-1.107100	-5.478943	-1.853683	Н	3.467209	1.192398	-3.123352
С	-0.465836	-4.194016	-1.465530	Н	5.842087	1.889800	-2.822403
N	0.866028	-4.150223	-1.086670	Н	6.435760	3.724426	-1.274216
С	1.173492	-2.884750	-0.700729	С	-0.527328	8.125610	-0.000702
N	0.102524	-2.112000	-0.805557	С	-1.775269	7.725647	-0.795227
C	-0.916900	-2.907990	-1.289474	C	-2.379547	6.377533	-0.385422
н	-3.086426	-4.679749	-1.477783	С	-1.424667	5.185333	-0.546280
H	-3.088089	-6.324768	-2.127991	0	-0.398117	5.252747	-1.257538
н	-2 729767	-4 893875	-3 214035	N	-1.798141	4.053421	0.085266
н	-1.003738	-6.134750	-0.974335	Н	0.203979	7.312439	-0.108307
н	-0 553085	-5 961380	-2 675064	н	-0.741333	8.268478	1.093445
н	1 523636	-4 944717	-1 114105	н	-0.040863	9.015778	-0.464355
н	2 141602	-2 546326	-0 349991	н	-2.547714	8.499435	-0.688522
н	-1 897629	-2 497589	-1 489685	н	-1.518250	7.647583	-1.858841
C	-7 350250	3 688751	-5 346710	н	-2.739471	6.405807	0.656403
C	-5 8/3079	3 667618	-5 022552	н	-3 263016	6 150787	-1 005173
C	-5 530010	3 167801	-3 552368	н	-1 164551	3 199417	0 231583
C	-6 163147	1 261/90	-2 585526	н	-2 623383	4 086655	0.680283
C	-5 906555	4.201490	-1 2258/5	C	5 222656	0 993088	1 175690
c	-5 004227	3 101540	-0 001/37	C	1 1891/8	0.043610	0 561905
0	- 1 757202	2 072424	0.5401457	C	2 7/3501	0.043010	1 006851
C	4.737202	2.072421	1 7/2501	0	2./43001	1 10/035	1 878967
C	-4.329041 1 E036E0	2.344000	-1.743391 2 102760	0	1 000016	-0 476776	0 351106
U U	-4.393030 7 0E1776	4 412102	-3.102/00	U Fo	1.000910	-0.4/0//0	0.000000
н II	-/.851//0	4.413193	-4.08/280 E 106100	re	-0.446289	1 010000	0.000000
H II	-/.82//89	2.709427	-5.126129	0	-0.440209 / 0E70E/	1.010290	1 106706
п	-7.010210 F 007F1F	4.034223	-0.403000	п 11	6 10/254	2.023004	1.100790
H II	-5.32/515	2.896255	-5.613647	п	0.10423U	0.929439	0.013090
H	-5.418091	4.632996	-5.343857	п	1 160760	0.132923	2.239024
H	-6.869308	5.028/1/	-2.897034	п	4.109/09	0.14/440	0.333004
H	-6.393112	4.750122	-0.490402	H	4.425323	-1.01/334	0./56592
H	-5.3/5549	3.433640	1.09//1/	Н	0.268127	2.002335	1.199219
H	-3.592529	1.014944	-1.410/9/	C	-1./39808	-3./54349	4.906097
н	-4.039291	1.931427	-3.828583	C	-2.853683	-3.083023	4.060135
C	1.6901/0	1.221146	-5.983/49	L	-2.424942	-2.03000/	3.008192
C	0.2/6855	0.646240	-5./41562	N	-2.859207	-0.716888	3.128235
C	-0.166229	0./124/9	-4.310837	C	-2.290665	-0.024124	2.09/916
N	-0.769424	1.841385	-3.776520	N	-1.555084	-0.832642	1.346878
C	-0.932480	1.665314	-2.439728	C	-1.633835	-2.083862	1.9393//
N	-0.467987	0.475769	-2.073334	H	-2.216217	-4.559494	5.489944
С	0.011078	-0.123413	-3.231155	H	-1.306351	-3.055695	5.651398
Н	2.396347	0.731705	-5.300079	Н	-0.944/48	-4.256/44	4.269638
Н	1.733383	2.316559	-5.750793	Н	-3.365372	-3.890671	3.514938
Н	2.016327	0.974380	-7.017883	Н	-3.600769	-2.653625	4.744766
Н	-0.437820	1.214661	-6.349640	Н	-3.323135	-0.269241	3.913559
H	0.218613	-0.394043	-6.081390	Н	-2.383881	1.044708	1.943695
Н	-1.155914	2.616318	-4.322159	H	-1.092453	-2.928406	1.522049
Н	-1.338287	2.421173	-1.779968				
Н	0.478745	-1.102417	-3.208679				
С	5.880035	5.453200	2.277283				
С	5.580704	5.841461	0.806931				
С	4.356033	5.218765	0.199463				
С	3.025284	5.493546	0.448868				
N	2.214447	4.604111	-0.228287				
С	3.008148	3.757782	-0.970000				
С	2.663696	2.699097	-1.819580				
С	3.697250	2.049911	-2.489685				
С	5.045700	2.437485	-2.314194				
С	5.386139	3.462158	-1.438431				
С	4.364395	4.133667	-0.742447				
Н	5.893387	4.363235	2.400162				
Н	5.093582	5.865067	2.955276				
Н	6.895386	5.863205	2.523560				
Н	5.514633	6.937286	0.741776				
Н	6.438019	5.556931	0.177704				
Н	2.588669	6.262558	1.080536				

**Table S7.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}(Mn)SOD^{OH-}$  (starting coordinates based on PDB file 1VEW).<sup>2</sup>

Atom	х	V	Z	Н	1.089615	4.840988	-1.073288
C	-2 383987	-5 657013	-1 638763	н	1.680374	2.355591	-2.299835
C	-0 919342	-5 635513	-1 175079	н	3 618408	1 075333	-3 221207
C	0.226752	1 201/10	0.006755	и и	5 046655	1 076/3/	-2 005056
C	-0.320732	-4.201410	-0.986755	п	C 401021	2.045060	1 506100
N	1.004/30	-4.156600	-0.629181	н	6.401031	3.945068	-1.586166
C	1.268326	-2.862976	-0.328979	C	-0.826630	8.098160	-1.31/520
N	0.166229	-2.137300	-0.488876	С	-2.023804	7.480240	-2.048355
С	-0.828812	-3.006622	-0.904892	С	-2.538498	6.175674	-1.428024
Н	-2.965225	-4.908173	-1.083145	С	-1.482880	5.072144	-1.324890
Н	-2.815598	-6.642258	-1.371048	0	-0.471664	5.030350	-2.062515
Н	-2.479660	-5.438980	-2.722870	N	-1.746002	4.105988	-0.417480
н	-0.852158	-6.096558	-0.176010	Н	-0.045975	7.326080	-1.248032
н	-0 289566	-6 243668	-1 843200	н	-1 085159	8 437469	-0 276688
и и	1 652267	-1 955933	-0 565/1/	н	-0 367355	8 902191	-1 946671
11	2 220057	2 /01500	0.000414	и и	-2 950311	0.1022151	-2 090554
п	2.230037	-2.401090	-0.011003 1 104771	п	1 727/11	0.19224J 7 0/E/20	2.009334
H	-1.830414	-2.663956	-1.124//1	н	-1./3/411	7.245438	-3.0/9/2/
C	-7.237488	2.526886	-6.257645	H	-2.9/45/9	6.349884	-0.429398
C	-5.718460	2.635590	-6.033508	Н	-3.352219	5.766235	-2.051346
С	-5.304855	2.574997	-4.579391	Н	-1.093400	3.322693	-0.179718
С	-5.903458	3.398972	-3.613495	Н	-2.531723	4.231552	0.211609
С	-5.572968	3.289825	-2.262924	С	5.046585	1.621262	1.200928
С	-4.642960	2.332779	-1.847672	С	4.084442	0.553085	0.675552
0	-4.327988	2,142242	-0.508942	С	2.621552	0.795868	0.999634
C	-4 007370	1 525742	-2 790756	0	2,200363	1.784698	1.606750
C	-1 332275	1 668137	-1 1/0808	0	1 833893	-0 169998	0 527206
	7 7/00/15	2 252002	4.140000 E 7/1///0	0	-0 310200	1 0/0762	0.31003/
п	-7.740243	1 505002	-5.741440	U	-0.510290	1.049702	0.310924
H	-7.652039	1.585938	-5.823196	re	0.000000	0.000000	0.000000
Н	-7.464005	2.639969	-7.349411	H	4.66/00/	2.620987	0.958298
Н	-5.191483	1.843857	-6.586411	Н	6.039520	1.490265	0.718200
Н	-5.381104	3.589203	-6.462814	Н	5.118332	1.520279	2.297623
Н	-6.660095	4.130020	-3.905579	Н	4.118393	0.499374	-0.426300
Н	-6.056259	3.937561	-1.524139	Н	4.341553	-0.461273	1.024948
Н	-4.930176	2.731995	0.014252	Н	0.458115	2.074203	0.902908
Н	-3.282425	0.781265	-2.465164	С	-1.619125	-3.123184	5.411758
н	-3.829269	1,033829	-4.867920	С	-2.698761	-2.617661	4.422546
C	1 8/9792	0 408569	-6 037613	C	-2.259400	-1.683151	3.326721
C	0 476700	-0 2311/0	-5 7/0/79	N	-2 864685	-0 447464	3 124130
C	0.470700	0.231140	1 240100	C C	-2.001009	0 161346	2 052070
C N	0.006271	0.072220	-4.340190	C NI	1 252200	0.101340	1 541670
IN G	-0.5555/3	1.293213	-3.997162	IN C	-1.33330Z	-0.019905	1.341072
С	-0./1682/	1.34//94	-2.658096	C	-1.319519	-1./66266	2.320908
N	-0.298294	0.210373	-2.108124	Н	-2.099930	-3.855316	6.077850
С	0.154541	-0.589722	-3.152512	Н	-1.247116	-2.307129	6.065796
Н	2.551773	0.101944	-5.246521	Н	-0.774002	-3.669846	4.891647
Н	1.828186	1.529617	-6.028717	Н	-3.166992	-3.498566	3.947906
Н	2.274445	0.009064	-6.975876	Н	-3.512726	-2.138458	4.987793
Н	-0.266525	0.135132	-6.461670	Н	-3.692017	-0.119293	3.614090
Н	0.523438	-1.319687	-5.861633	Н	-2.545120	1.156403	1.704208
н	-0.869400	2,006866	-4.658295	Н	-0.619904	-2.566437	2.100739
н	-1 112686	2 204224	-2 128281	-			
и и	0 569809	-1 5762/8	-2 978165				
	5 E 20762	6 220120	1 670010				
C	5.550762	0.230129	1.0/0010				
C r	5.346817	6.314/13	0.139709				
C	4.199005	5.538239	-0.432739				
C	2.833800	5./92435	-0.292938				
N	2.101654	4.805176	-0.891281				
С	2.966614	3.890671	-1.469254				
С	2.699463	2.715134	-2.169388				
С	3.792480	2.008469	-2.684616				
С	5.112747	2.460861	-2.495361				
С	5.373734	3.617767	-1.761490				
Ċ	4.294220	4.342484	-1.222885				
н	5 600342	5 193573	2 010651				
н ц	1 6000342	6 70070F	2.010001				
ц	4.000222 6 50/101	6 720751	1 000000				
11	0.004101	0.100201	T.)07007				

Н

Η

Η

5.247391

6.262604 2.339233 7.371948

5.954712 6.620102 -0.146866

-0.352112

0.207504

**Table S8.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{3+}(Mn)SOD$  (starting coordinates based on PDB file 1MMM).<sup>3</sup>

