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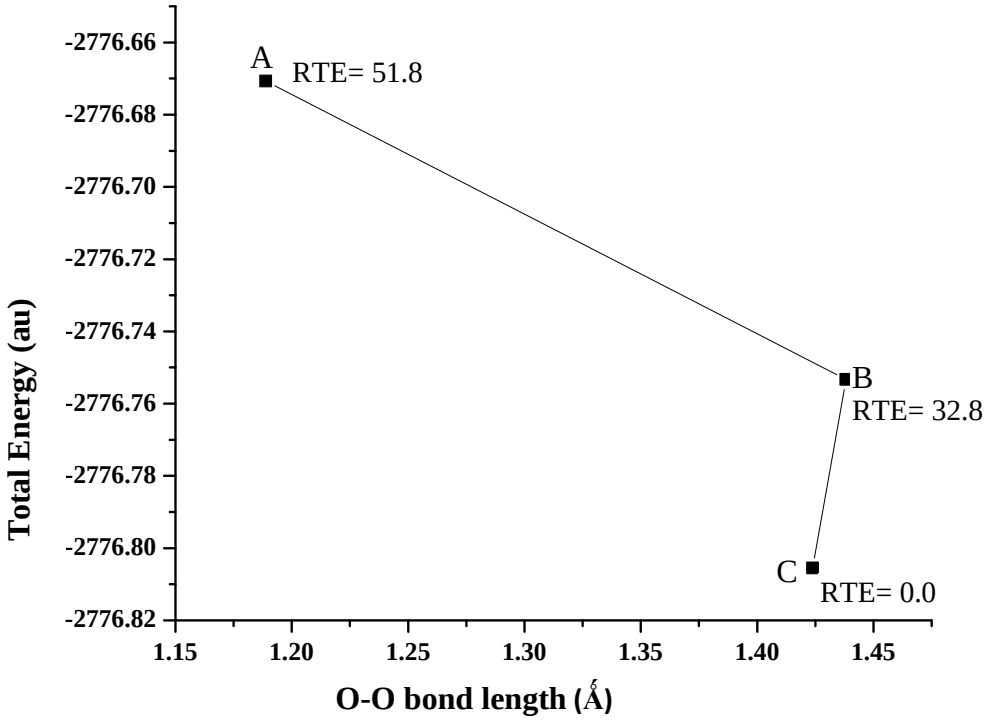

Fig. S1. Variation of total energy (a.u.) as a function of OO bond distance of superoxide radical anion moiety during the process of hydrogen abstraction from the (O3O4) sites of ascorbic acid. Relative total energies (RTE) are in kcal/mol. The point A corresponds to total energy of free reactants while the point C corresponds to the final product complex. The point B was obtained during search for transition state which was found not to exist. Thus the point B does not represent the optimized TS and its location does not follow any physical criterion e.g. that of minimum energy or one based on interatomic distances. All calculations were performed at the M06-2X/6-311+G(d) level of theory in gas phase.