C         -2.80243         -0.52050         -5.558541         H         1.003387         3.77097         1.70426           C         -0.615800         -0.26176         -4.267990         H         5.003189         4.26263         3.242660           C         -0.615800         -0.26176         -4.267990         H         5.003189         4.26263         3.242660           C         -0.73458         -0.356424         -2.291733         C         -2.952700         3.467556         7.107339           C         -0.74738         -0.726612         -2.791734         C         -2.922700         2.400146         6.059333           H         -3.10953         -0.132642         -6.64603         0         -1.134918         3.233304         4.425166           H         -0.93031         -0.15244         -5.699313         N         -1.864529         2.303344         4.425146           H         -0.93031         -0.15244         -2.932465         H         -2.989732         H         -3.83308         2.602477         5.72384           H         -0.930331         -0.15247         -2.3898912         H         -3.83308         2.602477         5.72384           H         -0.843613         0	Atom	х	У	Z	Н	0.675522	2.669632	4.454010
C         -1.267300         -0.073288         -5.56842         H         2.665364         4.263394         0.13861           N         0.763388         -0.26424         -4.267395         H         5.003189         4.267950         7.80107           N         0.04466         -0.55988         -2.26424         -4.121335         H         5.699585         4.262533         3.242426           N         0.04466         -0.55988         -2.119233         C         -2.158708         3.46766         7.107333           H         -0.0497462         -4.61137         C         -2.585708         3.257950         7.024750           H         -0.193034         -0.45217         H         -0.462025         3.184734         4.633400           H         -0.835513         0.041519         -6.439300         H         -1.211609         3.184766         7.80144           H         1.362522         -0.77256         -4.929666         H         -0.935032         4.173037         B.347471           H         1.362629         -0.767266         -4.929666         H         -0.935032         4.170517         B.42766         7.80148           H         -2.3628010         -0.618747         -2.3018971	С	-2.802643	-0.520050	-5.585861	Н	1.003387	3.370987	1.704926
C         -0.615800         -0.261785         -4.267990         H         5.031289         4.6631289         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.278138         0.228233         0.2284286           C         1.131124         -0.141144         -2.891488         C         -1.2318825         0.2292700         2.406168         6.09933           C         -1.047318         -0.126260         -2.911831         C         -2.922700         2.406168         6.09933           H         -3.149339         -1.1319464         -1.1319473         7.024730         H         -0.466205         1.1319474         4.289801           H         -0.843613         -0.061874         -2.531693         H         -1.211009         2.137203         8.419700           H         -2.052805         -0.61874         -2.503907         H         -3.038483         3.464766         7.845184           C         -7.10453         4.999164         H         -3.053482         1.405095         6.522964           C         -7.10453         4.999147         H         -1.069853         1.841973         7.224884 <t< td=""><td>С</td><td>-1.267900</td><td>-0.579208</td><td>-5.568542</td><td>Н</td><td>2.685364</td><td>4.398331</td><td>0.188614</td></t<>	С	-1.267900	-0.579208	-5.568542	Н	2.685364	4.398331	0.188614
A         0.763458         -0.25642         -4.181325         H         5.699885         4.262233         3.287280           D         0.044662         -0.05998         -2.119232         C         -2.585709         3.46766         7.107239           H         -3.20144         -0.992462         -4.681717         C         -1.285529         2.300364         4.93106           H         -3.19535         0.11348         -5.629913         N         -1.873444         1.11755         4.28884           H         -0.95033         -1.13204         -5.629913         N         -1.873444         1.11755         4.28884           H         -0.95033         -1.13204         -5.279090         H         -1.250022         4.170502         -1.24756           H         -2.952805         -0.05174         -2.603237         H         -2.5090902         4.450766         -5.73986           C         -6.728201         -2.92172         H         -1.039853         -2.602286         -5.639394         -6.6239399         C         5.518937         0.269526         -5.63934           C         -6.728221         -2.92420         -2.934433         H         -2.354631         0.228960         -5.723884	С	-0.615800	-0.261765	-4.267990	Н	5.003189	4.863159	0.978134
c         1.13122         -0.14114         -2.811835         c         -1.235825         3.22790         7.801407           c         -1.047318         -0.126622         -2.911933         c         -2.922700         2.40164         6.09433           c         -1.047318         -0.126622         -2.911834         c         -2.922700         2.40164         6.09433           H         -3.149536         -1.1361348         -5.707370         H         -0.46000         3.181756         4.621460           H         -0.950331         -1.613244         -5.7707370         H         -0.46000         3.181756         4.621460           H         -0.950323         -0.115956         -2.501031         H         -3.954943         3.49766         7.853954           H         -2.05247         H         -2.583902         H.451006         H         -3.053482         1.409565         6.523954           C         -6.375778         3.627723         1.491006         H         -3.053482         1.40106         C.401375         5.75238           C         -6.04269         1.97249         3.157939         C.5158737         0.729891         0.721181         0.62240           C         -6.092689	N	0.763458	-0.256424	-4.181335	Н	5.699585	4.262543	3.284286
N         0.04462         -0.059998         -2.119232         C         -2.885709         3.467566         7.107239           H         -3.210144         -0.922462         -4.681717         C         -1.885529         2.300588         4.983100           H         -3.179153         0.519348         -5.629313         N         -1.130415         -6.446503         0         -1.130415         -6.446503         0         -1.130415         -6.446503         1.811732         -0.245613         -1.615204         -7.044750           H         -0.843613         0.011519         -6.779070         H         -1.6460169         2.177108         8.414700           H         1.25470         -0.115936         -2.314939         H         -3.294403         3.40165         7.283154           H         -4.644975         -1.49106         H         -3.054482         1.401692         -7.7184         -6.723981         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273788         -7.273789         -7.273788         -7.273789         -7.273497         -7.273788         -7.2737	C.	1.131424	-0.141144	-2.881485	С	-1.235825	3.257950	7.801407
C         1.147318         0.1366002         2.271634         C         2.222700         2.400146         6.099433           H         3.149536         -1.130615         -6.466003         0         -1.134918         3.23304         4.943100           H         3.149536         -1.051294         -5.70737         H         -0.662025         3.11732         7.024750           H         0.845613         0.041519         -6.373900         H         -1.211609         2.317108         8.438700           H         1.366282         -0.374756         -4.929266         H         -0.955032         4.17503         8.334741           H         2.1664975         -4.929266         H         -2.958092         4.430595         6.232843           C         -6.648575         H         -2.958092         4.40695         6.232844           C         -6.47370         1.491806         H         -2.95431         0.927816         6.122848           C         -6.073707         H         -3.83408         2.640131         5.572843           C         -6.94269         1.572479         3.157959         C         5.158737         0.729980         1.711043           C         -6.943429	N	0 044662	-0 059998	-2 119232	C	-2.585709	3.467636	7.107239
H         -1.210144         -0.922462         -4.62177         C         -1.85529         2.300858         4.943100           H         -3.179153         0.519348         -5.629913         N         -1.8771344         1.19736         4.62160           H         -0.95031         -1.613204         -5.629913         N         -1.8771344         1.19736         4.62160           H         -0.642631         0.01519         -6.379300         H         -1.314169         2.3181732         7.024750           H         -2.662805         -0.015736         -2.501693         H         -3.299483         3.494766         7.843184           C         -6.4737078         3.622732         1.491806         H         -3.255482         1.406982         6.523954           C         -7.12483         4.899124         H         -1.999953         0.85111         3.619553           C         -6.373778         3.622732         2.8849472         H         -1.999953         0.732801         1.741443           C         -6.034269         1.572489         3.159559         C         3.181737         0.738980         1.741443           C         -6.0394269         1.572479         3.15975950         C	C	-1 047318	-0 126602	-2 971634	C	-2 922700	2 400146	6 059433
H       -1.1136115       -6.446503       0       -1.134918       3.23904       4.621460         H       -1.173153       0.519348       -5.629913       N       -1.463205       3.181732       7.024730         H       -0.460205       3.181732       7.024730       H       -0.460205       3.181732       7.024730         H       -1.366292       -0.374756       -4.992966       H       -0.955033       4.177003       8.374741         H       2.156472       -0.115936       -4.992966       H       -0.955033       4.147503       8.374741         H       2.156472       -0.0115936       -4.992966       H       -2.398902       4.430955       6.522964         C       6.732861       -0.728078       3.621732       H       -2.35493       3.494766       6.522964         C       -6.728821       2.794220       2.934433       H       -2.35431       0.320618       4.62140         C       -6.094269       1.572479       3.157959       C       5.158737       0.729803       0.620321         C       -6.728821       2.794220       2.934433       H       -2.354431       0.320618       4.62140         C       -6.7393061       1.36	ч	-3 210144	-0 992462	-1 681717	C	-1 885529	2 300858	4 943100
H         -0.519382         -5.629913         N         -1.747344         1.19776         4.228881           H         -0.950511         -1.615204         -5.70737         H         -0.46205         3.181732         4.228881           H         -0.845205         -0.374756         -4.99266         H         -1.211609         2.317108         8.374741           H         2.165472         -0.0115736         -2.531633         H         -3.994483         3.449766         7.6845184           C         -0.648575         4.728027         1.491065         H         -3.083402         2.460317         S.522864           C         -7.12453         4.728027         1.491065         H         -3.083408         2.660311         3.615953           C         -6.375778         3.622332         1.984472         H         -1.098953         0.855111         3.615953           C         -6.375778         3.622332         2.483443         H         -2.354431         0.320618         4.662140           C         -6.375778         3.622332         2.483443         H         -2.354431         0.320618         4.662140           C         -6.375778         3.622332         0.283462         0.277867	и П	-3 1/9536	-1 130615	-6 116503	0	-1 134918	3 239304	4 621460
H         -0.950031         -1.113328         -1.77034         H         -0.460035         -1.11132         7.024150           H         -0.831613         -0.041513         -6.373900         H         -1.211609         2.337108         6.418700           H         -1.55647         -0.0115936         -2.531693         H         -0.955032         4.105003         6.33944           H         -2.062805         -0.0115936         -2.531693         H         -2.380302         4.30095         6.53394           C         -6.468875         -0.115936         -1.621737         H         -3.833408         2.460137         5.573288           C         -6.738821         2.794220         2.934433         H         -2.334431         0.320618         4.662140           C         -6.738821         1.94260         1.217331         0         2.459213         -0.095164         2.19366           C         -3.33405         3.174698         1.023300         0         1.93338         0.000000         -0.000018           H         -9.019638         4.339905         2.452637         Pe         0.000000         0.000000         0.000001           H         -9.019638         4.339905         2.452619	11	2 170152	0 E10240	E 620012	N	-1 87/3//	1 119736	4.258881
n       -1.012204       -3.70731       n       -1.012020       1.410100       1.410100       1.410100       1.410100         H       -1.0643613       0.041519       -0.0129300       H       -0.0129301       4.175003       8.147401         H       1.06270       -0.011976       -0.012970       H       -0.02803       8.444766       7.465184         H       2.062805       -0.0161874       -2.660802       4.40695       6.523964         C       -7.120453       3.612732       1.949472       H       -3.033482       1.406982       6.523964         C       -7.120453       3.612732       1.949472       H       -1.098933       0.300184       4.67140         C       -6.094269       1.572479       3.157959       C       5.158737       0.729980       1.741043         C       -6.094269       1.572479       3.157959       C       5.158737       0.05318       2.193649         C       -6.094269       1.372479       3.157959       C       5.158737       0.05318       2.193649         C       -6.094269       1.374798       1.233400       0       2.45631       1.021200       2.45641         H       -0.3134341       1.341	п	-3.1/9103 0 0F0F21	1 (15204	-3.029913	11	-0 460205	2 101720	7 024750
H       1.386292       0.191319       0.19300       H       -1.212039       4.137003       6.112100         H       2.153472       -0.1374756       -4.992966       H       -0.95303       4.175033       6.177741         H       2.1562805       -0.161874       -2.663347       H       -2.369292       4.400695       6.93934         C       -1.120453       4.720077       1.91806       H       -2.363468       2.04017       5.572268         C       -6.7726861       2.992205       1.354453       H       -1.098453       0.930118       4.662130         C       -6.7726861       3.124679       2.283264       C       4.110062       0.728073       0.655330         C       -6.73451       0.101277       2.428406       C       2.47716       0.999069       C       -5.33465       0.000000       -0.000010       0.000010       0.000010       0.000010       0.000010       0.000000       0.0	п	-0.950551	-1.013204	-3.770737	11	1 211600	2 217100	0 110700
n       1.30622       -0.319363       -0.319363       -1.419463       -1.419463       -1.419463         h       -2.536363       H       -2.536363       H       -2.536363       -1.446685       -5.53644         h       -2.66687       -0.661874       -2.603367       H       -2.5363483       -1.446682       -5.53264         C       -6.4375778       4.8991271       1.661373       H       -3.83488       2.404137       5.572388         C       -6.375778       4.8991271       1.651377       H       -1.099533       0.395111       3.161853         C       -6.094269       1.572479       3.157959       C       5.158737       0.3000818       4.662140         C       -6.094269       1.572479       3.157959       C       5.158737       0.0729980       1.741041         C       -5.33405       3.174698       1.023300       0       1.933838       0.00000       0.000000         H       -9.194538       4.33905       2.452647       Fe       0.00000       0.000000       0.000000         H       -9.39643       3.976843       0.736574       Fe       0.00000       0.000000       0.000000         H       -9.396610       0.382	н	-0.843613	0.041519	-6.3/3900	п	-1.211009	2.31/100 / 17E002	0.410/00
H       2.1534/2       -0.113936       -2.331633       H       -3.33483       -1.334169       -1.68176         C       -8.668573       4.220077       1.491806       H       -3.033482       1.406983       6.533934         C       -7.120453       4.280377       1.491806       H       -3.033482       1.406983       6.522964         C       -7.120453       4.129122       1.849472       H       -1.098953       0.895111       5.77386         C       -6.092306       1.572479       3.157959       C       3.148767       0.3991618       4.612493         C       -1.09336       1.072479       3.157959       C       3.148767       0.3999169       0.655120         C       -4.70394       1.01470       2.232431       O       2.459213       0.009000       0.000001         C       -5.033465       3.147699       1.023200       D       2.459213       0.000000       0.000001         H       -6.47660       3.147698       1.232631       O       2.459213       0.000000       0.000000         H       -5.035627       0.326421       1.432200       H       5.792400       1.43341         H       -6.7268018       5.132642	п	1.300292	-0.3/4/30	-4.992900	п 11	2 200402	2 101766	0.J/4/41 7 0/E10/
n       -2.002005       -0.001014       -2.003207       n       -2.100402       1.420031       0.420032         C       -6.648875       4.720027       1.431806       m       -3.031402       1.420032       0.232964         C       -6.7120453       4.890124       1.561737       m       -3.863408       0.80953       0.89511       3.161553         C       -6.728821       2.7941220       2.934433       m       -2.354431       0.320618       4.662140         C       -6.094269       1.512479       3.157939       C       5.158737       0.724073       0.625320         C       -5.095306       1.136475       2.283264       C       4.110062       0.724073       0.625320         C       -5.333405       1.944260       1.217331       O       2.459213       0.093184       2.193669         C       -5.333405       5.3727143       1.342300       M       5.952400       1.321200       2.668411         H       -6.736808       5.332642       0.626190       H       5.952400       1.391206       1.433441         H       -6.736008       5.332642       0.626190       H       5.95052       0.020020       0.090600         H <td>н</td> <td>2.155472</td> <td>-0.115936</td> <td>-2.531093</td> <td>п</td> <td>-3.390403</td> <td>J.494/00</td> <td>7.040104 6 E020E1</td>	н	2.155472	-0.115936	-2.531093	п	-3.390403	J.494/00	7.040104 6 E020E1
C         -7.5.033422         1.403942         0.124341           C         -7.120453         4.891273         1.403942         0.124343           C         -6.375778         3.612732         1.849472         H         -1.098933         0.893111         3.613933           C         -6.094269         1.572479         3.157959         C         5.158737         0.729980         1.741043           C         -5.095306         1.136475         2.283264         C         4.10062         0.722980         1.265320           C         -4.473861         -0.101273         2.428406         C         2.767136         0.154770         0.999069           C         -5.333405         3.174698         1.021300         0         1.933838         0.000000         0.00000         0.000000	н	-2.062805	-0.061874	-2.605347	п	2.000902	4.430093	6 5005904
C       -1.12033       4.059124       1.561737       H       -5.053406       2.044157       3.07256         C       -6.728821       2.794220       2.934433       H       -2.354431       0.320618       4.662140         C       -6.094269       1.156475       2.283264       C       4.110662       0.728073       0.625330         C       -5.095306       1.136475       2.283264       C       4.110662       0.728073       0.625330         C       -5.095306       1.136475       2.283264       C       4.11062       0.728073       0.625330         C       -5.333405       1.944260       1.217331       O       2.456213       0.095184       2.193649         H       -9.019638       4.339905       2.452637       Fe       0.000000       0.000000       0.000000         H       -9.19638       4.339905       2.452637       Fe       0.000000       0.000000       0.000000         H       -6.306010       0.946350       0.714688       H       4.72762       1.121200       2.666411         H       -6.386010       0.946350       4.06058       C       -0.140717       6.197083       -1.31200         H       -6.396010	C	-8.648575	4./2802/	1.491806	п	-3.033462	1.400902	0.322904 E E73300
C         -6.3/37/8         3.612/32         1.8494/2         H         -1.09933         0.893111         3.61933           C         -6.094269         1.572479         3.157959         C         5.158737         0.729980         1.741043           C         -5.095306         1.136475         2.283244         C         4.110062         0.728073         0.625320           O         -4.475861         -0.101273         2.428406         C         2.167133         0.00000         0.000000         -0.000015           H         -9.019633         4.339905         2.452637         Fe         0.00000         0.000000         -0.000015           H         -9.139633         5.755143         1.342300         H         5.992400         1.331296         1.433441           H         -6.758908         5.332642         0.626190         H         5.903400         1.30292         1.330296           H         -6.390610         0.946354         4.006038         C         -1.45147         -5.43512         -1.032466           H         -6.2396610         0.946354         4.006038         C         -1.45147         -5.43512         -1.021466           H         -6.390610         0.946354	C	- /.120453	4.899124	1.561/3/	H	-3.883408	2.640137	2.2/2388
C         -6.728821         2.942420         2.934433         H         -2.35441         0.320518         4.864440           C         -6.094269         1.572479         3.157959         C         5.158737         0.728973         0.623320           O         -4.479861         -0.101273         2.428406         C         2.452136         0.095184         2.193649           C         -5.333405         1.744688         1.023300         0         1.933838         0.00000         0.000000           H         -9.019638         4.339905         2.452637         Fe         0.000000         0.000000         0.000000           H         -9.019638         0.716658         H         4.724762         1.121200         2.668411           H         -6.736906         5.332462         0.626190         H         5.903052         -0.306290         1.433441           H         -6.896132         5.62687         2.354919         H         3.668042         1.765152         0.328263           H         -4.92546         0.545904         3.618739         H         4.548495         0.272749         0.132816           C         1.46744         5.454875         0.272449         0.647639         1	C	-6.375778	3.612732	1.849472	H	-1.098953	0.895111	3.619553
C         -6.094269         1.572479         3.157959         C         5.158737         0.729980         1.741043           C         -5.095366         -1.01273         2.428406         C         2.767136         0.154770         0.999069           C         -4.475861         -0.101273         2.428406         C         2.767136         0.095184         2.193649           C         -5.333405         3.174698         1.023300         O         1.933838         0.000000         -0.000015           H         -9.019638         4.339905         2.452637         Fe         0.000000         0.000000         -0.000015           H         -9.139633         5.755143         1.342300         H         5.992400         1.391296         1.433441           H         -6.736908         5.332642         0.626190         H         5.903500         1.906800           H         -7.528809         3.065640         3.613739         H         4.454895         0.227249         -0.394266           H         -6.390610         0.46350         4.060538         C         -1.454147         -5.443512         -0.446794           H         -5.016632         3.94571         0.186462         N	С	-6.728821	2.794220	2.934433	Н	-2.354431	0.320618	4.662140
C         -5.09306         1.136475         2.283244         C         4.11002         0.728073         0.623320           C         -4.47586         -0.101273         2.422466         C         2.457136         0.154770         0.099069           C         -5.333405         1.944260         1.217331         0         2.4525230         0.00000         0.00000         0.00000           H         -9.019638         4.339905         2.452637         Fe         0.000000         0.000000         0.000000           H         -9.139633         5.725143         1.342300         H         5.992400         1.321206         1.433441           H         -7.528809         3.056842         0.626190         H         5.903052         -0.306290         1.391286           H         -6.898112         5.626587         2.354919         H         3.668042         1.765152         0.3226263           H         -6.390610         0.946350         4.006058         C         -0.140717         -6.197083         -1.331818           H         -3.922333         1.603867         0.537415         C         -1.334637         -4.053202         -0.416794           H         -3.922333         1.6328640	С	-6.094269	1.572479	3.157959	C	5.158737	0.729980	1.741043
0         -4.479861         -0.101273         2.428406         C         2.767136         0.154770         0.999069           C         -5.333405         3.174698         1.023300         0         1.93383         0.000000         -0.000015           H         -9.019638         4.339905         2.452637         Fe         0.000000         0.000000         0.000000           H         -9.139633         5.725143         1.342300         H         4.724762         1.121200         2.668411           H         -6.736908         5.332642         0.626190         H         5.592400         1.991296         1.433441           H         -6.736908         5.332642         0.626190         H         5.592400         1.991296         1.433441           H         -6.390510         0.94650         4.060598         C         -0.140717         -6.197083         -1.331818           H         -4.222546         -0.554900         3.189606         C         -1.454147         -5.443512         -1.012146           H         -5.016632         3.794571         0.186422         N         -2.133087         -0.667465           C         -1.005127         5.328689         -1.4452525         N	С	-5.095306	1.136475	2.283264	C	4.110062	0.728073	0.625320
C       -4.701935       1.944260       1.217331       O       2.459213       -0.099184       2.193649         C       -5.333405       3.174688       1.023300       O       1.933838       0.000000       0.000000         H       -9.105638       4.339905       2.452637       Fe       0.000000       0.000000       0.000000         H       -6.39608       5.735642       0.626100       H       5.593052       -0.36220       1.433441         H       -6.39601       0.946350       4.006058       C       -0.140717       -6.197083       -1.331818         H       -6.392061       0.946350       4.006058       C       -0.140717       -6.197083       -1.331818         H       -4.922546       -0.554900       3.189606       C       -1.454447       -5.445512       -0.046794         H       -5.016632       3.794571       0.166462       N       -2.133087       -3.679367       0.667455         C       -1.014660       4.052704       -0.796570       C       -1.04668091       -2.917068       -7.139221       -1.877811       0.032804       -0.467945         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.917066	0	-4.475861	-0.101273	2.428406	C	2.767136	0.154770	0.999069
C         -5.333405         3.174698         1.023300         O         1.933838         0.000000         -0.00001           H         -9.019638         4.339905         2.452637         Pe         0.000000         0.000000         0.000000           H         -9.139633         5.725143         1.342300         H         4.724762         1.121200         2.668411           H         -6.736908         5.332642         0.626190         H         5.592400         1.391296         1.433441           H         -6.736908         5.332642         0.626190         H         5.592400         1.9918961         1.931896           H         -6.390610         0.946350         4.006058         C         -0.140717         -6.197083         -1.331818           H         -4.3222333         1.603867         0.537415         C         -1.354303         -4.063202         -0.416794           H         -3.922333         1.603867         0.537415         C         -1.3454147         -2.365219         0.935043           C         0.106527         5.382889         -1.485245         N         -1.018723         -1.87871         0.186422         N         -1.018723         -1.87811         0.082870 <tr< td=""><td>C</td><td>-4.701935</td><td>1.944260</td><td>1.217331</td><td>0</td><td>2.459213</td><td>-0.095184</td><td>2.193649</td></tr<>	C	-4.701935	1.944260	1.217331	0	2.459213	-0.095184	2.193649
H       -9.019638       4.339905       2.452637       Fe       0.000000       0.000000       0.000000         H       -9.19633       5.725143       1.342300       H       5.929400       1.321206       2.666411         H       -6.736908       5.332642       0.626190       H       5.503052       0.306200       1.906800         H       -6.639061       0.946350       4.006058       C       -0.140717       -6.197083       -1.331818         H       -6.3202246       -0.554300       3.189606       C       -1.454147       -5.443512       -1.012146         H       -5.012632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214690       6.208450       -1.023209       C       -1.1914215       -2.355219       0.935043         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.917068       -7.59567         N       -1.63268       3.89324       0.478104       H       -0.418991       -7.139221       -1.827011         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.070640       -0.407333         N <td< td=""><td>С</td><td>-5.333405</td><td>3.174698</td><td>1.023300</td><td>0</td><td>1.933838</td><td>0.000000</td><td>-0.000015</td></td<>	С	-5.333405	3.174698	1.023300	0	1.933838	0.000000	-0.000015
H       -8.940643       3.976883       0.718658       H       4.724762       1.121200       2.666411         H       -6.736908       5.332642       0.626190       H       5.992400       1.331296       1.433441         H       -6.736908       5.332642       0.626190       H       5.503052       -0.306290       1.906800         H       -6.390610       0.946350       3.613739       H       4.464895       0.227249       -0.294266         H       -6.390610       0.946350       4.006058       C       -0.140717       -6.197083       -1.31818         H       -4.922546       -0.554900       3.189606       C       -1.454147       -6.467085       -0.140717         H       -5.016632       3.794571       0.186462       N       -2.133087       -0.667465         C       0.124890       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.005127       5.38289       -1.485245       N       -1.018723       -1.8771811       0.082870         C       -1.62568       3.89324       0.478619       H       -0.419891       -7.139221       -1.8271811         C       -1.466766	Н	-9.019638	4.339905	2.452637	Fe	0.000000	0.000000	0.000000
H       -9.139633       5.725143       1.342300       H       5.92400       1.391296       1.433441         H       -6.736908       5.332642       0.626190       H       3.686042       1.765152       0.302620       1.906800         H       -6.390610       0.946350       4.006058       C       -0.140717       -6.197083       -1.331818         H       -6.322246       -0.554900       3.189606       C       -1.454147       -5.443512       -1.012146         H       -5.922246       -0.554900       3.189606       C       -1.1346147       -5.443512       -1.012146         H       -5.922246       -0.554900       3.189606       C       -1.1346147       -5.443512       -1.012146         H       -5.922246       -0.224890       -1.023209       C       -1.914215       -2.352219       0.935043         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.89324       0.478104       H       -0.418981       -7.139221       -1.827011         C       -1.046676       2.612122       0.877869       H       0.3797049       -6.490402       -0.47733	Н	-8.940643	3.976883	0.718658	Н	4.724762	1.121200	2.668411
H       -6.736908       5.332642       0.626190       H       5.03052       -0.306290       1.906800         H       -6.898132       5.626587       2.354919       H       3.868042       1.765152       0.326263         H       -7.528809       3.095840       3.613739       H       4.464895       0.227249       -0.294266         H       -6.390610       0.966350       4.006058       C       -1.454147       -5.443512       -1.012146         H       -3.922333       1.603867       0.537415       C       -1.354630       -4.063202       -0.416794         H       -5.016623       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214890       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.05127       5.382809       -1.485258       N       -1.018723       -1.871811       0.082870         C       -1.466766       2.61222       0.877869       H       0.327049       -6.949042       -0.407333         N       -0.630291       1.913635       -0.080002       H       0.327144       -5.630966       -2.056625         C       -	Н	-9.139633	5.725143	1.342300	Н	5.992400	1.391296	1.433441
H       -6.898132       5.626587       2.354919       H       3.686042       1.765152       0.326263         H       -6.390610       0.946350       4.06058       C       -0.140717       -6.197083       -1.31818         H       -4.922546       -0.554900       3.189606       C       -1.454147       -5.443512       -1.012146         H       -3.922333       1.603867       0.537415       C       -1.354630       -4.063202       -0.416794         H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214890       6.208450       -1.023209       C       -1.914215       -2.355219       0.935043         C       -1.064660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.418991       -7.139221       -1.877011         C       -1.466766       2.612122       0.677869       H       0.397049       -6.490402       -0.407333         N       -0.86029       1.91355       -0.80002       H       0.52344       -5.361267       -1.946633         H <t< td=""><td>Н</td><td>-6.736908</td><td>5.332642</td><td>0.626190</td><td>Н</td><td>5.503052</td><td>-0.306290</td><td>1.906800</td></t<>	Н	-6.736908	5.332642	0.626190	Н	5.503052	-0.306290	1.906800
H       -7.528809       3.095840       3.613739       H       4.454895       0.227249       -0.229246         H       -6.390610       0.964350       4.006058       C       -0.140717       -6.197083       -1.3131818         H       -4.922546       -0.554900       3.189606       C       -1.454147       -5.443512       -1.012146         H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.6674455         C       0.214890       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.465766       2.612122       0.877869       H       0.397049       -6.490402       -0.477333         N       -0.66229       1.913635       -0.080002       H       0.53548       -5.61267       -1.945633         H       0.187073       6.492484       0.061646       H       -2.880920       -4.241180       1.067932         H	Н	-6.898132	5.626587	2.354919	Н	3.868042	1.765152	0.326263
H       -6.390610       0.946350       4.006058       C       -0.140717       -6.197083       -1.331818         H       -4.922546       -0.5554900       3.189606       C       -1.454147       -5.443512       -1.012146         H       -3.922333       1.603667       0.537415       C       -1.354630       -4.063202       -0.416794         H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214890       6.208450       -1.023209       C       -1.914215       -2.365219       0.9355043         C       -1.04660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.337049       -2.630966       -2.056625         C       -0.660291       1.913635       -1.126328       H       -2.039558       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.80920       -4.241180       1.067932         H	Н	-7.528809	3.095840	3.613739	Н	4.454895	0.227249	-0.294266
H       -4.922546       -0.554900       3.189606       C       -1.454147       -5.443512       -1.012146         H       -3.922333       1.603867       0.537415       C       -1.334630       -4.063202       -0.416794         H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214490       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.006127       5.38289       -1.485245       N       -1.018723       -1.871811       0.062870         C       -1.632568       3.89324       0.478104       H       -0.41991       -7.139221       -1.877011         C       -1.466766       2.612122       0.877869       H       0.337049       -6.490402       -0.407333         N       -0.632904       2.804535       -1.126328       H       -2.039658       -5.51267       -1.945633         H       0.187076       6.492844       0.61646       H       -2.80920       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H <t< td=""><td>Н</td><td>-6.390610</td><td>0.946350</td><td>4.006058</td><td>С</td><td>-0.140717</td><td>-6.197083</td><td>-1.331818</td></t<>	Н	-6.390610	0.946350	4.006058	С	-0.140717	-6.197083	-1.331818
H       -3.922333       1.603867       0.537415       C       -1.354630       -4.063202       -0.416794         H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214890       6.208450       -1.023209       C       -1.914215       -3.679367       0.667465         C       -1.0045127       5.382889       -1.485245       N       -1.018723       -1.871811       0.082870         C       -1.104660       4.052704       -0.795570       C       -0.668091       -2.917068       -0.795567         N       -1.466766       2.612122       0.877869       H       -0.419891       -7.139221       -1.827011         C       -1.666726       2.612122       0.877869       H       0.397049       -6.490402       -0.4407333         N       -0.663229       1.913635       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.039658       -5.361267       -1.9456378         H       0.187073       6.492844       0.061646       H       -2.280920       -4.241180       1.067932         H	Н	-4.922546	-0.554900	3.189606	С	-1.454147	-5.443512	-1.012146
H       -5.016632       3.794571       0.186462       N       -2.133087       -3.679367       0.667465         C       0.214890       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.005127       5.382889       -1.485245       N       -1.018723       -1.871811       0.082870         C       -1.104660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.662668       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       1.117798       5.92896       -1.157974       H       -2.071487       -6.05445       -0.345078         H       0.137073       6.492844       0.061646       H       -2.80920       -4.241180       1.075897         H       0.159504       7.084763       -1.684555       H       -2.0426422       -1.81480       1.715897         H	Н	-3.922333	1.603867	0.537415	С	-1.354630	-4.063202	-0.416794
C       0.214890       6.208450       -1.023209       C       -1.914215       -2.365219       0.935043         C       -1.005127       5.382889       -1.485245       N       -1.018723       -1.871811       0.082870         C       -1.104660       4.052704       -0.795570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.662291       1.913635       -0.080002       H       0.523544       -5.630966       -2.056625         C       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.80902       -4.241180       1.067932         H       0.385064       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -1.928421       5.950943       -1.309052       H       0.040085       2.753265       -1.564865         H	Н	-5.016632	3.794571	0.186462	N	-2.133087	-3.679367	0.667465
C       -1.005127       5.382889       -1.485245       N       -1.018723       -1.871811       0.082870         C       -1.104660       4.052704       -0.796570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.80920       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.00015       2.232485         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -0.136749       2.493408       -2.038986       -2.038986       -2.038986       -2.03897175       3.2655978       O       -0	С	0.214890	6.208450	-1.023209	С	-1.914215	-2.365219	0.935043
C       -1.104660       4.052704       -0.795570       C       -0.668091       -2.917068       -0.759567         N       -1.632568       3.893234       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.660229       1.913635       -0.080002       H       0.539544       -5.630966       -2.056625         C       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.809520       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -1.788162       2.237228       1.841049       H       -0.236938       -0.912613       2.525986         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829          C       2.016098	С	-1.005127	5.382889	-1.485245	N	-1.018723	-1.871811	0.082870
N       -1.632568       3.89324       0.478104       H       -0.419891       -7.139221       -1.827011         C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.860229       1.913635       -0.080002       H       0.523544       -5.630966       -2.056625         C       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.880920       -4.41180       1.07932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -1.788162       2.337228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -0.014254       -0.024292       2.296829         C       5.042160       3.013000       6.046616       -0.024292       2.296829       -0.024292       2.296829         N       1.694885<	С	-1.104660	4.052704	-0.796570	C	-0.668091	-2.917068	-0.759567
C       -1.466766       2.612122       0.877869       H       0.397049       -6.490402       -0.407333         N       -0.860229       1.913635       -0.080002       H       0.523544       -5.630966       -2.056625         C       -0.632304       2.804535       -1.126328       H       -2.036658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.036658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.880920       -4.241180       1.067932         H       0.159504       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -0.024593       -0.912613       2.55986         C       5.042160       3.013000       6.046616       -0.236938       -0.924292       2.296829         N       1.694885       2.725098	N	-1.632568	3.893234	0.478104	Н	-0.419891	-7.139221	-1.827011
N       -0.860229       1.913635       -0.080002       H       0.523544       -5.630966       -2.05625         C       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       0.187073       6.492844       0.061646       H       -2.880920       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -1.694885       2.725098       4.411362       2.61649       5.08820       -       -       -       -       -	С	-1.466766	2.612122	0.877869	Н	0.397049	-6.490402	-0.407333
C       -0.632904       2.804535       -1.126328       H       -2.039658       -5.361267       -1.945633         H       1.117798       5.592896       -1.157974       H       -2.071487       -6.055445       -0.345078         H       0.187073       6.492844       0.061646       H       -2.880920       -4.241180       1.067932         H       0.1359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -1.788162       2.237228       1.841049       H       -0.026938       -0.912613       2.255986         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829       2.296829         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829       2.296829         K       -0.136749       2.493408       -2.038986       -0.024292       2.296829       2.296829         N       1.694885       2.725098       4.411362       -0.024292       2.296829       2.296248       -1.14924       -0.024292       2.296829         C	N	-0.860229	1.913635	-0.080002	Н	0.523544	-5.630966	-2.056625
H       1.117798       5.592896       -1.157974       H       -2.071487       -6.065445       -0.345078         H       0.187073       6.492844       0.061646       H       -2.880920       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.84880       1.715897         H       -1.928421       5.950943       -1.309052       H       0.040085       -2.753265       -1.564865         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829       2.296829         C       5.663849       1.622314       6.333344       -0.024292       2.296829       2.296829         N       1.694885       2.725098       4.411362       -0.024292       2.296829       -0.024292       2.296829         C       2.962448       4.158	С	-0.632904	2.804535	-1.126328	Н	-2.039658	-5.361267	-1.945633
H       0.187073       6.492844       0.061646       H       -2.880920       -4.241180       1.067932         H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -1.928421       5.950943       -1.309052       H       0.040085       -2.753265       -1.564865         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -2.149454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829         C       5.042160       3.013000       6.046616       -0.024292       2.296829         C       2.531616       2.611649       5.508820       -0.1663132       -0.024292       2.296829         N       1.694885       2.725098       4.411362       -0.236938       -0.024292       -2.96248         C       2.962448       4.158142       1.215866       -0.2369337       -0.2369337       -0.2369337	Н	1.117798	5.592896	-1.157974	Н	-2.071487	-6.065445	-0.345078
H       0.359604       7.084763       -1.684555       H       -2.426422       -1.814880       1.715897         H       -1.928421       5.950943       -1.309052       H       0.040085       -2.753265       -1.564865         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -       -0.024292       2.296829         C       5.63849       1.622314       6.333344       -       -0.024292       2.296829         N       1.694885       2.72598       4.411362       -       -       -       -       -       -       -       -       -       -       -       -       -       - <td>Н</td> <td>0.187073</td> <td>6.492844</td> <td>0.061646</td> <td>Н</td> <td>-2.880920</td> <td>-4.241180</td> <td>1.067932</td>	Н	0.187073	6.492844	0.061646	Н	-2.880920	-4.241180	1.067932
H       -1.928421       5.950943       -1.309052       H       0.040085       -2.753265       -1.564865         H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -       -0.024292       2.296829         C       5.663849       1.622314       6.333344       -       -0.024292       2.296829         K       -0.024160       3.013000       6.046616       -	Н	0.359604	7.084763	-1.684555	Н	-2.426422	-1.814880	1.715897
H       -0.951630       5.201157       -2.565979       O       -0.036453       0.000015       2.232483         H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       H       -0.236938       -0.024292       2.296829         C       5.663849       1.622314       6.333344       H       1.049454       -0.024292       2.296829         N       0.663849       1.622314       6.333344       H       1.049454       -0.024292       2.296829         N       1.694885       2.725098       4.411362       - <th< td=""><td>Н</td><td>-1.928421</td><td>5.950943</td><td>-1.309052</td><td>Н</td><td>0.040085</td><td>-2.753265</td><td>-1.564865</td></th<>	Н	-1.928421	5.950943	-1.309052	Н	0.040085	-2.753265	-1.564865
H       -2.144363       4.611465       0.996628       H       -0.236938       -0.912613       2.525986         H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       H       1.049454       -0.024292       2.296829         H       -0.236938       1.049454       -0.024292       2.296829       2.296829         H       -0.531616       2.611649       5.508820       F       - </td <td>Н</td> <td>-0.951630</td> <td>5.201157</td> <td>-2.565979</td> <td>0</td> <td>-0.036453</td> <td>0.000015</td> <td>2.232483</td>	Н	-0.951630	5.201157	-2.565979	0	-0.036453	0.000015	2.232483
H       -1.788162       2.237228       1.841049       H       1.049454       -0.024292       2.296829         H       -0.136749       2.493408       -2.038986       -0.024292       2.296829         C       5.663849       1.622314       6.333344       -0.024292       2.296829         C       5.042160       3.013000       6.046616       -0.024292       2.296829         C       5.042160       3.013000       6.046616       -0.024292       2.296829         C       3.042160       3.013000       6.046616       -0.024292       2.296829         N       1.694885       2.725098       4.411362       -0.024292       2.296829         C       2.531616       2.611649       5.508820       -0.024292       2.296829         N       1.694885       2.725098       4.411362       -0.024292       -0.024292       2.296829         C       2.410324       3.260086       3.362442       -0.055145       -0.024292       -0.024292       -0.024292       -0.024292       -0.024292       -0.024292       2.296829         C       2.016098       3.572769       2.055145       -0.05145       -0.024292       -0.024292       -0.024292       -0.024292       -0.024292 <td>Н</td> <td>-2.144363</td> <td>4.611465</td> <td>0.996628</td> <td>Н</td> <td>-0.236938</td> <td>-0.912613</td> <td>2.525986</td>	Н	-2.144363	4.611465	0.996628	Н	-0.236938	-0.912613	2.525986
H       -0.136749       2.493408       -2.038986         C       5.663849       1.622314       6.333344         C       5.042160       3.013000       6.046616         C       3.807175       3.029053       5.188278         C       2.531616       2.611649       5.508820         N       1.694885       2.725098       4.411362         C       2.410324       3.260086       3.362442         C       2.016098       3.572769       2.055145         C       2.962448       4.158142       1.215866         C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	Н	-1.788162	2.237228	1.841049	Н	1.049454	-0.024292	2.296829
C5.6638491.6223146.333344C5.0421603.0130006.046616C3.8071753.0290535.188278C2.5316162.6116495.508820N1.6948852.7250984.411362C2.4103243.2600863.362442C2.9624484.1581421.215866C4.2773444.4227001.663132C3.7424323.4826203.822861H5.8251041.0705115.397293H4.9981381.0001536.987137H6.6639401.7993936.806015H4.8315283.5104227.004425H2.1492772.2191626.448380	Н	-0.136749	2.493408	-2.038986				
C5.0421603.0130006.046616C3.8071753.0290535.188278C2.5316162.6116495.508820N1.6948852.7250984.411362C2.4103243.2600863.362442C2.0160983.5727692.055145C2.9624484.1581421.215866C4.2773444.4227001.663132C4.6732644.0833742.953537C3.7424323.4826203.822861H5.8251041.0705115.397293H4.9981381.0001536.987137H6.6639401.7993936.806015H4.8315283.5104227.004425H5.7915343.6447455.545776H2.1492772.2191626.448380	С	5.663849	1.622314	6.333344				
C3.8071753.0290535.188278C2.5316162.6116495.508820N1.6948852.7250984.411362C2.4103243.2600863.362442C2.0160983.5727692.055145C2.9624484.1581421.215866C4.6732644.0833742.953537C3.7424323.4826203.822861H5.8251041.0705115.397293H4.9981381.0001536.987137H6.6639401.7993936.806015H4.8315283.5104227.004425H5.7915343.6447455.545776H2.1492772.2191626.448380	С	5.042160	3.013000	6.046616				
C       2.531616       2.611649       5.508820         N       1.694885       2.725098       4.411362         C       2.410324       3.260086       3.362442         C       2.016098       3.572769       2.055145         C       2.962448       4.158142       1.215866         C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	С	3.807175	3.029053	5.188278				
N       1.694885       2.725098       4.411362         C       2.410324       3.260086       3.362442         C       2.016098       3.572769       2.055145         C       2.962448       4.158142       1.215866         C       4.277344       4.422700       1.663132         C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	С	2.531616	2.611649	5.508820				
C       2.410324       3.260086       3.362442         C       2.016098       3.572769       2.055145         C       2.962448       4.158142       1.215866         C       4.277344       4.422700       1.663132         C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	N	1.694885	2.725098	4.411362				
C2.0160983.5727692.055145C2.9624484.1581421.215866C4.2773444.4227001.663132C4.6732644.0833742.953537C3.7424323.4826203.822861H5.8251041.0705115.397293H4.9981381.0001536.987137H6.6639401.7993936.806015H4.8315283.5104227.004425H5.7915343.6447455.545776H2.1492772.2191626.448380	С	2.410324	3.260086	3.362442				
C2.9624484.1581421.215866C4.2773444.4227001.663132C4.6732644.0833742.953537C3.7424323.4826203.822861H5.8251041.0705115.397293H4.9981381.0001536.987137H6.6639401.7993936.806015H4.8315283.5104227.004425H5.7915343.6447455.545776H2.1492772.2191626.448380	C	2.016098	3.572769	2.055145				
C       4.277344       4.422700       1.663132         C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	C	2,962448	4.158142	1,215866				
C       4.673264       4.083374       2.953537         C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	C	4,277344	4.422700	1.663132				
C       3.742432       3.482620       3.822861         H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	Ċ	4,673264	4.083374	2.953537				
H       5.825104       1.070511       5.397293         H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	Ċ	3.742432	3,482620	3.822861				
H       4.998138       1.000153       6.987137         H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	H	5.825104	1.070511	5.397293				
H       6.663940       1.799393       6.806015         H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	H	4,998138	1.000153	6,987137				
H       4.831528       3.510422       7.004425         H       5.791534       3.644745       5.545776         H       2.149277       2.219162       6.448380	H	6.663940	1.799393	6.806015				
H 5.791534 3.644745 5.545776 H 2.149277 2.219162 6.448380	н	4,831528	3.510422	7 004425				
H 2.149277 2.219162 6.448380	H	5.791534	3.644745	5.545776				
	Н	2.149277	2.219162	6.448380				