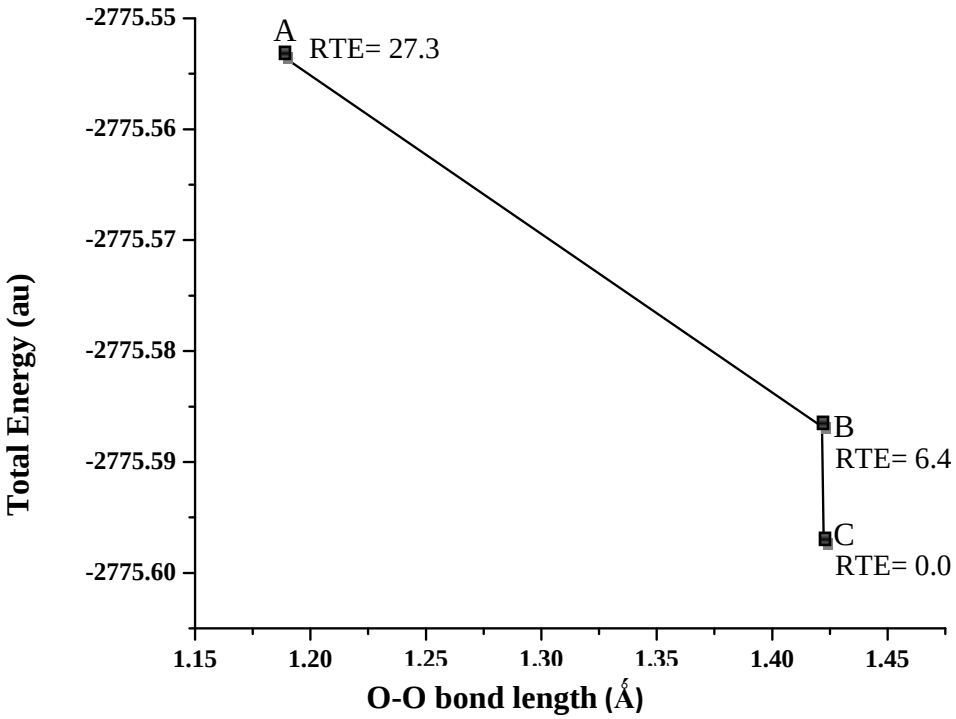

Fig. S2. Variation of total energy (a.u.) as a function of OO bond distance of superoxide radical anion moiety during the process of hydrogen abstraction from the (O6O7) site of ascorbic acid. Relative total energies (RTE) are in kcal/mol. The point A corresponds to total energy of free reactants while the point C corresponds to the final product complex. The point B was obtained during search for transition state which was found not to exist. Thus the point B does not represent the optimized TS and its location does not follow any physical criterion e.g. that of minimum energy or one based on interatomic distances. All calculations were performed at the M06-2X/6-311+G(d) level of theory in gas phase.

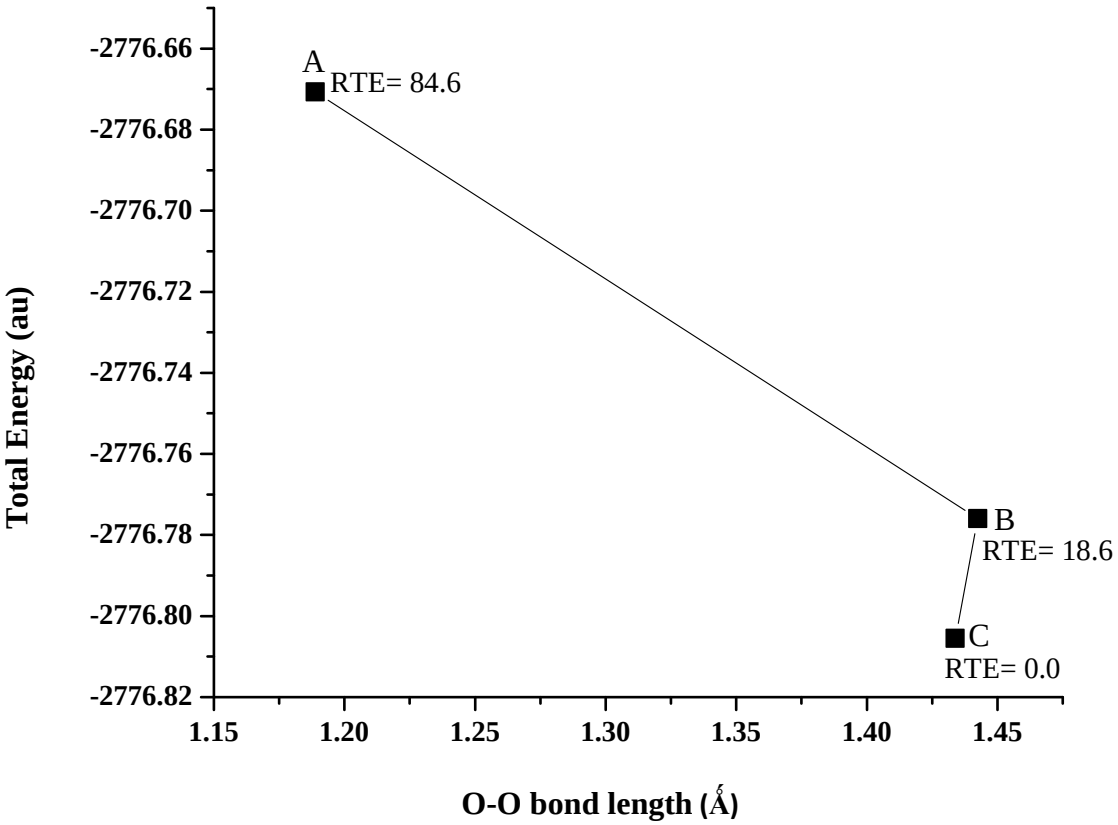

Fig. S3. Variation of total energy (a.u.) as a function of OO bond distance of superoxide radical anion moiety during the process of hydrogen abstraction from the (C6C7) site of ascorbic acid. Relative total energies (RTE) are in kcal/mol. The point A corresponds to total energy of free reactants while the point C corresponds to the final product complex. The point B was obtained during search for transition state which was found to exist with a negative barrier energy. All calculations were performed at the M06-2X/6-311+G(d) level of theory in gas phase.

Table S4. NBO charge distribution in ascorbic acid obtained at M06-2X/6-311+G(d) level of theory in aqueous media.[a]

Sl. No.	Atoms	NBO Charge	Total
1	O1	-0.568	Total positive NBO charge= 4.151
2	C2	0.784	
3	O2	-0.644	
4	C3	0.104	
5	O3	-0.693	Total negative NBO charge= -4.150
6	H3	0.504	
7	C4	0.312	
8	O4	-0.673	
9	H4	0.510	
10	C5	0.075	
11	H5′	0.236	
12	C6	0.078	Net charge=0.001
13	H6′	0.205	
14	O6	-0.773	
15	H6	0.489	
16	C7	-0.043	
17	H7′	0.195	
18	H7″	0.179	
19	O7	-0.756	
20	H7	0.478	

[a]The optimized structure of ascorbic acid is shown in Fig. 1.

Table S5. NBO charge distribution in Fe-SOD model complexed with super oxide anion obtained at M06-2X/6-11+G(d) level of theory in aqueous media.

Sl. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	Fe10	1.156	1.156	19	H19	0.247	
2	O8	0.023	$O_2^{\cdot -}$:0.115	20	C20	-0.064	
3	O9	0.092		21	H20	0.235	
4	N11	-0.586	Ring 1: Charge= (-1.19)+ (1.439)= 0.249	22	N21	-0.589	Ring 3: Charge= (-1.200)+ (1.445)= 0.245
5	C12	0.262		23	C22	0.263	
6	H12	0.235		24	H22	0.240	
7	N13	-0.508		25	N23	-0.509	
8	H13	0.457		26	H23	0.456	
9	C14	-0.040		27	C24	-0.039	
10	H14	0.249		28	H24	0.248	
11	C15	-0.056		29	C25	-0.063	
12	H15	0.236		30	H25	0.238	
13	N16	-0.596	Ring 2: Charge= (-1.213)+ (1.446)= 0.233				
14	C17	0.272		Total	Negative	-3.603	
15	H17	0.237			Positive	5.601	
16	N18	-0.510			Net	1.998	
17	H18	0.455					
18	C19	-0.043					

Table S6. NBO charge distribution on different atoms of TS2 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the O6 and C6 sites to form product complex PC2 in aqueous media at M06-2X/6-311+G(d) level.[a]

Sl. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.561	Ascorbic acid Charge= (-3.925)+ (4.085) =0.150	27	N13	-0.515	Ring1 Charge= (-1.243)+ (1.430)=0.187
2	C2	0.793		28	H13	0.455	
3	O2	-0.590		29	C14	-0.051	
4	C3	0.129		30	H14	0.246	
5	O3	-0.683		31	C15	-0.060	
6	H3	0.511		32	H15	0.235	
7	C4	0.304		33	N16	-0.602	Ring2 Charge= (-1.228)+ (1.436)=0.208
8	O4	-0.662		34	C17	0.261	
9	H4	0.510		35	H17	0.239	
10	C5	-0.003		36	N18	-0.515	
11	H5′	0.266		37	H18	0.454	
12	C6	0.628		38	C19	-0.050	
13	O6	-0.598		39	H19	0.246	
14	C7	-0.115		40	C20	-0.061	
15	O7	-0.723		41	H20	0.236	
16	H7	0.494		42	N21	-0.624	Ring3 Charge= (-1.264)+ (1.448)=0.184
17	H7′	0.228		43	C22	0.281	
18	H7″	0.222		44	H22	0.238	
19	O8	-0.526	Charge= (-0.974)+ (0.946)= -0.028	45	N23	-0.520	
20	H6	0.504		46	H23	0.452	
21	O9	-0.448		47	C24	-0.055	
22	H6′	0.442		48	H24	0.244	
23	Fe10	1.301	1.301	49	C25	-0.065	
24	N11	-0.617		50	H25	0.233	
25	C12	0.265		Net Charge=2.002			
26	H12	0.229					

[a]The optimized structure of TS2 is shown in Fig. 4.

Table S7. NBO charge distribution on different atoms of TS3 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C5 and C6 sites to form product complex PC3 in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.521	Ascorbic acid Charge: (-3.782)+ (4.395)= 0.613	27	N13	-0.522	Ring1 Charge= (-1.208)+ (1.427)=0.219
2	C2	0.797		28	H13	0.450	
3	O2	-0.465		29	C14	-0.052	
4	C3	0.267		30	H14	0.242	
5	O3	-0.622		31	C15	-0.071	
6	H3	0.523		32	H15	0.229	
7	C4	0.200		33	N16	-0.549	Ring2 Charge= (-1.195)+ (1.414)=0.219
8	O4	-0.666		34	C17	0.255	
9	H4	0.526		35	H17	0.230	
10	C5	0.619		36	N18	-0.519	
11	C6	-0.051		37	H18	0.451	
12	O6	-0.726		38	C19	-0.048	
13	H6	0.499		39	H19	0.243	
14	C7	-0.024		40	C20	-0.079	
15	O7	-0.707		41	H20	0.235	
16	H7	0.517		42	N21	-0.563	Ring3 Charge= (-1.204)+ (1.426)=0.222
17	H7′	0.226		43	C22	0.263	
18	H7″	0.221		44	H22	0.241	
19	O8	-0.480	Charge= (-1.028)+ (0.825)= -0.203	45	N23	-0.519	
20	H5′	0.492		46	H23	0.450	
21	O9	-0.548		47	C24	-0.052	
22	H6′	0.333		48	H24	0.242	
23	Fe10	0.921	0.921	49	C25	-0.070	
24	N11	-0.563		50	H25	0.230	
25	C12	0.267		Net charge=1.991			
26	H12	0.239					

[a]The optimized structure of TS3 is shown in Fig. 4.