**Table S9.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}(Mn)SOD^{HOH}$  (starting coordinates based on PDB file 1MMM).<sup>3</sup>

Atom	х	v	7.	Н	0.619186	3.849777	-2.847153
	2 720270	1 20000	1 000700	11	1 020075	1 052625	2 240250
C	-2./283/8	-5./22290	1.029/09	Н	1.030975	1.053635	-3.249359
С	-1.190094	-5.691742	1.067581	Н	2.743851	-0.514038	-4.142044
С	-0.563339	-4,401642	0.656433	Н	5.040543	0.278778	-4.683151
NT	0 017017	1 205072	0 6 5 0 5 0 5	ц	5 686325	2 645477	-1 295120
IN	0.81/91/	-4.2858/3	0.038383	п	5.000525	2.045477	-4.293120
С	1.151443	-2.986832	0.432846	C	-1.323822	1.224/4/	-3./50412
N	0.054000	-2.264023	0.270172	С	-2.660568	6.487839	-3.896042
C	-1 016449	-3 129913	0 401291	C	-2 980713	5 519882	-2 751678
	1.010449	3.129915	1 400000	0	1 047402	1 205002	2.751070
н	-3.130188	-4.//839/	1.422/60	C	-1.94/403	4.395996	-2.564041
Н	-3.080963	-6.520950	1.716949	0	-1.145538	4.074982	-3.470856
н	-3.114487	-5.868088	-0.000137	N	-2.008789	3.747513	-1.385162
11	0 956506	E 020240	2 107024	ц	-0 545532	6 463028	-3 598038
п	-0.838308	-3.030340	2.10/034		0.545552	0.405020	5.550050
H	-0.775238	-6.529251	0.482605	Н	-1.308762	7.929672	-2.868454
Н	1.450729	-5.071213	0.866608	Н	-1.044540	7.713882	-4.717651
н	2 159805	-2 592163	0 390182	н	-3.491638	7.202164	-3.983475
11	2 027506	2 702066	0 204220	п.	-2 630252	5 005/37	- 1 010067
п	-2.03/508	-2.703900	0.304230	п	-2.039232	5.005457	-4.010007
С	-8.613953	0.641754	-4.880142	Н	-3.102539	6.056335	-1.795853
С	-7.075745	0.693817	-5.005219	Н	-3.946152	5.023788	-2.950607
C	-6 358261	1 170166	-3 754883	н	-1.304672	3.015717	-1.032303
c	6.350201	2 226721	2.00005	11	2.001072	4 111212	1.052505
C	-0./01001	2.336/31	-3.080055	п	-2.042022	4.111313	-0.0/9002
С	-6.129990	2.757004	-1.916702	С	5.142853	1.513504	-0.637878
С	-5.090027	2.001968	-1.365173	С	4.144806	0.362091	-0.473572
0	-4,529373	2,318481	-0.140930	С	2.786194	0.729752	0.117371
o a	1.525575	2.0101	0.110550	0	2 505179	1 000707	0 400522
C	-4.63/939	0.862137	-2.033/3/	0	2.505478	1.000/07	0.409552
С	-5.264984	0.471924	-3.220459	0	1.961960	-0.297546	0.154755
Н	-8.985687	1.622070	-4.548431	0	-0.436615	1.882614	-0.321121
н	-8 933700	-0 090042	-4 099930	Fe	0 00000	0 000000	0 00000
11	0.005202	0.00042		10	4 657050	2 267447	1 105671
н	-9.095383	0.426/12	-5.8/9654	п	4.05/959	2.30/44/	-1.1230/1
H	-6.678619	-0.289276	-5.296982	Н	5.976303	1.162445	-1.286423
Н	-6.831009	1.378357	-5.832077	Н	5.512512	1.827286	0.353027
ч	-7 592361	2 936400	-3 169971	н	3 908722	-0 079971	-1 455902
11	7.JJZJ01	2.550400	1 412742	11	4 5565722	0.075571	0 100010
н	-6.453522	3.6/8116	-1.413/42	Н	4.556503	-0.466080	0.129013
Н	-5.103149	3.013123	0.277435	Н	0.430344	2.273117	-0.059448
Н	-3.815200	0.281174	-1.615936	С	-0.271973	-0.981705	6.390488
н	-4 887680	-0 414139	-3 731384	С	-1.570847	-0.747910	5.573273
0	1.007000	1 027402	C 1E2702	c	-1 423050	-0 200177	1 117010
C	0.348526	-1.837402	-0.153/93	C	-1.423030	-0.200177	4.14/042
С	-0.858719	-2.260086	-5.289261	N	-1.934830	0.923325	3.700439
С	-1.000061	-1.476242	-4.016174	C	-1.658188	1.056473	2.372070
N	-1.512695	-0.187195	-3,990280	Ν	-0.994064	-0.003571	1.933319
C	-1 396699	0 311560	-2 733505	Ċ	-0 8/5779	-0 845108	3 02/551
C	-1.390098	0.511509	-2.755505		0.045775	0.045100	J.024JJI
N	-0.855179	-0.593811	-1.928055	Н	-0.56/245	-1.3/5351	1.3/6038
С	-0.603638	-1.709946	-2.718246	Н	0.262222	-0.030304	6.589996
н	1,259491	-1.918488	-5.542694	Н	0.411972	-1.752151	5.912308
11	0 200509	0 772644	6 502441	ц	-2 1/2007	-1 692429	5 576736
п	0.300398	-0.772644	-0.302441	п	-2.142807	-1.092429	5.570750
H	0.485992	-2.549133	-6.993500	Н	-2.208405	-0.031006	6.114883
Н	-1.777573	-2.146866	-5.877823	Н	-2.530700	1.554688	4.229645
Н	-0.780991	-3.322311	-5.030350	Н	-1.876648	1.935928	1.776993
 u	-1 9/0003	0 200700	-1 700107	н	-0 320496	-1 790634	2 928406
11	1 (2000)	1 210700	4./OULJ/		0.520190		2.520100
н	-1.0/2836	1.319/02	-2.454224				
Н	-0.139236	-2.601685	-2.310150				
С	5.553421	5.982071	-2.022812				
C	1 913921	5 513687	-3 367172				
C	1.943924	5.513007	2.007172				
C	3./34268	4.623200	-3.28/003				
С	2.446335	4.949371	-2.907593				
N	1.642410	3.827698	-2.908371				
C.	2.386108	2.750671	-3,333588				
č	2.000100	1 /10007	_2 E10EEE				
C	2.023529	1.410202	-2.010000				
С	2.988388	0.542465	-4.022202				
С	4.295166	0.990341	-4.322632				
C.	4.662888	2,312927	-4.098709				
č	2 7002000	2 9 1 0 2 9 2	1.000/00				
	J./U8∠∠⊥	3.410343	-3.590430				
Н	5.722504	5.123825	-1.35/941				
Н	4.868454	6.694626	-1.496689				
н	6,549271	6.443924	-2.246628				
 u	1 711504	6 101070	-3 075720				
п 	4./11094	0.4013/0	- 3 . 3 / 3 / 3 / 3				
Н	5.710907	4.961304	-3.931686				
Н	2.039185	5.914505	-2.616409				

**Table S10.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of  $Fe^{2+}(Mn)SOD^{OH-}$  (starting coordinates based on PDB file 1MMM).<sup>3</sup>

Atom	х	V	Z	N	1.901428	2.471954	5.168365
C	-2.424316	-0.567902	-5.722229	С	2.309372	2.819489	3.887726
C.	-0.888245	-0.613129	-5.716217	C	1.542664	3.061630	2.756348
C.	-0.291260	-0.335602	-4.374069	C	2.224396	3,469131	1.600693
N	1 073593	-0 418533	-4 136230	C	3,619263	3.629761	1.593445
C	1 308884	-0 228745	-2 815643	C	4.385834	3.355576	2.727737
N	0 160812	-0 044586	-2 175339	C	3 726913	2 933929	3 894653
C	-0 835342	-0 093094	-3 133270	н	6 251434	0 601898	4 980057
ц	-2 778763	-1 050079	-1 803787	н	5 580170	0.531876	6 641678
и П	-2 865/63	-1 157135	-6 560837	н	7 206100	1 288528	6 351746
п 11	2.000400	-1.137133	-0.J000J7	11 U	5 584442	3 085968	6 687561
п	-2.792330	1 62472040	- 0.079123	11 U	6 215027	3 13/070	5 0/6021
н	-0.539322	-1.624/10	-5.9/1954	п 11	0.210027	2 120202	7 015001
н	-0.477859	0.060898	-6.4/9034	п	2.914000	2.120392	7.013091 E 200002
H II	1.829010	-0.638900	-4.802078	п	0.690330	2.2//433	2.200092
H	2.291382	-0.2218/8	-2.361588	н	0.459320	2.953857	2.//4/19
н	-1.86/035	0.089432	-2.868378	н	1.003498	3.070645	0.689835
C	-8.737228	4.752335	1.976685	H	4.108017	3.9/9645	0.686432
С	-7.231323	4.789810	2.308975	H	5.4/1//1	3.466/21	2./05338
С	-6.577942	3.425278	2.280365	С	5.330872	0.255951	1.433975
С	-7.069412	2.333862	3.014084	С	4.178360	0.423325	0.443115
C	-6.512787	1.062012	2.864655	C	2.823792	-0.054276	0.947800
С	-5.452300	0.874100	1.974442	0	2.596130	-0.434647	2.099335
0	-4.908249	-0.403778	1.769150	0	1.888885	0.000000	0.000046
С	-4.948288	1.942764	1.238464	Fe	0.00000	0.000000	0.00000
С	-5.511139	3.207489	1.402908	Н	5.034439	0.645813	2.415756
Н	-9.311325	4.398514	2.846481	Н	6.238861	0.805496	1.089417
Н	-8.925644	4.032852	1.152267	Н	5.559067	-0.821045	1.535828
Н	-9.105362	5.768570	1.745132	Н	4.020355	1.484680	0.191040
Н	-6.699509	5.405685	1.571609	Н	4.376007	-0.078354	-0.518082
Н	-7.081512	5.275711	3.283768	С	-0.165894	-6.030975	-1.529053
Н	-7.910706	2.472763	3.697632	С	-1.533554	-5.361954	-1.212357
Н	-6.892853	0.216187	3.439285	С	-1.452957	-3.993347	-0.589539
Н	-4.312500	-0.576889	2.548843	N	-1.959030	-3.668213	0.666519
н	-4.118347	1.774078	0.553238	С	-1.660538	-2.379135	0.949753
н	-5.119873	4.065384	0.850586	N	-0.987854	-1.837708	-0.061417
С	-2.396194	5,283493	4,285034	С	-0.861633	-2.826828	-1.023071
C.	-3.372787	4.090988	4.248993	Н	-0.367966	-6.958740	-2.085739
C.	-2.985657	2.879303	5.126358	Н	0.352798	-6.338486	-0.592087
C.	-1.745422	2.095200	4.654709	Н	0.459915	-5.372147	-2.210403
0	-0.710159	2.157974	5.370865	Н	-2.101624	-5.282242	-2.150818
0	-1.856628	1.376694	3,581039	Н	-2.125092	-6.022217	-0.560425
н	-1 362717	4 892548	4 316833	Н	-2.587891	-4.210388	1.262375
н	-2 462433	5 958267	5 179276	Н	-1.890000	-1.888382	1.884766
н	-2 494598	5 885788	3 336121	н	-0.326080	-2.627930	-1.944824
н	-4 386032	4 409500	4 533432	0	-0.200241	-0.000015	2.125000
н	-3 476929	3 715652	3 218231	H	0.746582	-0.138947	2.409393
н	-2 798660	3 188873	6 162735	н	-0.698975	0.604309	2.808151
н	-3 831284	2 174393	5 122360				
C	0 775330	5 978745	-0 898529				
C	-0 583282	5 376465	-1 315247				
C	-0.867126	1 016342	-0 766205				
N	-1 100166	3 073605	0.700203				
	1 505460	3.02300J 3.E17334	0.440000				
L NI	-1.303403	2.017074	0.700230				
IN O	-0.940394	1.021///	1 107500				
C II	-0.548600	2.750330	-1.18/500				
н	1.338131	5.218979	-1.038936				
H II	0.848/55	6.330688	0.100/94				
H	0.995438	6./83646	-1.019019				
H	-1.392731	6.054321	-1.018021				
H	-0.618958	5.295273	-2.409225				
H	-1./46/35	4.588943	1.080124				
H	-1.881012	2.130493	1./18460				
Н	-0.034729	2.454041	-2.093842				
C	6.181458	1.145523	5.929077				
C	5.570800	2.558304	5.725891				
C	4.166504	2.608688	5.216705				
С	2.995056	2.354630	5.956772				

**Table S11.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E  $Fe^{3+}SOD^{HOH}$  with Glu69 deprotonated (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	х	У	Z	С	2.326600	2.302185	6.282532
С	-1,949646	-0.490829	-5.885468	N	1.286255	2.368668	5.399292
C	-0 416580	-0 387100	-5 850784	C	1.769852	2.716949	4.149551
C	0 102/32	-0 131027	-1 176110	Ċ	1 093948	2 943024	2 953445
N	1 4502432	0.101027	4.4/0440	C	1 050050	2 370570	1 961053
N	1.450348	-0.1818/0	-4.148651	C	2 220202	2 = 0211=	1 067575
C	1.581207	-0.038467	-2.804581	C	3.238297	3.383115	1.96/5/5
N	0.388062	0.092072	-2.241500	С	3.914581	3.328064	3.159424
С	-0.533279	0.053818	-3.270630	C	3.178329	2.882523	4.272186
Н	-2.289215	-1.019302	-4.985382	H	5.711945	0.665695	5.480835
Н	-2.290146	-1.102539	-6.742218	Н	4.851471	0.516678	7.041946
Н	-2.422500	0.516449	-5.871521	Н	6.503265	1.326996	6.961884
Н	0.035721	-1.340561	-6.166489	Н	4.855469	3.086472	7.189758
Н	-0.065918	0.370865	-6.563950	Н	5.568176	3.173630	5.587402
н	2.251587	-0.374969	-4.765823	Н	2,148193	2,068192	7.328949
н	2 526810	-0.031326	-2 279282	Н	0.299500	2.190628	5.596146
н	-1 589035	0 184875	-3 077500	н	0 017288	2 803070	2 879288
	2.305033	1 162002	0 000000	и Ц	1 355972	3 58/808	0 910248
C	-0.030903	4.402902	1 256105	11	2 700070	2 05554000	1 104520
Ĉ	-7.334671	4.508438	1.256195	п	3.790070	3.955551	1.104000
С	-6./04010	3.142136	1.433472	H	4.994858	3.4/8302	3.22/142
C	-7.265350	2.162613	2.268478	С	5.194473	0.455400	1.695328
С	-6.675995	0.905594	2.409637	С	4.145111	0.569733	0.588058
С	-5.514343	0.597794	1.693161	С	2.796326	-0.011826	0.996567
0	-4.932587	-0.665222	1.736755	0	2.561142	-0.445175	2.120407
С	-4.942291	1.550278	0.852661	0	1.906067	0.000000	0.000015
С	-5.529114	2.811478	0.748077	Fe	0.000000	0.000000	0.000000
Н	-9.408676	4.052567	1.742294	0	-0.614563	0.000015	1.827713
н	-9 031097	3 786118	0 032181	Н	4.765366	0.815384	2.637878
н	-9 232452	5 483688	0.751282	н	6 107956	1 048279	1 468460
и и	-6 77110/	5 046707	0./79700	и Ц	5 /62631	-0 608337	1 825272
п 	-0.771194	5.040707	0.470700	11	2 046020	1 6200557	0 225012
H	-7.205811	5.090607	2.184479	п	3.940930	1.020950	0.323012
Н	-8.188751	2.364517	2.811752	Н	4.461533	0.0851/5	-0.350845
Н	-7.124832	0.158173	3.068207	Н	0.211472	-0.178711	2.335449
Н	-5.012207	-0.986877	2.677139	С	0.099838	-5.872726	-2.103912
Н	-4.023788	1.312073	0.318649	С	-1.308243	-5.254349	-1.901428
Н	-5.041245	3.579147	0.146378	С	-1.326630	-3.942841	-1.165771
С	-3.324203	5.113922	4.186096	N	-1.962662	-3.742477	0.054794
С	-4.252914	3.890060	4.113251	С	-1.739548	-2.469818	0.471573
C	-3.841370	2.698914	5.019821	N	-1.002900	-1.827423	-0.431046
C	-2 566025	2 004471	4 584030	C	-0.747223	-2.727783	-1.450882
0	-1 /71283	2.004471	5 101730	н	-0 014832	-6 779373	-2 718323
0	2 720027	1 100000	2 550200	и и	0.014032	-6 203506	-1 130/79
0	-2./3093/	1.120090	3.009280	п	0.333330	-0.203300 E 171014	-1.130478
H	-2.2/8091	4./596/4	4.234421	H	0.766037	- 5.1/1814	-2.69/968
Н	-3.432938	5.765686	5.091003	Н	-1./58682	-5.104248	-2.893997
Н	-3.411453	5.704285	3.233566	Н	-1.957108	-5.975281	-1.381531
Н	-5.289948	4.161652	4.359406	H	-2.483734	-4.435120	0.583557
Н	-4.308990	3.504242	3.083435	H	-2.073059	-2.046143	1.411789
Н	-3.670761	3.024826	6.051788	H	-0.147476	-2.439300	-2.307220
Н	-4.654709	1.958405	5.010040				
Н	-1.855804	0.749405	3.267471				
С	0.501129	6.140198	-0.739273				
С	-0.757706	5,470856	-1.332016				
C	-0 966049	4 065323	-0 873184				
N	-1 662552	3 700101	0 205050				
0	1 5700/1	2 4702101	0.200000				
	-1.5/9941	2.4/0322	0.062404				
N	-0.888992	1.856842	-0.395/21				
C	-0.501053	2.843307	-1.29///5				
Н	1.347366	5.448303	-0.860764				
H	0.459793	6.407806	0.355362				
Н	0.734604	7.011963	-1.369278				
Н	-1.653290	6.055862	-1.084564				
Н	-0.680176	5.453003	-2.426834				
Н	-2.079025	4.489746	0.894089				
Н	-2.007217	2.004517	1.438889				
Н	0,103638	2,617584	-2.167587				
C C	5 507250	1 171036	6 437005				
c	1 001100	1.1/1000 0 570617	6 22250				
	4.7U11U8	2.3/201/	0.222300				
C	3.526550	∠.589508	5.630646				