Table S8. NBO charge distribution on different atoms of TS5 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C6 and C7 sites to form product complex PC5 in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.559	Ascorbic acid Charge= (-4.085) +(4.476) =0.391	27	N13	-0.522	Ring1 Charge= (-1.208)+ (1.427)= 0.219
2	C2	0.789		28	H13	0.450	
3	O2	-0.628		29	C14	-0.052	
4	C3	0.113		30	H14	0.242	
5	O3	-0.684		31	C15	-0.071	
6	H3	0.510		32	H15	0.229	
7	C4	0.341		33	N16	-0.549	Ring2 Charge= (-1.195)+ (1.414)= 0.219
8	O4	-0.657		34	C17	0.255	
9	H4	0.517		35	H17	0.230	
10	C5	0.027		36	N18	-0.519	
11	H5′	0.279		37	H18	0.451	
12	C6	0.581		38	C19	-0.048	
13	O6	-0.598		39	H19	0.243	
14	H6	0.538		40	C20	-0.079	
15	C7	-0.209		41	H20	0.235	
16	O7	-0.750		42	N21	-0.563	Ring3 Charge= (-1.204)+ (1.426) =0.222
17	H7	0.512		43	C22	0.263	
18	H7″	0.269		44	H22	0.241	
19	O8	-0.462	Charge= (-0.962)+ (0.909)= -0.052	45	N23	-0.519	
20	H6′	0.504		46	H23	0.450	
21	O9	-0.500		47	C24	-0.052	
22	H7′	0.405		48	H24	0.242	
23	Fe10	1.006	1.006	49	C25	-0.070	
24	N11	-0.563		50	H25	0.230	
25	C12	0.267		Net Charge=2.005			
26	H12	0.239					

[a]The optimized structure of TS5 is shown in Fig. 5.

Table S9. NBO charge distribution on different atoms of TS6 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C7 and O7 sites to form product complex PC6 in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.561	Ascorbic acid Charge=(-3.830)+(4.028)=0.198	27	N13	-0.519	Ring 1 Charge=(-0.208)+(1.420)=0.212
2	C2	0.789		28	H13	0.451	
3	O2	-0.616		29	C14	-0.053	
4	C3	0.114		30	H14	0.243	
5	O3	-0.686		31	C15	-0.061	
6	H3	0.508		32	H15	0.231	
7	C4	0.306		33	N16	-0.567	Ring 2 Charge=(-1.187)+(1.427)=0.240
8	O4	-0.674		34	C17	0.261	
9	H4	0.515		35	H17	0.236	
10	C5	0.083		36	N18	-0.516	
11	H5′	0.241		37	H18	0.453	
12	C6	-0.000		38	C19	-0.051	
13	O6	-0.737		39	H19	0.245	
14	H6	0.509		40	C20	-0.053	
15	H6′	0.243		41	H20	0.232	
16	C7	0.518		42	N21	-0.580	Ring 3 Charge=(-1.216)+(1.425)=0.209
17	O7	-0.556		43	C22	0.261	
18	H7″	0.202		44	H22	0.233	
19	O8	-0.444	Charge=(-0.930)+(1.020)=0.090	45	N23	-0.518	
20	H7′	0.498		46	H23	0.453	
21	O9	-0.486		47	C24	-0.050	
22	H7	0.522		48	H24	0.245	
23	Fe10	1.054	1.054	49	C25	-0.068	
24	N11	-0.575		50	H25	0.233	
25	C12	0.259		Net charge=2.003			
26	H12	0.236					

[a]The optimized structure of TS6 is shown in Fig. 5.

Table S10. NBO charge distribution on different atoms of product complex PC1 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the O3 and O4 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.542	Ascorbic acid Charge= (-3.655)+ (3.707)= 0.052	27	N13	-0.503	Charge= (-1.180)+ (1.414) =0.234
2	C2	0.732		28	H13	0.448	
3	O2	-0.460		29	C14	-0.025	
4	C3	0.470		30	H14	0.253	
5	O3	-0.526		31	C15	-0.061	
6	C4	0.535		32	H15	0.233	
7	O4	-0.534		33	N16	-0.578	Ring 3: Charge= (-1.166)+ (1.424-1.192)= 0.232
8	C5	0.020		34	C17	0.265	
9	H5′	0.258		35	H17	0.229	
10	C6	0.095		36	N18	-0.503	
11	H6′	0.206		37	H18	0.447	
12	O6	-0.781		38	C19	-0.029	
13	H6	0.516		39	H19	0.254	
14	C7	-0.054		40	C20	-0.056	
15	O7	-0.758		41	H20	0.236	
16	H7	0.491		42	N21	-0.594	Ring 3 Charge= (-1.192)+ (1.424-1.192)= 0.232
17	H7′	0.190		43	C22	0.263	
18	H7″	0.194		44	H22	0.227	
19	O8	-0.418	H_2O_2 Charge= (-0.839) +(1.078) =0.239	45	N23	-0.510	
20	H3	0.533		46	H23	0.447	
21	O9	-0.421		47	C24	-0.028	
22	H4	0.545		48	H24	0.252	
23	Fe10	0.991	0.991	49	C25	-0.060	
24	N11	-0.591	Ring 1	50	H25	0.235	
25	C12	0.249		Net Charge=1.980			
26	H12	0.231					

[a]The optimized structure of PC1 is shown in Fig. 6.

Table S11. NBO charge distribution on different atoms of PC2 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C6 and O6 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.571	Ascorbic acid Charge= (-4.026)+ (4.073)= 0.047	27	N13	-0.515	Ring1 Charge= (-1.204)+ (1.418) =0.214
2	C2	0.793		28	H13	0.452	
3	O2	-0.598		29	C14	-0.047	
4	C3	0.127		30	H14	0.245	
5	O3	-0.685		31	C15	-0.062	
6	H3	0.510		32	H15	0.233	
7	C4	0.304		33	N16	-0.570	Ring2 Charge= (-1.193)+ (1.435)= 0.242
8	O4	-0.699		34	C17	0.269	
9	H4	0.519		35	H17	0.233	
10	C5	0.007		36	N18	-0.513	
11	H5′	0.261		37	H18	0.452	
12	C6	0.626		38	C19	-0.051	
13	O6	-0.603		39	H19	0.245	
14	C7	-0.127		40	C20	-0.059	
15	O7	-0.743		41	H20	0.236	
16	H7	0.491		42	N21	-0.591	Ring3 Chrage= (-1.205)+ (1.419)= 0.214
17	H7′	0.227		43	C22	0.261	
18	H7″	0.211		44	H22	0.232	
19	O8	-0.424	Charge= (-0.851)+ (1.079) =0.228	45	N23	-0.511	
20	H6′	0.534		46	H23	0.452	
21	O9	-0.427		47	C24	-0.028	
22	H6	0.545		48	H24	0.242	
23	Fe10	1.051	1.051	49	C25	-0.075	
24	N11	-0.580		50	H25	0.232	
25	C12	0.253		Net Charge=1.996			
26	H12	0.235					

[a]The optimized structure of PC2 is shown in Fig. 6.

Table S12. NBO charge distribution on different atoms of PC3 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C5 and C6 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.539	Ascorbic acid Charge= (-3.972)+ (4.184)=0.212	27	N13	-0.512	Ring1 Charge= (-1.181)+ (1.424)= 0.243
2	C2	0.770		28	H13	0.453	
3	O2	-0.612		29	C14	-0.044	
4	C3	0.144		30	H14	0.246	
5	O3	-0.675		31	C15	-0.060	
6	H3	0.511		32	H15	0.235	
7	C4	0.264		33	N16	-0.531	Ring2 Charge= (-1.155)+ (1.423)= 0.268
8	O4	-0.692		34	C17	0.262	
9	H4	0.526		35	H17	0.234	
10	C5	0.163		36	N18	-0.515	
11	C6	0.302		37	H18	0.452	
12	O6	-0.696		38	C19	-0.048	
13	H6	0.522		39	H19	0.245	
14	C7	-0.063		40	C20	-0.061	
15	O7	-0.695		41	H20	0.230	
16	H7	0.521		42	N21	-0.561	Ring3 Charge= (-1.17)+ (1.411)= 0.241
17	H7′	0.231		43	C22	0.235	
18	H7″	0.230		44	H22	0.233	
19	O8	-0.383	Charge= (-0.767)+ (1.044)= 0.277	45	N23	-0.507	
20	H5′	0.514		46	H23	0.459	
21	O9	-0.384		47	C24	-0.034	
22	H6′	0.530		48	H24	0.247	
23	Fe10	0.762	0.762	49	C25	-0.068	
24	N11	-0.565		50	H25	0.237	
25	C12	0.246		Net Charge=2.003			
26	H12	0.244					

[a]The optimized structure of PC3 is shown in Fig. 7.