**Table S12.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E Fe<sup>3+</sup>SOD<sup>OH-</sup> with Glu69 protonated (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	х	V	Z	N	1.164719	2.963135	5.019974
С	-1.820251	-1.022995	-5,998291	С	1.706741	3.180481	3.772110
C	-0.297684	-1.049911	-5.800461	C	1.064697	3.341888	2.547073
C	0.152603	-0.626511	-4.443512	C	1.864029	3.619110	1.437378
N	1.485413	-0.704636	-4.059891	C	3.263504	3.732056	1.557175
C	1.583191	-0.363907	-2.748276	C	3.904114	3.544922	2.779465
N	0 385681	-0.083710	-2 259796	C.	3.121094	3.258300	3.911362
C	-0 506836	-0 229691	-3 304672	н	5 546295	1 082520	5 280853
н	-2 301636	-1 444702	-5 106293	н	4 729950	1 081818	6 877930
н	-2 131363	-1 673019	-6 848831	н	6 382400	1 828644	6 722931
и и	-2.191303	0.016403	-6 110333	н	4 707184	3 588745	6 873611
п u	0 07/020	-2 079766	-5 010000	н	5 457794	3 628723	5 287491
п	0.074029	-2.070700	-3.919090	11 U	1 072026	2 001170	6 99/736
п	0.109/30	1 000075	-0.372230	п 11	1,973230	2.001170	0.994730 E 16EE27
п	2.290344	-1.022075	-4.01/300	п 11	0.132107	2.970490	2 400000
H	2.300332	-0.330139	-2.183436	п	1 40740	3.203243	2.400990
H	-1.5580/5	-0.015488	-3.1/0/46	H	1.40/480	3./55905	0.456300
C	-8.826/06	4.695465	-0.014526	H	3.855972	3.961975	0.0/3553
С	-7.354462	4.768967	0.408096	Н	4.992920	3.615448	2.852219
С	-6.766037	3.492279	0.968246	C	5.224884	0.433670	1.659195
С	-7.356354	2.830582	2.060913	C	4.163513	0.497025	0.561676
C	-6.687988	1.822647	2.751465	С	2.797211	-0.037109	0.999832
С	-5.380127	1.448090	2.371933	0	2.557907	-0.458115	2.124863
0	-4.632935	0.654602	3.162308	0	1.910461	0.000000	0.000000
С	-4.860489	1.986160	1.176529	Fe	0.000000	0.000000	0.000000
С	-5.534119	3.007950	0.512238	0	-0.829422	0.000000	1.665436
Н	-9.438858	4.397659	0.851791	Н	4.832230	0.907745	2.568069
Н	-9.005234	3.933746	-0.813339	Н	6.159866	0.964645	1.361420
Н	-9.191208	5.703186	-0.304092	Н	5.447403	-0.624039	1.891739
Н	-6.721786	5.113922	-0.423935	Н	3.988327	1.534531	0.236679
Н	-7.266083	5.535278	1.196869	Н	4.470108	-0.053497	-0.344131
Н	-8.324631	3.178619	2.440536	Н	-0.212585	0.062286	2.425461
Н	-7.115173	1.404388	3.666718	С	0.128052	-6.165558	-1.403931
Н	-3.877914	1.657562	0.839325	С	-1.273926	-5.496552	-1.405502
Н	-5.043045	3.512833	-0.322021	С	-1.315353	-4.094925	-0.861832
н	-3.685791	1.191437	3.335022	Ν	-1.995956	-3.737259	0.297195
С	-3.138794	5,906967	3.398056	С	-1.772018	-2.424988	0.558655
C	-4.107544	4,713058	3.424805	N	-0.974548	-1.910095	-0.370392
Ċ	-3 831680	3 678894	4 543304	C	-0.694138	-2.931046	-1.259674
C	-2 510071	2 943222	4 308395	н	0.027039	-7.153152	-1.881638
0	-1 464584	3 452072	4 795837	н	0.478973	-6.360916	-0.365204
0	-2 512207	1 874680	3 578522	н	0.852676	-5.555359	-2.032425
о н	-2 118317	5 530289	3 590103	н	-1.639496	-5.485443	-2.443893
н	-3 307129	6 662827	4 203812	н	-1.981766	-6.124008	-0.842500
и и	-3 1/5721	6 372559	2 376724	н	-2 681290	-4 299454	0 812668
и и	-5 15/69/	5 0/9515	3 / 88510	н	-2 139557	-1 882339	1 422485
и и	-1 055283	1 165619	2 169772	н	-0 041382	-2 761566	-2 110718
и и	-3 757010	4.166590	5 5010/0		0.011502	2.701500	2.110/10
и П	-1 654739	2 950790	1 566986				
C	4.034733	6 007065	-1 380981				
C	-0 736176	5 331095	-1 940637				
C	-0.976669	3 000063	-1 196030				
N	-1 5/3001	3 959017	-1.190030				
N	-1.040991	3.03091/ 3.571015	0.060959				
C NI	-1.403023	2.5/1915	0.40030				
N	-0.906265	1.844803	-0.513916				
C	-0.59/229	2.726349	-1.543396				
H	1.3/2940	5.251434	-1.3/68//				
H	0.540955	6.438431	-0.3454/4				
н	0.8/8693	6./53891	-2.132294				
H	-1.592651	5.991302	-1.647751				
H	-0.700150	5.161118	-2.924500				
H 	-1.863800	4.642319	0.635208				
H 	-1.773300	2.199341	1.431381				
H	-0.082520	2.402695	-2.440231				
С	5.399826	1.655640	6.204208				
С	4.772522	3.046097	5.923584				
С	3.413361	3.061722	5.298264				
С	2.181381	2.913132	5.933136				

**Table S13.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E Fe<sup>3+</sup>SOD<sup>OH-</sup> with Glu69 deprotonated (starting coordinates based on PDB file 1ISA).<sup>1</sup>

Atom	x	V	7	C	3 324936	2 540909	5 531403
7100111	A	<u>y</u>	5 010166		9.524950	2.540909	3.331403 4 815051
C	-2.660172	-1.389313	-5.318466	N	2.214752	2.547836	4.715851
С	-1.130600	-1.385284	-5.404633	С	2.605103	2.870193	3.442932
C	-0 458054	-0 942627	-4 140182	С	1.849548	3.003143	2.271393
NT	0 007707	1 077007	2 021010	C	2 5100/5	3 312221	1 101501
IN	0.897797	-1.0//08/	-3.931010	C	2.510045	3.542224	1.121321
C	1.203125	-0.624313	-2.727600	C	3.913193	3.549820	1.11419/
N	0.094635	-0.198669	-2.148727	С	4.661423	3.416885	2.274933
C	-0 959579	-0 386398	-3 011261	С	4.003372	3.071411	3.466064
11	0.0000000	1 710207	A 21EAAE	U U	6 59/213	1 005600	1 571060
п	-2.952556	-1./1030/	-4.515445	п	0.304213	1.003000	4.371900
H	-3.076355	-2.078766	-6.053009	Н	5.931168	0.964462	6.227539
Н	-3.047806	-0.375961	-5.422974	Н	7.515411	1.729980	5.910187
н	-0.775970	-2.392044	-5.625595	Н	5.834839	3.461411	6.233536
TT	0 010561	0 706741	6 106126	U	6 116211	3 171070	4 551620
п	-0.012301	-0./06/41	-0.190130	п	0.410214	5.471970	4.551020
Н	1.564102	-1.459610	-4.587112	Н	3.40//15	2.333481	6.598236
Н	2.236313	-0.650574	-2.381271	Н	1.251404	2.501343	5.025955
Н	-1.966644	-0.094955	-2.712692	Н	0.772247	2.838745	2.296036
C	- 9 612570	1 532691	1 222207	н	1 971466	3 456726	0 185883
C	-0.012379	4.552004	1.0100	11	1 10005	2 010120	0.107040
C	-/.090012	4.69/861	1.401/03	н	4.419205	3.819138	0.18/042
С	-6.344879	3.507172	1.973618	Н	5.738907	3.580017	2.250519
С	-6.658813	3.003891	3.240875	С	5.482681	0.204620	1.039139
C	-5 92/057	1 964050	3 806244	C	4 290268	0 329285	0 081604
c	1.005000	1 412625	2 102745	C	2.002105	0.000771	0.001004
C	-4.865860	1.413635	3.103/45	C	2.983185	-0.208771	0.000508
0	-4.116898	0.407349	3.674377	0	1.938538	0.000000	-0.000107
С	-4.538284	1.885864	1.840164	0	2.984375	-0.826996	1.752197
Ċ	-5 280151	2 930344	1 280167	Fe	0 00000	0 000000	0 00000
	0.052401	4 115241	2.2700107	10	E 261002	0.000000	1 005152
Н	-8.953491	4.115341	2.2/9800	Н	5.261093	0.698547	1.985153
H	-8.899765	3.868042	0.517654	H	6.349121	0.676941	0.576309
Н	-9.079849	5.505295	1.178284	Н	5.731552	-0.844711	1.197327
н	-6 695800	4 861649	0 398773	н	4 129440	1 378952	-0 164474
11	0.0000	4.001040	0.000775	11	1 106120	0 00050	0 021024
н	-6.84504/	5.552/80	2.031967	п	4.490429	-0.229838	-0.031024
H	-7.491150	3.425903	3.804108	C	-0.340302	-6.247131	-1.029510
Н	-6.183731	1.588577	4.796066	С	-1.642380	-5.440277	-0.825714
н	-3 740250	-0 141205	2 953796	С	-1.440033	-4.050705	-0.301178
TT	2 707226	1 442740	1 201214	N	-1 076563	-3 626633	0 005300
п	-3.707330	1.442/49	1.291214	IN	-1.970303	-3.020033	0.095509
H	-5.029938	3.305588	0.287811	C	-1.675812	-2.354600	1.086502
С	-2.660980	5.813156	3.835297	N	-0.961166	-1.937439	0.057159
C	-3 528519	4 560547	3 961807	С	-0.798019	-2.978729	-0.824997
c	2 067010	2 522026	4 021000	U U	-0 623611	-7 106000	-1 193063
C	-2.90/010	3.323020	4.951900	п	-0.023011	-7.190900	-1.403003
C	-1.700043	2.856018	4.409622	Н	0.16/526	-6.433060	-0.083084
0	-0.614212	3.425110	4.414398	Н	0.300186	-5.738510	-1.750061
0	-1.758362	1.587357	3,934967	Н	-2.164398	-5.345230	-1.777924
U	-1 621262	5 196313	3 953720	н	-2 282669	-5 957260	-0 110962
11	1.021202	5.400545	1.655080	11	2.202009	4 100500	1 526026
н	-2.842//3	6.495239	4.6658/8	н	-2.51/410	-4.189590	1.536026
H	-2.815521	6.287537	2.866135	H	-2.018677	-1.842682	1.985672
Н	-4.519196	4.838928	4.321213	Н	-0.230637	-2.830841	-1.743790
н	-3 617783	4 079865	2 987671	0	0.280319	0.00000	2.134430
11	2 724762	1.075005	E 070240	U U	0 522569	0 006070	2 176669
н	-2./24/62	4.004410	5.8/9349	п	0.522508	0.000070	2.4/0009
Н	-3.709686	2.743225	5.100632	Н	1.188812	-0.461304	2.142197
Н	-2.668793	1.196365	4.030487				
С	0.393326	5.994888	-1.380203				
Ċ	-0 915/05	5 252335	-1 670014				
C	-0.913403	3.232333	-1.070914				
C	-1.029297	3.954//3	-0.935455				
N	-1.398376	3.881912	0.391998				
С	-1.309097	2.629974	0.804413				
N	-0 900711	1 886780	-0 200366				
	0.700/11	1.000700	1 200075				
L	-0./22183	2.089636	-1.3098/5				
Н	1.191116	5.255081	-1.446136				
Н	0.383621	6.431503	-0.381470				
н	0.603973	6.721146	-2.165176				
 TT	1 70100	5 0 7 / F 0 7	1 275102				
п	-T./OTDZ	5.0/452/	-1.3/3183				
Н	-0.981018	5.034302	-2./36923				
Н	-1.692719	4.656357	0.969650				
Н	-1.558350	2.376434	1.834702				
н	-0 380633	2 255707	-2 252822				
	0.000000	2.200/0/	2.2J202J				
C	6.515976	1.546814	5.515579				
С	5.851929	2.908279	5.294540				
С	4,441849	2,851730	4,806717				

**Table S14.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E  $Fe^{2+}SOD^{HOH}$  with Glu69 and Tyr34 protonated (starting coordinates based on PDB file 2BKB)<sup>4</sup>

Atom	x	v	7.	N	1,706848	5,440338	-1,060669
-	0 00 00 10	5 630.045	0 1 5 0 1 0 6	a a	2 040210	4 202400	1 0 0 0 4 4 0
C	-2.33/219	-5.63984/	-0.150436	C	2.048218	4.383408	-1.862442
С	-0.829880	-5.616013	-0.423019	С	1,291702	3,279526	-2.274948
- -	0 050704	4 024121	0 407401	0	1 004000	2 2 2 2 4 1 1	2 002011
C	-0.253/84	-4.234131	-0.49/421	C	1.904068	2.362411	-3.092911
N	1,103241	-3,993011	-0.512314	С	3.242828	2.520538	-3.505173
0	1 21 221 5	2 600117	0 550720	C	3 002210	3 613900	-3 005303
C	1.310315	-2.08911/	-0.559/38	C	5.992210	3.013800	- 3 . 0 9 3 3 8 3
N	0.146393	-2.075851	-0.578644	С	3.391708	4.568115	-2.258759
0	0 050707	2 010720	0 540543	TT	6 275055	E 072761	0 267522
C	-0.852/0/	-3.019/30	-0.540543	п	0.2/5955	3.0/3/01	-0.30/323
Н	-2.558533	-4.830231	0.545197	Н	5.624420	6.567719	0.348450
TT	2 622566	6 501010	0 206402	ч	7 059334	6 639504	-0 717056
п	-2.023300	-0.391919	0.296402	п	7.050554	0.038304	-0.717030
H	-2.890457	-5.418030	-1.062973	Н	5.105194	7.419312	-1.942612
U	-0 307343	-6 142960	0 375301	н	5 691513	5 885391	-2 628342
п	-0.307343	-0.142900	0.373301	11	5.051515	5.005551	2.020342
H	-0.624588	-6.104965	-1.375381	Н	2.901810	7.212387	-0.393921
ц	1 830811	-1 693116	-0 490800	н	0 734161	5 644958	-0 817276
11	1.050011	4.000140	0.490000		0.754101	5.044550	0.017270
Н	2.335754	-2.303665	-0.576355	Н	0.257813	3.173813	-1.946060
н	-1 897308	-2 708252	-0 548782	н	1.353653	1.487427	-3.438812
	1.057500	2.700252	0.010702		2 704117	1 777466	4 1 5 5 7 6 9
С	-9.269302	2.215469	-2.381256	Н	3./0411/	1.///466	-4.155/62
С	-7.797577	2,439529	-2.747665	Н	5.026505	3.719330	-3.422958
0	6 066100	2.100025	1 564202	0	E 2E047E	1 412071	0 604007
C	-0.800180	2.619476	-1.564392	C	5.3584/5	1.4139/1	-0.684097
С	-7.101471	3.614502	-0.609268	С	4.171005	0.478409	-0.946182
Ċ	6 205972	2 920066	0 122015	C	2 969147	0 7/0269	-0 043229
C	-0.2058/2	3.839066	0.433945	C	2.909147	0.749200	-0.043220
С	-5.063217	3.063965	0.533035	0	1.910233	0.130707	-0.302841
0	-1 150333	3 305030	1 5//015	$\cap$	3 065/91	1 561691	0 907913
0	-4.139332	3.303939	1.344013	0	5.005491	1.301091	0.907913
С	-4.809204	2.062729	-0.394241	Fe	0.00000	0.000000	0.000000
C	-5 712602	1 9//300	-1 130736	ц	5 047668	2 151559	-0 776932
C	- 3.712092	1.044500	-1.438730	11	5.047000	2.454555	0.770952
H	-9.542862	2.938141	-1.612610	Н	6.136276	1.199800	-1.417053
н	-9 431946	1 205353	-2 005447	н	5 780716	1 220795	0 302155
	5.451540	1.205555	2.003447		3.000710	1.220799	1.0002100
Н	-9.893585	2.371460	-3.261017	Н	3.836395	0.595230	-1.977005
H	-7.427872	1.581802	-3.309631	Н	4,477371	-0.554169	-0.779007
	F F0F1F0	2.001002	0.050001		0 725412	2 121002	E 400.00
Н	-/./0/153	3.338/91	-3.3569/9	C	0./35413	-3.121002	5.469986
Н	-7,998489	4,230438	-0.673462	С	-0.686569	-2.742264	4.998444
	C 40C021	4 (21204	1 1 ( 5 0 0 4	C	0 700050	1 762402	2 961761
н	-6.406921	4.021384	1.165894	C	-0.728038	-1./02402	3.004/01
H	-3.292587	3.540421	1.047119	N	-1.339645	-0.532211	3.972794
U	-3 0101/1	1 /52001	-0 305374	C	-1 261124	0 101593	2 816422
п	-3.910141	1.452001	-0.303374	C	-1.201124	0.101393	2.010422
H	-5.520859	1.058945	-2.169968	N	-0.618454	-0.672760	1.961044
C	-3 611638	5 400604	-3 623856	C	-0 272797	-1 844208	2 591278
C	3.044030	5.400004	5.025050	0	0.272797	1.011200	2.351270
С	-4.287842	5.033066	-2.286453	Н	0.621/19	-3.889542	6.23446/
C	-3 566986	5 626160	-1 077560	н	1 258896	-2 262924	5 891830
-	5.500500	5.020100	1.077500		1.000000	2.202521	5.051050
C	-2.200470	4.994308	-0.840576	Н	1.286667	-3.5/9605	4.649094
0	-1.198700	5.470764	-1.425629	Н	-1.208496	-3.637772	4.660843
~	0 140700	2 0 0 1 7 0 0	0 000017		1 000145	2 201000	E 00E010
0	-2.140/93	3.961/00	-0.02691/	н	-1.236145	-2.291900	5.825012
Н	-2.564743	5.376495	-3.477737	Н	-1.782730	-0.160248	4.800644
	2 047205	C 200010	2 027110	п	-1 60/122	1 096191	2 709610
н	-3.94/205	0.399918	-3.93/119	п	-1.094122	1.090191	2.709010
H	-3.868759	4.643661	-4.375458	Н	0.269485	-2.616852	2.046234
U	- 5 314575	5 300170	-2 263077	0	-0 328354	2 106781	0 766571
11	5.514575	5.550170	2.205577	0	0.520554	2.100/01	0./005/1
H	-4.285248	3.949692	-2.167038	Н	-0.833710	2.908463	0.411179
н	-3 418655	6 695100	-1 230804	Н	0.590576	2,404922	0.950089
 TT	1 1 1 7 0 0 0	E 400010	0 101040				
н	-4.10/892	5.468018	-0.181946				
С	-0.618561	0.779327	-6.083435				
C	-1 770/24	0 164002	- 5 202762				
C	-1.19434	0.104993	-2.293/02				
С	-1.677841	0.403748	-3.820511				
N	-2 0/1153	1 598/0/	-3 233765				
IN	2.041155	1.320404	5.255705				
С	-1.744141	1.563660	-1.946869				
N	-1 206300	0 387100	-1 676331				
10	1.156056	0.507100	1.070551				
C	-1.1208./0	-0.358475	-2.829285				
Н	0.293915	0.518723	-5.547104				
	0 711400	1 0 ( 1 0 1 1	6 120102				
н	-0./11426	1.864014	-0.138123				
Н	-0.527267	0.305573	-7.060776				
п	-2 720245	0 507676	-5 62/100				
п	-2./20245	0.09/020	-0.034109				
Н	-1.797363	-0.913254	-5.452805				
н	-2 468010	2 381552	-3 702712				
	2.100010	2.304332	1 015113				
Н	-1.956055	2.426193	-1.315125				
н	-0.746857	-1.368195	-2.808136				
	C 100105	1 0 0 1 0 0 1 0 J	2.000100				
C	P.T08T82	6.138535	-0.528885				
С	5.224487	6.351334	-1.760635				
Ċ	3 010000	5 770507	-1 657745				
C	2.040909	5.119581	-1.00//40				
C	2.794632	6.277466	-0.943924				