Table S13. NBO charge distribution on different atoms of PC4 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the O6 and O7 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.533	Ascorbic acid	27	C14	-0.049	
2	C2	0.792		28	H14	0.245	
3	O2	-0.599		29	C15	-0.063	
4	C3	0.123		30	H15	0.233	
5	O3	-0.681	Charge= (-3.563)+ (3.629)= 0.066	31	N16	-0.565	Ring2 Charge= (-1.186)+ (1.431)= 0.245
6	H3	0.508		32	C17	0.265	
7	C4	0.303		33	H17	0.235	
8	O4	-0.680		34	N18	-0.514	
9	H4	0.520		35	H18	0.452	
10	C5	0.006		36	C19	-0.050	
11	H5′	0.262		37	H19	0.245	
12	C6	0.518		38	C20	-0.057	
13	O6	-0.528		39	H20	0.234	
14	C7	0.416		40	N21	-0.580	Ring3 Charge= (-1.205)+(1.420)=0.215
15	O7	-0.542		41	C22	0.263	
16	H7″	0.181		42	H22	0.225	
17	O8	-0.421	Charge= (-0.848)+ (1.072)= 0.224	43	N23	-0.515	
18	H6	0.536		44	H23	0.453	
19	O9	-0.427		45	C24	-0.048	
20	H7	0.536		46	H24	0.245	
21	Fe10	1.055	1.055	47	C25	-0.062	
22	N11	-0.586	Ring1 Charge= (-1.214)+ (1.428)= 0.214	48	H25	0.234	
23	C12	0.263		Net Charge=2.019			
24	H12	0.234					
25	N13	-0.516					
26	H13	0.453					

[a]The optimized structure of PC4 is shown in Fig. 7.

Table S14. NBO charge distribution on different atoms of PC5 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C6 and C7 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.571	Ascorbic acid Charge= (-4.047)+ (4.13) =0.083	27	N13	-0.526	Ring1 Charge= (-1.209) (1.412)= 0.203
2	C2	0.794		28	H13	0.463	
3	O2	-0.599		29	C14	-0.047	
4	C3	0.125		30	H14	0.245	
5	O3	-0.697		31	C15	-0.057	
6	H3	0.516		32	H15	0.233	
7	C4	0.303		33	N16	-0.564	Ring2 Charge= (-1.183)+ (1.43)= 0.247
8	O4	-0.718		34	C17	0.262	
9	H4	0.530		35	H17	0.236	
10	C5	0.056		36	N18	-0.515	
11	H5′	0.255		37	H18	0.453	
12	C6	0.208		38	C19	-0.051	
13	O6	-0.726		39	H19	0.245	
14	H6	0.504		40	C20	-0.053	
15	C7	0.100		41	H20	0.234	
16	O7	-0.736		42	N21	-0.582	Ring3 Charge= (-1.213)+ (1.433)= 0.220
17	H7	0.517		43	C22	0.266	
18	H7″	0.222		44	H22	0.234	
19	O8	-0.435	Charge= (-0.859)+ (1.073) =0.214	45	N23	-0.516	
20	H6′	0.541		46	H23	0.453	
21	O9	-0.424		47	C24	-0.048	
22	H7′	0.532		48	H24	0.246	
23	Fe10	1.026	1.026	49	C25	-0.067	
24	N11	-0.579		50	H25	0.234	
25	C12	0.229		Net Charge=1.993			
26	H12	0.242					

[a]The optimized structure of PC5 is shown in Fig. 8.

Table S15. NBO charge distribution on different atoms of PC6 in presence of Fe-SOD involving double hydrogen abstraction by superoxide radical anion from the C7 and O7 sites of ascorbic acid in aqueous media at M06-2X/6-311+G(d) level.[a]

S. No.	Atoms	NBO Charge	Total	S. No.	Atoms	NBO Charge	Total
1	O1	-0.580	Ascorbic Acid Charge= (-3.927)+ (3.980) =0.052	27	N13	-0.518	Ring1 Charge= (-1.216)+ (1.431)= 0.215
2	C2	0.795		28	H13	0.450	
3	O2	-0.625		29	C14	-0.053	
4	C3	0.107		30	H14	0.243	
5	O3	-0.695		31	C15	-0.061	
6	H3	0.506		32	H15	0.232	
7	C4	0.323		33	N16	-0.567	Ring2 Charge= (-1.193) +(1.431) =0.238
8	O4	-0.667		34	C17	0.265	
9	H4	0.515		35	H17	0.235	
10	C5	0.076		36	N18	-0.514	
11	H5′	0.248		37	H18	0.452	
12	C6	0.018		38	C19	-0.050	
13	H6′	0.236		39	H19	0.245	
14	O6	-0.775		40	C20	-0.062	
15	H6	0.511		41	H20	0.234	
16	C7	0.482		42	N21	-0.579	Ring3 Charge= (-1.204)+ (1.418) =0.214
17	O7	-0.585		43	C22	0.251	
18	H7″	0.163		44	H22	0.240	
19	O8	-0.425	Charge=(-0.851)+(1.082) =0.231	45	N23	-0.515	
20	H7′	0.533		46	H23	0.451	
21	O9	-0.426		47	C24	-0.049	
22	H7	0.549		48	H24	0.244	
23	Fe10	1.051	1.051	49	C25	-0.062	
24	N11	-0.584		50	H25	0.232	
25	C12	0.261		Net Charge=2.001			
26	H12	0.245					

[a]The optimized structure of PC6 is shown in Fig. 8.

Table S16**:** Imaginary frequencies ν^{TS} (cm^{-1}) and Wigner transmission coefficients ($\Gamma(T)$) for hydrogen abstraction from the different pairs of sites of ascorbic acid by $O_2^{\cdot -}$ calculated using the barrier energies given in Tables 1 and 2 obtained at M06-2X/6-311+G(d) level of theory in gas phase at room temperature (298.15K).

Sl. No.	Reaction sites[a]	Without Fe-SOD		With Fe-SOD[b]	
		Freq.(ν^{TS})	$\Gamma(T)$	Freq.(ν^{TS})	$\Gamma(T)$
1	(O3,O4)	i2021.51	4.94		
2	(O6,C6)	i1261.44	2.54	i946.78	1.86
3	(C5,C6)	i959.49	1.89	i457.94	1.20
4	(O6,O7)	i511.97	1.25		
5	(C6,C7)	i2109.40	5.29		
6	(C7,O7)	i360.44	1.13	i384.35	1.14

[a]Numbering of atomic sites is shown in Fig. 1.
[b]Entries in these columns are irrelevant for barrierless reactions.

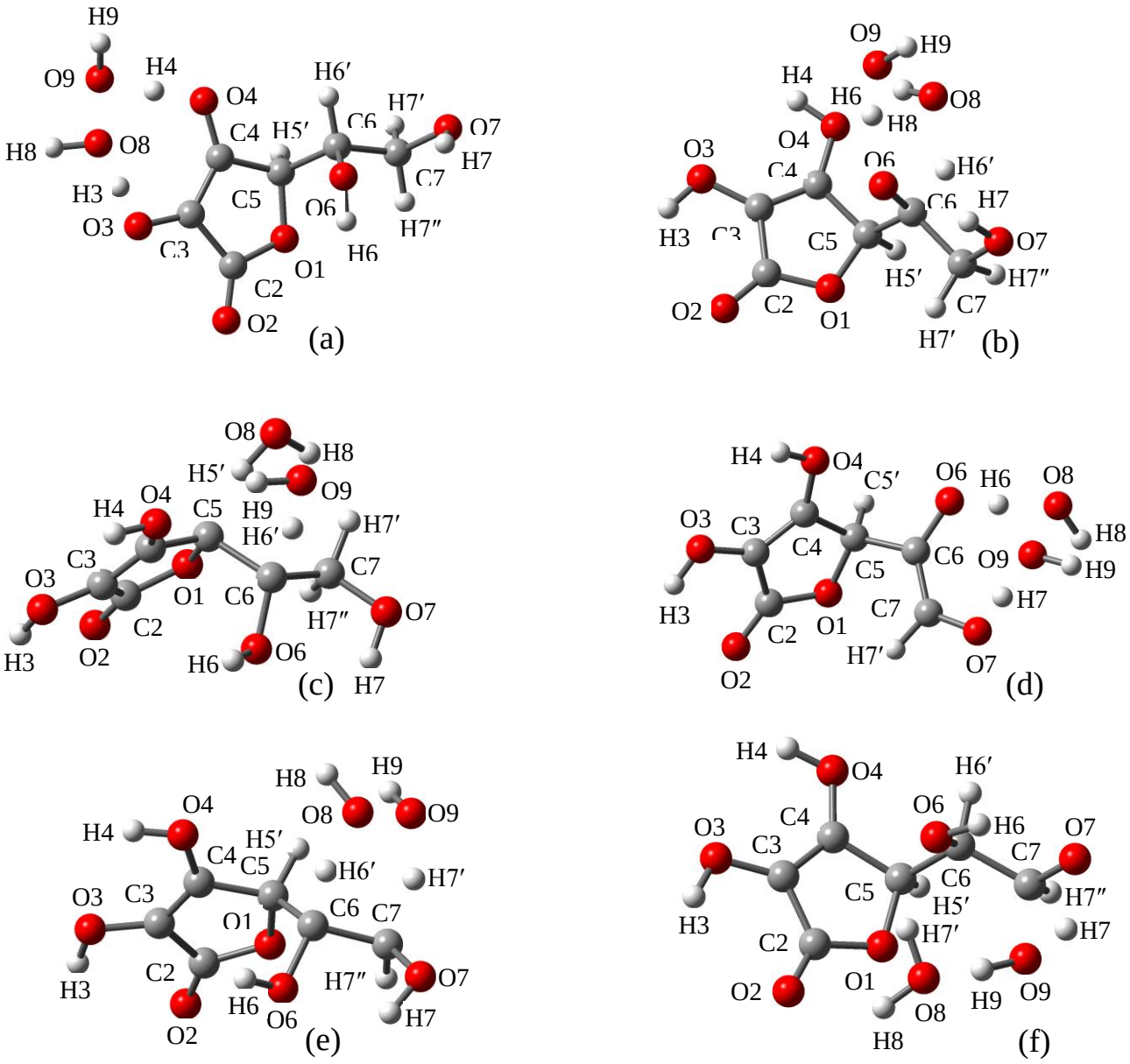

Fig. S17 (a-f). Optimized geometries of transition states involved in the double hydrogen abstraction from the different pairs of sites of ascorbic acid by H_2O_2 in absence of Fe-SOD obtained at the M062X/6-311+G(d) level of theory in aqueous media.