**Table S15.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E  $Fe^{2+}SOD^{HOH}$  with Glu69 protonated and Tyr34 deprotonated (starting coordinates based on PDB file 2BKB).<sup>4</sup>

7 + 0 m				D.T.	1 100710	F 400004	1 400750
ALOIII	X	У	Z	IN	1.120/12	5.499084	-1.462/53
C	-1.878479	-5.800125	0.349731	C	1.443466	4.435303	-2.263290
С	-0.423431	-5.675827	-0.113297	C	0.732422	3.260208	-2.536438
С	0.026428	-4.259430	-0.309692	С	1.309952	2.355377	-3.392532
N	1.347397	-3.918228	-0.505859	С	2.570190	2.594452	-3.977310
С	1.447784	-2.605484	-0.626526	С	3.274689	3.758423	-3.705460
N	0.239258	-2.083221	-0.518173	С	2.708191	4.702042	-2.833847
C	-0 668564	-3 096588	-0 319473	Н	5.755112	5.507919	-1.344452
U U	-2 075992	-1 979607	1 030/00	и Ц	5 079956	6 979889	-0 605072
п 11	2.073002	-4.9/000/	1.030490	11	6 260160	7 100406	1 0/6/51
п	-2.029938	-0.749710	0.003000	п	4 010700	7.109400	-1.0404JI
н	-2.556/32	-5.662155	-0.492294	H	4.213700	7.685104	-2.840347
Н	0.234680	-6.125290	0.630386	Н	4.831329	6.169800	-3.539993
Н	-0.299530	-6.190781	-1.065964	Н	2.243408	7.384216	-1.017303
Н	2.125732	-4.560165	-0.552170	Н	0.166077	5.639450	-1.118698
Н	2.423080	-2.145889	-0.786514	Н	-0.240784	3.092407	-2.075073
Н	-1.727631	-2.864975	-0.205719	Н	0.792740	1.426743	-3.634018
С	-9.640594	1.403763	-1.259109	Н	3.005127	1.859207	-4.654358
C	-8.248474	1.720688	-1.817703	Н	4.248444	3.926117	-4.165665
C	-7 194824	2 023560	-0 769852	C	5 101532	1 779083	-1 410858
C	-7 300506	2.025500	0.171371	C	3 969/37	0 7/6185	-1 486084
C	-7.300390	2.040373	1 002274	C	2 071216	0.740105	1.400004
C	-6.391296	3.3/8830	1.083374	C	2.0/1210	0.966995	-0.44/032
С	-5.186829	2.696915	1.063/21	0	1.841217	0.259628	-0.548111
0	-4.186600	3.051743	1.942917	0	3.019516	1.826782	0.453888
С	-4.970505	1.676392	0.147964	Fe	0.000000	0.000000	0.000000
С	-5.976288	1.343521	-0.764496	Н	4.699265	2.788162	-1.500427
Н	-9.873627	2.138153	-0.488205	Н	5.796890	1.590698	-2.228760
Н	-9.673935	0.402496	-0.829880	Н	5.657013	1.663147	-0.480194
н	-10.379791	1,472427	-2.057266	Н	3.501144	0.790604	-2.469376
н	-7 883911	0 868423	-2 391190	н	4.375931	-0.251831	-1.322525
и П	-9 306763	2 505505	-2 165296	C	1 656555	-2 805008	5 439667
п т	-0.00700	2.595505	-2.405200	C	0 161255	-2 555862	5 139786
H	-8.333100	3.384015	0.200012	C	0.101255	1 624445	2 006200
H	-6.561905	4.1/6315	1.806610	C	-0.098984	-1.634445	3.986389
Н	-3.415329	3.319504	1.322815	N	-0./88986	-0.449860	4.12/4/2
Н	-4.021454	1.140350	0.143311	C	-0.905685	0.134781	2.948624
Н	-5.814484	0.542358	-1.485687	N	-0.314270	-0.627304	2.046585
С	-4.487091	4.941803	-3.320709	С	0.199677	-1.739700	2.669052
С	-4.927734	4.588303	-1.899994	Н	1.700607	-3.544373	6.239319
С	-4.112198	5.288116	-0.814651	Н	2.157898	-1.891891	5.760513
С	-2.680649	4.771927	-0.731171	Н	2.136566	-3.257935	4.572144
0	-1.797882	5.313843	-1.441589	Н	-0.325134	-3.502350	4.903549
0	-2 432114	3 788300	0 106247	н	-0.315720	-2.110794	6.013016
ч	-3 398972	5 005356	-3 312485	н	-1.154266	-0.074890	4.991165
и П	-1 005272	5 900314	-3 620265	н	-1 426849	1 088257	2 862396
п 11	4.903273	4 120740	- 3.020203	11	1,120019	2 102160	2.002330
H	-4./41455	4.136749	-4.010100	П	0.730223	-2.495469	2.00/341
H	-5.969681	4.8/6038	-1./59995	0	-0.40/86/	2.114059	0.707184
Н	-4.823654	3.514664	-1.743300	Н	-1.033005	2.849700	0.39/308
Н	-4.070160	6.357086	-1.023590	H	0.493134	2.502243	0.749649
Н	-4.582642	5.126251	0.155243				
С	-1.429535	0.453262	-5.979065				
С	-2.430374	-0.209839	-5.026566				
С	-2.166107	0.102631	-3.587769				
N	-2.548279	1.292175	-3.002472				
C	-2.091965	1.338333	-1.763519				
N	-1 432175	0 218933	-1 521835				
C	-1 466705	-0 572470	-2 611333				
C	-1.400705	-0.372479	-2.044333				
H	-0.439575	0.286453	-5.554367				
H	-1.614990	1.52430/	-0.060150				
Н	-1.422653	-0.056305	-6.942581				
Н	-3.437759	0.135117	-5.259552				
Н	-2.381485	-1.292511	-5.143478				
Н	-3.091629	2.021957	-3.441086				
Н	-2.292145	2.210403	-1.141098				
Н	-0.977707	-1.546646	-2.639557				
С	5.483856	6.548706	-1.521072				
С	4.439896	6.638428	-2.637054				
C	3.138016	5.970444	-2.339539				
С	2.143997	6.419846	-1.515488				
			· · · ·				

**Table S16.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E  $Fe^{2+}SOD^{HOH}$  with Glu69 deprotonated and Tyr34 protonated (starting coordinates based on PDB file 2BKB).<sup>4</sup>

7 ± om			-	NT	2 21/271	2 260271	1 000700
ALOIII	Х	У	Z	IN	2.214371	2.3082/1	4.808/00
С	-2.659805	-1.187820	-5.367172	C	2.604828	2.738403	3.548874
С	-1.130188	-1.180664	-5.453033	С	1.849380	2.915390	2.383118
С	-0.457764	-0.785934	-4.172760	С	2.518784	3.297546	1.246887
N	0 000007	-0 020177	-3 060330	Ċ	3 913086	3 505280	1 247498
IN C	1 202070	0.520177	2.740004	C	4 661200	2 220600	2 402466
C	1.203278	-0.521149	-2./49084	C	4.001209	3.320090	2.402400
N	0.094757	-0.117554	-2.154602	C	4.003113	2.938553	3.579697
С	-0.959351	-0.272583	-3.023727	Н	6.583893	0.832504	4.607178
Н	-2.932068	-1.554474	-4.377380	Н	5.930664	0.729050	6.259903
н	-3 075912	-1 849228	-6 127228	н	7.514954	1.505951	5.971771
TT	2 047204	0 171200	E 422472	и	5 83/351	3 224000	6 360000
п	-3.04/394	-0.171200	-3.433472	11	C 41E0C2	2 207020	4 (70740
н	-0.//5543	-2.1/8391	-5./11/46	н	6.415863	3.29/836	4.6/9/49
H	-0.812103	-0.472717	-6.218475	H	3.407242	2.083115	6.681778
H	1.564438	-1.285736	-4.638687	Н	1.229752	2.379608	5.089966
Н	2.236481	-0.560364	-2.403946	Н	0.772095	2.750198	2.401505
н	-1.966446	0.007324	-2.714432	н	1.971481	3,447220	0.316193
	-9 612640	1 170305	1 501617	н	4 419235	3 809326	0 331177
C	-0.012040	4.4/9000	1.501017	11	E 7207E4	2 402560	0.001000
C	-7.090057	4.641/54	1.5//164	п	5.758754	5.492509	2.304323
C	-6.345062	3.430359	2.103943	С	5.482574	0.165237	1.0465/0
С	-6.659027	2.879700	3.351273	С	4.290222	0.325943	0.094315
С	-5.924332	1.819275	3.877106	C	2.983124	-0.233505	0.652512
С	-4.866135	1.295715	3.154434	0	1.938492	0.000000	0.000031
0	-4.117203	0.268616	3.686844	0	2,984161	-0.892487	1,720032
c	-1 539391	1 015047	1 000561	Fo	0 000000	0 000000	0 000000
C	4.JJ0JJ1	2 000001	1 200220	10	E 26002E	0 600100	2 010544
C	-3.280238	2.880081	1.389328	п	5.260925	0.623123	2.010344
Н	-8.953659	4.026627	2.432617	Н	6.349060	0.654648	0.601898
H	-8.899796	3.845932	0.662369	H	5.731522	-0.889328	1.165039
Н	-9.079910	5.457123	1.384186	Н	4.129425	1.384125	-0.112045
Н	-6.695816	4.843292	0.581223	Н	4.496445	-0.198456	-0.838730
н	-6.845184	5.472351	2.239273	С	-0.340240	-6.203888	-1.264236
н	-7 /0130/	3 280243	3 9299275	Ċ	-1 642380	-5 405273	-1 030289
11	C 104000	1 400704	1 050000	C	1 440063	1 026494	0 452674
п	-0.104002	1.400/04	4.052000		1 076660	-4.030404	-0.455074
н	-3.1/3203	0.6668/0	3.729980	IN	-1.976669	-3.65//91	0./5/858
Н	-3.707458	1.393112	1.344406	C	-1.675980	-2.393890	0.996887
Н	-5.029953	3.292465	0.411835	N	-0.961227	-1.938217	-0.015900
С	-2.661240	5.664505	4.051422	С	-0.797989	-2.945496	-0.936661
С	-3.528732	4.408020	4.130585	Н	-0.623627	-7.135941	-1.753250
C	-2 967316	3 334702	5 060959	Н	0.167450	-6.425369	-0.325424
c	-1 700363	2 607066	1 514039	и	0 300278	-5 668503	-1 96/996
0	1.700303	2.007000	4.514050	11	2 164269	5.000505 E 274400	1 070000
0	-0.58/814	3.200928	4./82455	н	-2.164368	-5.2/4400	-1.9/8226
0	-1.835236	1.599380	3.785614	Н	-2.282/30	-5.948822	-0.335510
Н	-1.621521	5.337234	4.057632	H	-2.517593	-4.244537	1.376892
Н	-2.843079	6.314850	4.907089	Н	-2.018860	-1.916200	1.914688
Н	-2.815689	6.175034	3.100922	Н	-0.230606	-2.763123	-1.849197
н	-4.519485	4.672700	4.500153	0	-0.322327	0.000000	2.246277
н	-3 617950	3 961117	3 139069	н	-0 729935	0 663147	2 895600
11	2 725220	2 700020	C 005070	и 11	0 567169	-0 233200	2.699000
п	-2.723220	5.700029	0.023079		0.307105	0.233200	2.30331
н	-3./10114	2.549103	5.200058				
С	0.393463	6.042648	-1.153198				
С	-0.915237	5.311569	-1.471848				
С	-1.029175	3.987152	-0.785797				
N	-1.398392	3.864410	0.537933				
C	-1 309082	2 597778	0 902802				
N	-0 900696	1 893311	-0 138168				
10	0.7000000	2 727001	1 207011				
C	-0.722107	2.737091	-1.207611				
н	1.191315	5.30584/	-1.246964				
Н	0.383667	6.441330	-0.138748				
Н	0.604218	6.797958	-1.910233				
Н	-1.759995	5.922195	-1.152969				
Н	-0.980789	5.133865	-2.545334				
Н	-1,692734	4.616562	1.144348				
н	-1 558/56	2 305610	1 922929				
11 11	T.220420	J JJ00000	16604F				
л	-0.389430	4.330909	-2.100240				
C	0.515518	1.33/738	5.5/0435				
С	5.851517	2.706604	5.400803				
С	4.441422	2.668488	4.911179				
С	3.324509	2.330627	5.623520				

**Table S17.** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E Fe<sup>2+</sup>SOD<sup>OH-</sup> with Glu69 protonated and Tyr34 protonated (starting coordinates based on PDB file 2BKB).<sup>4</sup>

Atom	х	V	Z	С	3.146973	4.044052	-0.787521
C	-3 263070	-1 963379	-1 /15000	C	2 29/968	3 181000	-1 /87700
C	-3.203070	-4.903379	-1.415909	C	2.294900	5.101000	-1.407700
C	-1.754379	-5.224900	-1.424698	C	2.875183	2.259491	-2.323944
С	-0.929596	-3.996231	-1.185500	С	4.274445	2.180344	-2.476105
N	0 121835	-1 015975	-0 934830	C	5 118134	3 034958	-1 781296
IN G	0.424055	4.0433773	0.554050	õ	4 552505	2 007005	0.010000
C	0.880280	-2.819778	-0.742416	C	4.552505	3.98/885	-0.919220
N	-0.129471	-1.976425	-0.861679	Н	7.054077	3.647202	1.484451
C	-1 273636	-2 686737	-1 139069	н	6 562637	5 148895	2 304520
	2.462455	1 01000	1.155005	11	0 1 ( 51 ) 1	E 040C10	1 510045
Н	-3.463455	-4.213882	-0.650009	н	8.103131	5.042618	1.518845
Н	-3.802948	-5.880203	-1.177109	Н	6.667892	6.356735	0.119553
н	-3 577300	-4 523361	-2 362656	Н	7.083176	4.826385	-0.688217
11	1 504600	E 041040	0 641705	 ц	1 204727	6 135303	1 225206
н	-1.504608	-5.941040	-0.641/85	п	4.204/2/	0.433303	1.225290
Н	-1.460861	-5.629395	-2.393402	H	1.886932	5.410828	0.188019
н	0.991959	-4.880920	-0.900772	Н	1.215393	3.256775	-1.357483
 TT	1 026600	2 CE0100	0 507500	п	2 250992	1 567261	-2 000100
п	1.930000	-2.030188	-0.527588		2.230552	1.307201	2.000100
H	-2.220520	-2.163818	-1.273849	Н	4.708572	1.439560	-3.147568
С	-8.052460	4.382248	-3.528625	Н	6.197800	2.958755	-1.910263
C	-6 521073	1 333710	-3 603500	C	5 555984	0 326385	0 453033
C	0.521575	4.555710	5.005500	õ	1.000610	0.320505	0.135055
C	-5.823059	4.171875	-2.267395	C	4.290619	-0.300537	-0.146881
С	-6.052536	5.073380	-1.222290	С	3.006592	0.107788	0.572632
C	-5 352417	4 979019	-0 021545	0	1 923187	-0 238983	0 046005
0	4 414505	2.074700	0.021919	0	2 0 6 2 5 2 0	0.760040	1 641060
C	-4.414505	3.9/4/92	0.146057	0	3.063538	0./62848	1.641068
0	-3.697098	3.899277	1.320236	Fe	0.00000	0.000000	0.00000
C	-4.173615	3.059921	-0.869812	Н	5.467087	1.412537	0.472366
0	4 070000	2 1 6 2 0 6 4	0.000012		6 109920	0 042052	0 162215
C	-4.8/9883	3.162064	-2.0/2113	п	0.400029	0.042055	-0.103313
Н	-8.332718	5.049713	-2.713821	H	5.734055	-0.067032	1.453873
Н	-8,469345	3,391602	-3.347229	Н	4.191452	0.005630	-1.188324
ц.	-0 152027	1 769500	-1 165516	ц	1 362228	-1 386871	-0 093353
п	-0.452527	4.709500	-4.405540		4.302220	1.300071	0.055555
H	-6.214554	3.490433	-4.221985	C	-0.937943	-3.833160	4.962814
Н	-6.149582	5.259766	-4.041687	С	-2.145370	-3.110626	4.324005
н	-6 790100	5 867371	-1 339462	С	-1.782562	-2.016357	3.365875
11	5.7J0100	5.007371	1.555402	NT	2 1 ( 5 2 5 0 2	0 70(741	2 550014
н	-5.544586	5.693359	0.//8946	IN	-2.165359	-0./06/41	3.559814
Н	-3.437759	2.268463	-0.727295	С	-1.746552	0.029160	2.545914
н	-4.697357	2,446533	-2.873900	N	-1.103424	-0.755783	1.700562
C	1 902665	6 127905	2 200122	C	-1 110245	-2 040161	2 100035
C	-T.002002	0.437803	-2.299133	C	-1.110245	-2.040101	2.109055
С	-2.752548	6.057510	-2.162262	Н	-1.338974	-4.645935	5.568359
С	-2.185104	6.337784	-0.772202	Н	-0.357727	-3.160767	5.594711
C	-1 032013	5 409042	-0 /10/92	н	-0 331284	-4 296631	4 184784
0	1.052015	5.405042	0.410452	11	0.551204	2.020601	3.709709
0	0.145584	5.90/181	-0.452957	Н	-2./4/528	-3.829681	3./68509
0	-1.281326	4.199219	-0.086960	Н	-2.753082	-2.656189	5.106522
н	-0.796646	6.169922	-2.979462	Н	-2.685242	-0.350983	4.349213
	1 040167	7 500016	2 400212	 TT	1 0 5 9 9 2 2	1 000020	2 524002
н	-1.84910/	7.508316	-3.499313	п	-1.950052	1.090030	2.524002
Н	-2.012482	5.839645	-4.186096	Н	-0.624146	-2.839157	1.630081
Н	-3.678406	6.625076	-2.255844	0	-0.083800	2.051834	0.995804
ч	-2 97369/	1 991170	-2 21/096	н	-0 430756	2 946930	0 639175
п	-2.973094	4.991470	-2.214090	11	0.430730	2.940950	1 200112
н	-1.814697	7.362045	-0./30209	H	0.824249	2.209076	1.322113
H	-2.968124	6.204269	-0.025818				
C	0.737747	1,609192	-5,904633				
0	0.(10070	1 1 ( 2 2 0 4	E 40C004				
C	-0.648270	1.163284	-5.426224				
С	-0.794357	1.198593	-3.937897				
N	-1.038223	2.364624	-3.241806				
C	-1 010254	2 115463	-1 911656				
C	-1.010254	2.115405	-1.944050				
N	-0.762527	0.828522	-1.774078				
С	-0.627274	0.231598	-3.004074				
н	1 463531	1 100677	-5 269989				
11	1.405551	2.2000//	5.205505				
п	0.85949/	2.08//44	-5.804/03				
Н	0.929184	1.246384	-6.914459				
Н	-1.407913	1.821457	-5.848083				
 ц	-0 000000	0 120604	-5 751000				
п 	-0.033/23	0.139094	- J . / D T 8 U U				
H	-1.212372	3.272964	-3.647690				
Н	-1.178375	2.921997	-1.231003				
н	-0 423111	-0 836945	-3 071793				
	7 100004	4 734055	1 4 6 4 0 4 4				
C	1.120804	4./34955	1.464844				
С	6.549850	5.273636	0.150574				
С	5.099289	4.995850	-0.069000				
C	4 036101	5 615952	0 526505				
C	4.030194 0.056600	J.010902	0.100100				
N	2.856689	5.046280	0.100189				

**Table S18** Cartesian coordinates (Å) for QM/MM geometry-optimized active-site model of Q69E Fe<sup>2+</sup>SOD<sup>HOH</sup> with Glu69 deprotonated and Tyr34 deprotonated (starting coordinates based on PDB file 2BKB).<sup>4</sup>

	Fe <sup>3+</sup> SOD
Bond lengths (Å)	
Fe–O (Sol)	1.92
Fe–O (Asp)	1.90
Fe–N (His26)	2.25
Fe-N (His160)	2.12
Fe–N (His73)	2.11
H–bond distances (Å)	
O(Sol)…N(Gln/Glu)	2.96
O(Sol)…O(Asp)	3.18
O(Tyr)…N(Gln/Glu)	3.34
O(Gln/Glu)····N(Trp)	2.76
Bond angle (deg)	
His–Fe–His	123

**Table S19.** Structural parameters (Å) of the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>SOD derived from PDB file 1ISB.

Table S20. INDO/S-CI c	omputed electronic	excitation	energies (	cm <sup>-1</sup> ) and	zero-field	splitting	parameters	for the
Fe <sup>3+</sup> SOD model derived fr	rom PDB file 1ISB.							

	Fe <sup>3+</sup> SOD
$d \rightarrow d$	5591.7
transitions	5672.4
	9877.8
	10 523.0
	16 849.2
	20 745.5
	21 197.7
	23 554.8
$Asp \rightarrow Fe^{3+}$	27 870 ( $f = 0.0028$ )
CT transitions	28 763 ( $f = 0.015$ )
	29 537 ( $f = 0.040$ )
	29 681 ( $f = 0.011$ )
	$33\ 812\ (f=0.017)$
$D(cm^{-1})$	-0.915
E/D	0.032

**Table S21.** Structural parameters (Å) of QM/MM geometry-optimized active-site models for the oxidized and reduced states of Fe(Mn)SOD derived from PDB file 1MMM.

	Fe <sup>3+</sup> (Mn)SOD	Fe <sup>2+</sup> (Mn)SOD <sup>HOH</sup>	Fe <sup>2+</sup> (Mn)SOD <sup>OH-</sup>
Bond lengths (Å)			
Fe–O (Sol)	1.90	2.23	1.96
Fe–O (Asp)	1.92	1.93	1.99
Fe–N (His26)	2.20	2.12	2.28
Fe-N (His160)	2.14	2.13	2.17
Fe–N (His73)	2.14	2.10	2.19
H–bond distances (Å)			
O(Sol)…N(Gln/Glu)	2.77	2.96	2.66
O(Sol)…O(Asp)	2.83	2.50	3.05
O(Tyr)…N(Gln/Glu)	3.25	3.41	3.15
O(Gln/Glu)····N(Trp)	2.84	2.88	2.86
Bond angles (deg)			
His–Fe–His	131	127	127

	Q69E Fe <sup>3+</sup> SOD <sup>a</sup>	Q69E Fe <sup>3+</sup> SOD <sup>b</sup>
Bond lengths (Å)		
Fe–O (Sol)	1.86	2.13
Fe–O (Asp)	1.91	1.89
Fe–N (His26)	2.29	2.18
Fe-N (His160)	2.18	2.09
Fe–N (His73)	2.12	2.07
H–bond distances (Å)		
O(Sol)…N(Gln/Glu)	3.16	2.60
O(Sol)…O(Asp)	3.45	2.83
O(Tyr)…N(Gln/Glu)	2.48	3.97
O(Gln/Glu)…N(Trp)	2.68	2.64
Bond angles (deg)		
His-Fe-His	122	124

**Table S22.** Structural parameters (Å) of QM/MM geometry-optimized active-site models for the oxidized and reduced states of Q69E FeSOD.

<sup>*a*</sup> In this model the solvent ligand is OH<sup>-</sup> and Glu69 is deprotonated.

<sup>b</sup> In this model the solvent ligand is HOH and Glu69 is deprotonated.

**Table S23.** Structural parameters (Å) derived from the partially QM/MM-optimized models of the Q69E Fe<sup>2+</sup>SOD species based on the PDB files 2BKB.

	Q69E	Q69E	Q69E	Q69E	Q69E
	Fe <sup>2+</sup> SOD <sup>a</sup>	$Fe^{2+}SOD^{b}$	Fe <sup>2+</sup> SOD <sup>c</sup>	$Fe^{2+}SOD^{d}$	Fe <sup>2+</sup> SOD <sup>e</sup>
Bond lengths (Å)					
Fe–O (Sol)	2.27	2.27	2.27	2.28	2.28
Fe–O (Asp)	1.94	1.94	1.94	1.94	1.94
Fe–N (His26)	2.16	2.16	2.16	2.16	2.16
Fe–N (His160)	2.10	2.10	2.10	2.10	2.10
Fe–N (His73)	2.16	2.16	2.16	2.16	2.16
C(Glu)–O(H-bonds W122)	1.26	1.25	1.25	1.25	1.28
C(Glu)–O(H-bonds sol/Y34)	1.32	1.32	1.32	1.32	1.28
H-bond distances (Å)					
O(Sol)…O(Glu)	2.70	2.71	2.69	2.69	2.69
O(Sol)…O(Asp)	3.45	3.44	3.47	3.48	3.46
O(Tyr)···O(Glu)	2.65	2.64	2.64	2.62	2.81
O(Glu)····N(Trp)	2.93	2.93	2.92	2.92	2.90
Bond angles (deg)					
His–Fe–His	128	128	128	128	128

<sup>*a*</sup> Initial protonation state: the solvent ligand and Tyr34 are protonated and Glu69 is deprotonated.

Final protonation state: the solvent ligand and Tyr34 are protonated and Glu69 is deprotonated.

<sup>b</sup> Initial protonation state: the solvent ligand and Glu69 are protonated and Tyr34 is deprotonated.

Final protonation state: the solvent ligand and Tyr34 are protonated and Glu69 is deprotonated.

<sup>c</sup> Initial protonation state: Glu69 and Tyr34 are protonated and the solvent ligand is deprotonated.

Final protonation state: the solvent ligand and Tyr34 are protonated and Glu69 is deprotonated.

<sup>d</sup> Initial protonation state: the solvent ligand, Glu69 and Tyr34 are protonated and a solvent molecule is OH<sup>-</sup>. Final protonation state: the solvent ligand and Tyr34 are protonated and Glu69 is deprotonated and the solvent molecule is HOH.

<sup>e</sup> Initial protonation state: Glu69 and Tyr34 are deprotonated and the solvent molecule is protonated.

Final protonation state: Glu69 and Tyr34 are deprotonated and the solvent molecule is protonated.

	Fe <sup>2+</sup> SOD	$Fe^{2+}(Mn)SOD^{a}$	$Fe^{2+}(Mn)SOD^{b}$	Q69E Fe <sup>2+</sup> SOD
$3d_{yz} \rightarrow 3d_{x^2-y^2}$	814	722	592	729
$3d_{yz} \rightarrow 3d_{xz}$	2535	2506	2322	2638
$3d_{yz} \rightarrow 3d_{xy}$	3050	2874	3069	2984
$3d_{yz} \rightarrow 3d_{z^2}$	9187	8239	8724	7986
_				
$D(cm^{-1})$	-4.630	-5.450	-4.231	-5.217
$E/D (cm^{-1})$	0.098	0.140	0.117	0.145

**Table S24.** INDO/S-CI computed electronic transition energies (cm<sup>-1</sup>) and zero-field splitting parameters for the QM/MM geometry-optimized active-site models of the Fe<sup>2+</sup>-bound SOD species.

<sup>*a*</sup> This model is based upon the PDB file 1VEW. <sup>*b*</sup> This model is based upon the PDB file 1MMM.

**Table S25**. INDO/S-CI computed electronic transition energies (cm<sup>-1</sup>) and zero-field splitting parameters for the <u>QM/MM geometry-optimized active-site model</u> of  $Fe^{3+}(Mn)SOD$  derived from the PDB file 1MMM.

	Fe <sup>3+</sup> (Mn)SOD
$d \rightarrow d$	4942
transitions	5042
	8505
	10 109
	15 944
	21 178
	24 192
$Asp \rightarrow Fe^{3+}$	28 632 ( $f = 0.011$ )
CT transitions	29 383 ( $f = 0.043$ )
	29 610 ( $f = 0.010$ )
	$33\ 569\ (f=0.011)$
	$33\ 637\ (f=0.010)$
$D(cm^{-1})$	-1.214
E/D	0.050

Table S26. TD-DFT and DFT/Slater computed transition energies (cm<sup>-1</sup>) for the QM/MM geometry-optimized active-site model of  $Fe^{2+}(Mn)SOD$  derived from the PDB file 1MMM.

	Fe <sup>2+</sup> (Mn)SOD
TD-DFT <sup>a</sup>	
$1 (3d_{yz} \rightarrow 3d_{x^2-y^2})$	1875
$2 (3d_{yz} \rightarrow 3d_{xz})$	4942
$3 (3d_{yz} \rightarrow 3d_{xy})$	5305
$4 (3d_{yz} \rightarrow 3d_{z^2})$	14 515
Slatar mathe $d^b$	12 022
Stater method	12 032

**Table S27.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>SOD, obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

				Fe		O (Sol)	O/O (Asp)		
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>	_	
194b	-9.0402	1	1.5	1.6	0.0	4.7	0.0	7.0	54.8
195b	-8.7236	1	0.2	0.0	0.1	0.4	4.0	1.6	70.0
196b	-8.5740	1	0.1	0.2	13.7	0.1	0.0	65.1	0.7
199b	-7.8290	1	0.2	1.0	0.0	0.1	0.0	0.5	57.3
200b	-7.7999	1	0.2	0.3	0.0	0.0	0.0	0.6	16.8
208b	-4.1230	0	5.8	38.9	14.9	19.1	5.6	2.9	4.2
209b	-4.0881	0	2.1	14.0	43.7	4.6	16.0	10.9	3.0
210b	-3.8362	0	0.1	1.0	19.3	1.7	57.3	2.6	5.2
211b	-3.7582	0	4.5	24.6	1.6	50.3	1.5	1.8	3.3
212b	-2.6040	0	58.5	9.9	0.0	0.0	0.0	9.7	3.7

**Table S28.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>(Mn)SOD (derived from PDB file 1VEW), obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

				Fe		O (Sol)	O/O (Asp)		
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	dyz	d <sub>x2-y2</sub>	d <sub>xy</sub>	_	
194b	-9.1011	1	1.3	0.7	0.0	2.4	0.0	6.2	30.0
195b	-8.8155	1	0.3	0.0	0.0	0.5	3.6	1.0	69.3
196b	-8.6665	1	0.4	0.9	12.6	0.4	0.0	67.9	1.1
197b	-7.9588	1	0.3	0.7	0.0	0.1	0.0	1.1	41.3
198b	-7.9525	1	0.0	0.8	0.0	0.0	0.0	0.9	36.9
208b	-4.1969	0	0.0	0.1	59.5	0.1	22.0	11.1	2.0
209b	-4.1898	0	5.2	58.1	0.5	21.1	0.0	0.9	5.1
210b	-3.9607	0	0.1	1.3	19.8	4.2	55.0	2.3	4.5
211b	-3.9007	0	1.8	23.6	1.0	50.6	3.6	3.3	4.0
212b	-2.6399	0	62.5	5.7	0.0	0.0	0.0	9.5	4.0

**Table S29.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>(Mn)SOD (derived from PDB file 1MMM), obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

		_		Fe		O (Sol)	O/O (Asp)			
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>	_		
193b	-9.1556	1	2.1	0.9	0.1	2.9	0.0	11.6	39.1	
195b	-8.8079	1	0.3	0.0	0.3	0.7	3.7	3.1	65.7	
196b	-8.5812	1	0.3	0.9	13.2	0.4	0.0	67.8	1.3	
197b	-7.9777	1	0.4	1.6	0.1	0.1	0.1	2.6	76.2	
208b	-4.1501	0	1.3	16.3	44.1	3.1	16.1	10.8	2.7	
209b	-4.1431	0	2.5	50.6	11.9	11.3	10.3	1.6	4.3	
210b	-3.9642	0	0.4	2.7	23.8	1.7	52.2	2.8	4.7	
211b	-3.8167	0	2.0	14.8	0.5	58.7	2.6	2.6	5.0	
212b	-2.6011	0	63.5	4.8	0.0	0.4	0.1	9.6	3.2	

**Table S30.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Q69E Fe<sup>3+</sup>SOD, obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

				Fe		O (Sol)	O/O (Asp)		
MO	E (eV)	Occ	d <sub>z2</sub>	$d_{xz}$	dyz	d <sub>x2-y2</sub>	d <sub>xy</sub>	_	
195b	-9.0792	1	0.9	1.8	0.0	4.5	0.0	4.8	55.0
196b	-8.7679	1	0.0	0.0	0.4	0.2	3.9	2.1	68.0
197b	-8.6779	1	0.3	0.2	12.0	0.2	0.0	66.6	2.4
199b	-7.8421	1	0.4	1.0	0.0	0.0	0.0	0.6	65.7
208b	-4.2650	0	9.0	46.6	6.1	21.3	1.7	0.8	4.7
209b	-4.2512	0	1.4	4.6	56.4	1.4	17.5	12.1	2.2
210b	-3.9214	0	0.3	1.6	16.5	3.1	57.2	1.8	5.8
211b	-3.8887	0	5.0	22.3	2.1	49.8	3.1	1.4	3.3
212b	-2.8603	0	56.4	12.7	0.0	0.0	0.0	9.4	3.7

**Table S31.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>SOD, obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

				Fe		O (Sol)	O/O (Asp)		
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>	_	
111b	-9.690	1	0.0	1.8	0.0	6.1	1.6	3.9	57.9
113b	-9.437	1	0.0	0.0	5.2	0.0	4.9	15.9	50.3
114b	-9.336	1	0.0	0.0	12.2	0.0	0.0	49.2	19.4
119b	-8.241	1	0.0	3.9	0.0	0.0	0.0	0.0	80.6
123b	-6.993	0	9.1	62.2	4.6	4.2	2.9	1.3	6.3
124b	-6.834	0	1.3	6.7	42.4	0.0	25.3	14.2	2.5
125b	-6.539	0	0.0	4.6	5.3	60.0	5.8	0.0	5.4
126b	-6.533	0	0.0	0.0	22.4	9.4	43.2	3.8	4.0
127b	-5.223	0	57.6	9.0	0.0	0.0	0.0	3.0	11.4

**Table S32.** Energies, occupations, and composition (%) of the  $Fe^{3+}$  3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of  $Fe^{3+}(Mn)SOD$  (derived from PDB file 1VEW), obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

			O (Sol)	O/O (Asp)					
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>vz</sub>	$d_{x2-y2}$	$d_{xy}$		
109b	-9.685	1	2.4	1.6	0.0	5.3	0.0	7.9	51.9
111b	-9.437	1	0.0	0.0	2.7	0.0	4.5	7.8	61.1
112b	-9.318	1	0.0	1.2	13.0	0.0	0.0	56.3	7.4
118b	-8.323	1	0.0	3.5	0.0	0.0	0.0	1.3	71.8
123b	-6.966	0	4.2	58.5	14.3	1.9	3.2	2.8	6.4
124b	-6.829	0	1.8	14.4	34.7	0.0	25.1	12.8	2.4
125b	-6.582	0	0.0	0.0	11.7	41.8	22.9	1.5	4.9
126b	-6.490	0	0.0	3.9	14.5	29.7	26.8	3.7	5.8
127b	-5.128	0	61.1	5.2	0.0	0.0	0.0	10.0	3.2

**Table S33.** Energies, occupations, and composition (%) of the Fe<sup>3+</sup> 3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>(Mn)SOD (derived from PDB file 1MMM), obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

				Fe	O (Sol)	O/O (Asp)			
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>	_	
108b	-9.738	1	2.9	1.3	0.0	4.7	0.0	9.2	55.0
111b	-9.433	1	0.0	0.0	2.7	0.0	4.6	8.4	56.3
113b	-9.257	1	0.0	1.0	13.2	0.0	0.0	51.6	5.9
118b	-8.348	1	0.0	2.5	0.0	0.0	0.0	2.1	53.0
123b	-6.953	0	3.5	65.0	9.4	1.4	4.2	1.6	4.8
124b	-6.815	0	1.4	11.9	34.4	0.0	28.9	12.8	2.8
125b	-6.601	0	0.0	0.0	26.7	13.5	36.7	4.6	3.9
126b	-6.423	0	0.0	2.2	4.4	58.3	8.5	2.7	7.0
127b	-5.125	0	62.2	4.3	0.0	0.0	0.0	10.3	2.7

**Table S34.** Energies, occupations, and composition (%) of the  $Fe^{3+}$  3d-, Asp-, and Sol-based spin-down MOs for the QM/MM geometry-optimized active-site model of Q69E  $Fe^{3+}$ SOD, obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

				Fe		O (Sol)	O/O (Asp)		
MO	E (eV)	Occ	d <sub>z2</sub>	$d_{xz}$	$d_{yz}$	$d_{x2-y2}$	d <sub>xy</sub>		
110b	-9.786	1	0.0	1.9	0.0	5.3	0.0	1.3	51.2
112b	-9.563	1	0.0	0.0	8.5	0.0	4.4	29.4	35.6
113b	-9.466	1	0.0	0.0	7.3	0.0	1.1	35.6	34.5
119b	-8.304	1	1.1	3.7	0.0	0.0	0.0	0.0	80.7
123b	-7.190	0	11.6	61.3	6.3	3.7	2.1	0.0	5.8
124b	-7.065	0	1.8	5.7	49.3	0.0	19.4	15.0	2.1
125b	-6.732	0	0.0	5.0	0.0	68.3	0.0	0.0	5.0
126b	-6.677	0	0.0	0.0	20.5	0.0	54.1	2.5	6.2
127b	-5.552	0	55.5	11.3	0.0	0.0	0.0	11.1	2.9

**Table S35.** Energies, occupations, and composition (%) of the Fe<sup>2+</sup> 3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>2+</sup>SOD, obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

			Fe <sup>2+</sup> 3d-based MOs								
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>				
208b	-5.7668	1	0.1	0.1	91.4	0.0	0.1				
209b	-1.8690	0	0.3	6.4	0.0	48.9	1.2				
210b	-1.6164	0	0.7	83.7	0.0	7.9	0.0				
211b	-1.3669	0	0.8	0.2	0.0	0.0	59.8				
222b	-0.0070	0	15.6	0.2	0.7	0.2	1.1				
225b	0.4528	0	12.9	0.2	0.1	8.4	1.5				
227b	0.5397	0	13.4	0.1	0.1	1.2	0.0				

**Table S36.** Energies, occupations, and composition (%) of the Fe<sup>2+</sup> 3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>(Mn)SOD (derived from PDB file 1VEW), obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

		_		Fe	e <sup>2+</sup> 3d-based M	Os	
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
208b	-5.8181	1	0.8	0.1	90.4	0.3	0.0
209b	-1.8834	0	0.8	10.5	0.0	47.7	1.7
210b	-1.7090	0	1.1	79.4	0.1	11.3	0.8
211b	-1.4765	0	0.4	0.2	0.0	0.9	62.4
219b	-0.0872	0	21.5	0.0	0.6	0.5	2.7
224b	0.3043	0	11.5	0.4	0.3	5.5	0.4

**Table S37.** Energies, occupations, and composition (%) of the Fe<sup>2+</sup> 3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of Fe<sup>3+</sup>(Mn)SOD (derived from PDB file 1MMM), obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

			1	Fe	e <sup>2+</sup> 3d-based M	Os	,
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
207b	-5.7873	1	0.1	1.0	88.4	0.4	0.0
209b	-1.8355	0	1.8	8.8	0.0	50.5	0.4
210b	-1.7191	0	1.0	78.1	1.2	8.1	2.8
211b	-1.5955	0	0.5	3.1	0.1	1.7	62.6
219b	-0.1130	0	11.7	0.2	0.2	0.2	2.9
222b	0.1545	0	17.5	0.1	0.2	0.7	4.0

**Table S38.** Energies, occupations, and composition (%) of the Fe<sup>2+</sup> 3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of Q69E Fe<sup>2+</sup>SOD, obtained from a spin-unrestricted DFT/COSMO computation using ORCA 2.4 (B3LYP functional) and  $\varepsilon = 4.0$ .

			Fe <sup>2+</sup> 3d-based MOs				
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
208b	-4.6907	1	0.6	0.1	90.8	0.3	1.1
209b	-0.8047	0	0.5	13.0	0.6	43.2	3.2
210b	-0.5445	0	3.7	74.6	0.0	11.4	0.1
211b	-0.3208	0	0.4	0.0	0.8	1.8	62.2
220b	0.9027	0	12.5	0.8	0.3	1.4	0.9
227b	1.5336	0	13.5	0.0	0.3	6.1	0.2
228b	1.6094	0	10.3	0.0	0.1	0.4	0.2

**Table S39.** Energies, occupations, and composition (%) of the  $Fe^{2+}$  3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of  $Fe^{2+}$ SOD, obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

				Fe	e <sup>2+</sup> 3d-based M	Os	
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
151b	-5.862	1	0.0	0.0	91.9	0.0	0.0
152b	-5.232	0	0.0	91.6	0.0	0.0	0.0
153b	-5.088	0	0.0	0.0	0.0	69.8	0.0
154b	-4.726	0	0.0	0.0	0.0	3.3	76.8
155b	-3.711	0	36.0	0.0	0.0	0.0	0.0
156b	-3.588	0	15.6	0.0	0.0	0.0	0.0

**Table S40.** Energies, occupations, and composition (%) of the  $Fe^{2+}$  3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of  $Fe^{3+}(Mn)SOD$  (derived from PDB file 1VEW), obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

			Fe <sup>2+</sup> 3d-based MOs				
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
151b	-6.007	1	0.0	0.0	90.7	0.0	0.0
152b	-5.169	0	5.0	87.2	0.0	0.0	0.0
153b	-5.169	0	8.9	2.8	0.0	55.8	7.4
154b	-4.875	0	1.6	0.0	0.0	5.4	71.9
155b	-3.657	0	44.8	1.6	0.0	13.0	0.0
159b	-3.159	0	17.2	0.0	0.0	0.0	0.0

**Table S41.** Energies, occupations, and composition (%) of the  $Fe^{2+}$  3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of  $Fe^{3+}(Mn)SOD$  (derived from PDB file 1MMM), obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

		4	Fe <sup>2+</sup> 3d-based MOs				
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
151b	-6.074	1	0.0	0.0	89.7	0.0	0.0
152b	-5.495	0	0.0	89.4	1.1	2.1	0.0
153b	-5.224	0	3.0	1.7	0.0	68.4	0.0
154b	-5.110	0	0.0	0.0	0.0	0.0	79.9
155b	-3.753	0	53.2	0.0	0.0	0.0	0.0
156b	-3.547	0	11.4	0.0	1.2	1.8	0.0

**Table S42.** Energies, occupations, and composition (%) of the  $Fe^{2+}$  3d-based spin-down MOs for the QM/MM geometry-optimized active-site model of Q69E  $Fe^{2+}$ SOD, obtained from a spin-unrestricted DFT computation using ADF 2006 (BP functional).

		_		Fe	e <sup>2+</sup> 3d-based M	Os	
MO	E (eV)	Occ	d <sub>z2</sub>	d <sub>xz</sub>	d <sub>yz</sub>	d <sub>x2-y2</sub>	d <sub>xy</sub>
151b	-3.481	1	0.0	0.0	90.4	0.0	1.4
152b	-2.923	0	0.0	85.3	0.0	1.1	1.0
153b	-2.701	0	7.7	2.4	0.0	60.7	8.8
154b	-2.467	0	0.0	0.0	1.0	9.6	70.3
155b	-1.455	0	28.1	2.2	0.0	1.1	0.0
156b	-1.152	0	34.6	0.0	0.0	1.4	0.0

**Table S43.** DFT/COSMO ( $\varepsilon = 4.0$ ) computed total energies (kcal/mol),  $\varepsilon_{PT}$ ,  $\varepsilon_{ET}$ , p*K*, and  $E^{\circ}$  values for Fe(Mn)SOD obtained with the QM/MM geometry-optimized active-site models derived from the PDB file 1MMM.

	Fe(Mn)SOD
Fe <sup>3+</sup> /OH <sup>-</sup>	-2281808
Fe <sup>2+</sup> /HOH	-2282198
Fe <sup>2+</sup> /OH <sup>-</sup>	-2281900
$IP \\ \epsilon_{ET}(eV)$	92.0 -0.44
ε <sub>deprot</sub>	298
$pK[Fe^{2+}SOD^{HOH}]$	18.3
$\epsilon_{\rm PT} (eV)$	0.67
$E^{\circ}\left(\mathrm{V} ight)$	0.23

	FeSOD	$Fe(Mn)SOD^{a}$	$Fe(Mn)SOD^{b}$	Q69E FeSOD
Fe <sup>3+</sup> /OH <sup>-</sup>	-2281813	-2281820	-2281819	-2294266
Fe <sup>2+</sup> /HOH	-2282207	-2282204	-2282209	-2294634
Fe <sup>2+</sup> /OH <sup>-</sup>	-2281898	-2281907	-2281907	-2294363
IP	85.1	86.8	87.6	96.8
$\epsilon_{ET}\left(eV\right)$	-0.74	-0.66	-0.63	-0.23
Edeprot	309	298	302	271
$pK[Fe^{2+}SOD^{HOH}]$	25.9	17.9	21.2	-1.96
$\varepsilon_{\rm PT}  (eV)$	1.12	0.65	0.85	-0.53
$E^{\circ}(\mathbf{V})$	0.38	-0.02	0.22	-0.77

**Table S44.** DFT/COSMO ( $\varepsilon = 10.0$ ) computed total energies (kcal/mol),  $\varepsilon_{PT}$ ,  $\varepsilon_{ET}$ , pK, and  $E^{\circ}$  values for the QM/MM geometry-optimized FeSOD, Fe(Mn)SOD, and Q69E FeSOD active-site models.

<sup>*a*</sup> This model is derived from the PDB file 1VEW. <sup>*b*</sup> This model is derived from the PDB file 1MMM.

Table S45. DFT/COSMO computed solvation energies (kcal/mol) for the QM/MM geometry-optimized FeSOD, Fe(Mn)SOD, and Q69E FeSOD active-site models.

	$\varepsilon = 4.0$	$\varepsilon = 10.0$	1 <sup>st</sup> sphere model
WT FeSOD			
Fe <sup>3+</sup> /OH <sup>-</sup>	-38.429	-39.361	-34.234
Fe <sup>2+</sup> /HOH	-35.446	-36.546	-34.317
Fe <sup>2+</sup> /OH <sup>-</sup>	-23.352	-24.420	-21.190
Fe(Mn)SOD <sup>a</sup>			
Fe <sup>3+</sup> /OH <sup>-</sup>	-39.361	-52.6909	-34.593
Fe <sup>2+</sup> /HOH	-36.546	-48.7216	-33.556
Fe <sup>2+</sup> /OH <sup>-</sup>	-24.420	-33.7103	-21.819
$Fe(Mn)SOD^b$			
Fe <sup>3+</sup> /OH <sup>-</sup>	-39.894	-53.510	-34.912
Fe <sup>2+</sup> /HOH	-38.743	-51.882	-33.211
Fe <sup>2+</sup> /OH <sup>-</sup>	-24.739	-34.204	-22.832
Q69E FeSOD			
Fe <sup>3+</sup> /OH <sup>-</sup>	-36.668	-48.843	-34.392
Fe <sup>2+</sup> /HOH	-38.472	-51.319	-36.265
Fe <sup>2+</sup> /OH <sup>-</sup>	-25.419	-35.011	-39.321

<sup>*a*</sup> This model is derived from the PDB file 1VEW. <sup>*b*</sup> This model is derived from the PDB file 1MMM.



Wavenumbers (cm<sup>-1</sup>) **Figure S1.** Absorption (top), CD (middle), and MCD (bottom) spectra at 4.5 K (solid lines) of Fe<sup>3+</sup>(Mn)SOD. Individual Gaussian bands (…) and their sums (---) obtained from an iterative fit are shown for each spectrum. Sample conditions: [Fe<sup>3+</sup>(Mn)SOD] = 1.1 mM in 55% (v/v) glycerol and 50 mM MES buffer (pH 7.0).



Wavenumbers (cm<sup>-1</sup>) **Figure S2.** Absorption (top), CD (middle), and MCD (bottom) spectra at 4.5 K (solid lines) of Q69E Fe<sup>3+</sup>SOD. Individual Gaussian bands (...) and their sums (---) obtained from an iterative fit are shown for each spectrum. Sample conditions:  $[Q69E Fe^{3+}SOD] = 0.85 \text{ mM} \text{ in } 55\%$  (v/v) glycerol and 50 mM phosphate buffer (pH 7.0).

**Supplementary Calculations.** Effect of  $OH^-$  binding to  $Fe^{3+}(Mn)SOD$  and Q69E  $Fe^{3+}SOD$  on experimental  $E^{\circ}$  values.

The following scheme was used to estimate how coordination of an exogenous OH<sup>-</sup> ion to the putative substrate-binding site of  $\text{Fe}^{3+}(\text{Mn})\text{SOD}$  and Q69E  $\text{Fe}^{3+}\text{SOD}$  under physiological conditions (i.e., at pH 7.0) affects the measured reduction potential  $E_m$ . In this scheme,  $E^{\circ}$  corresponds to the proton-coupled metal ion reduction potential of the wild type-like 5-coordinate state; this is the quantity of interest that we computed using the DFT/COSMO methodology as outlined in the manuscript.



$$Ox, Tot + e^{-} \xleftarrow{E_{m}} Red, Tot$$

$$[OxOH] = [Ox]I0^{pH-pK_{ox}} \qquad [RedOH] = [Red]I0^{pH-pK_{red}}$$

$$-nFE_{m} = \Delta G = -RT \ln K = -RT \ln \left(\frac{[Red] + [RedOH]}{[Ox] + [OxOH]}\right)$$

$$E_{m} = \frac{RT}{F} \ln \left(\frac{[Red](1+10^{pH-pK_{red}})}{[Ox](1+10^{pH-pK_{red}})}\right)$$

$$E_{m} = \frac{RT}{F} \left[ \ln \left(\frac{[Red]}{[Ox]}\right) + \ln \left(\frac{1+10^{pH} \times 10^{-pK_{red}}}{1+10^{pH} \times 10^{-pK_{ox}}}\right) \right]$$

$$E_{m} = E^{\circ} + \frac{RT}{F} \ln \left(\frac{10^{-pH} + 10^{-pK_{red}}}{10^{-pH} + 10^{-pK_{red}}}\right)$$

## Fe(Mn)SOD

$$E_{m} = E^{\circ} + \frac{RT}{F} \ln\left(\frac{\left[H^{+}\right] + \left[H^{+}\right]_{\text{at 50\% OH free Red}}}{\left[H^{+}\right] + \left[H^{+}\right]_{\text{at 50\% OH free Ox}}}\right)$$
$$E_{m} = E^{\circ} + \frac{RT}{F} \ln\left(\frac{10^{-7} + (<10^{-12})}{10^{-7} + 10^{-6.5}}\right) \text{ where the pK of OH}^{-1} \text{ binding to Ox is 6.5}^{5}$$
$$E_{m} = E^{\circ} + \frac{RT}{F} \ln\left(\frac{10^{-7}}{4.2 \times 10^{-7}}\right) = E^{\circ} - \frac{RT}{F} \times 1.4 = E^{\circ} - 38 \text{ mV}$$

<u>Q69E FeSOD</u>

$$E_m = E^\circ + \frac{RT}{F} \ln \left( \frac{\left[H^+\right] + \left[H^+\right]_{\text{at 50\% OH free Red}}}{\left[H^+\right] + \left[H^+\right]_{\text{at 50\% OH free Ox}}} \right)$$

 $E_{m} = E^{\circ} + \frac{RT}{F} \ln\left(\frac{10^{-7} + (<10^{-12})}{10^{-7} + 10^{-5}}\right) \text{ where the pK of OH}^{-1} \text{ binding to Ox is estimated to be 5}$ 

$$E_m = E^\circ + \frac{RT}{F} \ln\left(\frac{10^{-7}}{10^{-5}}\right) = E^\circ - \frac{2.3RT}{F} \log 10^2 = E^\circ - 120 \text{ mV}$$

- (1) Lah, M. S.; Dixon, M. M.; Pattridge, K. A.; Stallings, W. C.; Fee, J. A.; Ludwig, M. L. *Biochemistry* **1995**, *34*, 1646-1660.
- (2) Edwards, R. A.; Baker, H. M.; Whittaker, M. M.; Whittaker, J. W.; Jameson, G. B.; Baker, E. N. J. Biol. Inorg. Chem. 1998, 3, 161-171.
- (3) Edwards, R. A.; Whittaker, M. M.; Whittaker, J. W.; Jameson, G. B.; Baker, E. N. J. Am. Chem. Soc. 1998, 120, 9684-9685.
- (4) Yikilmaz, E.; Porta, J.; Grove, L. E.; Vahedi-Faridi, A.; Bronshteyn, Y.; Brunold, T. C.; Borgstahl, G. E. O.; Miller, A.-F. J. Am. Chem. Soc.. 2007, 129, 9927-9940.
- (5) Vance, C. K.; Miller, A.-F. Biochemistry 1998, 37, 5518-5527.