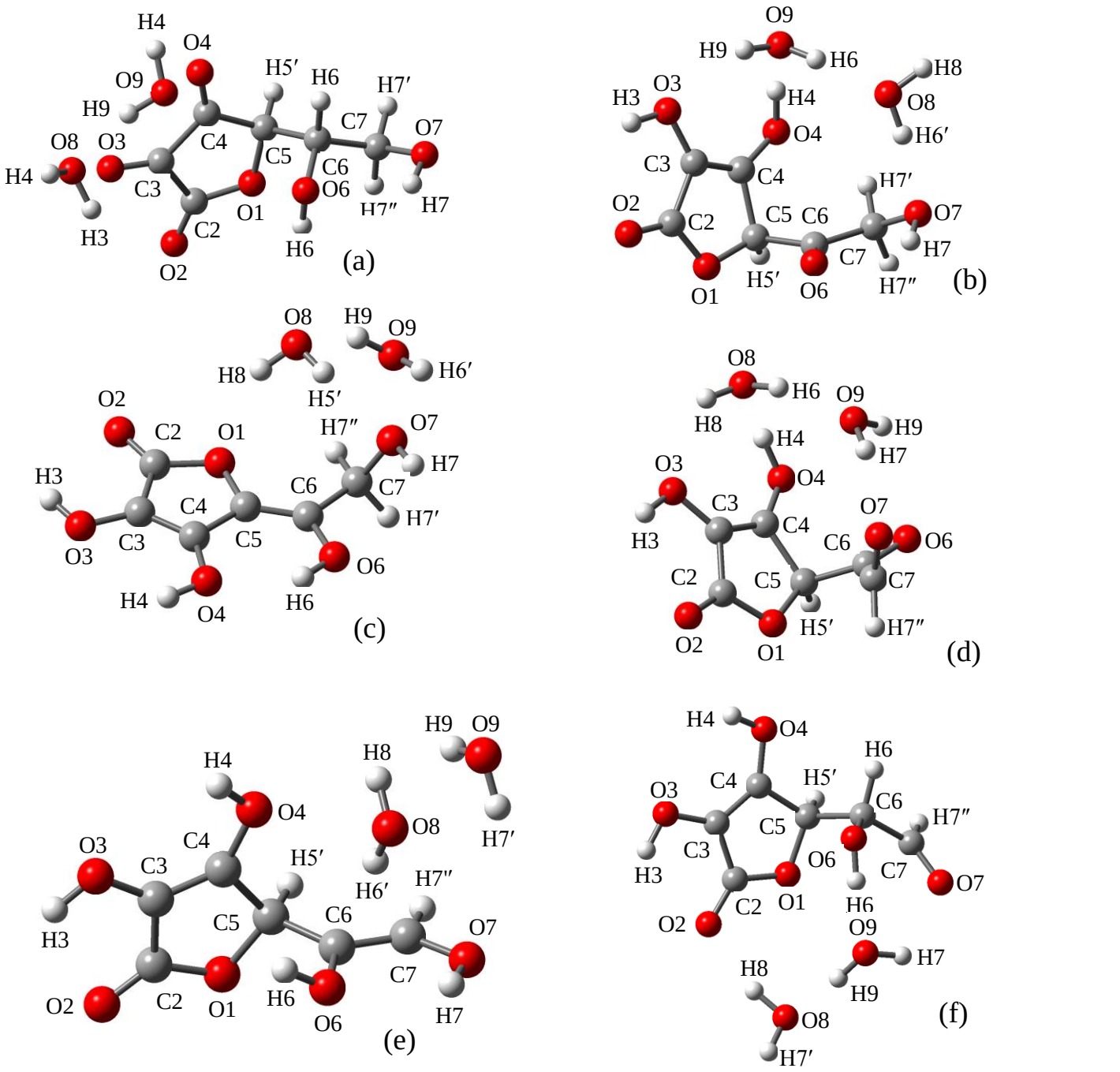

Fig S18 (a-f). Optimized geometries of product complexes formed due to double hydrogen abstraction from the different pairs of sites of ascorbic acid by H_2O_2 in absence of Fe-SOD obtained at the M062X/6-311+G(d) level of theory in aqueous media.

1. Cartesian coordinates of TS1 for double hydrogen abstraction from (O3,O4) pair of site of AA in absence of Fe-SOD

C	1.52078000	-1.55869400	-0.20103100
C	1.56559500	-0.19318300	0.34006800
C	0.38271900	0.04913600	1.03731900
C	-0.51101000	-1.15423400	0.78257700
O	0.31667100	-2.13129800	0.15611900
O	2.61595900	0.59335400	0.19214600
O	-0.02447900	1.09756700	1.62767400
O	2.34517300	-2.18249900	-0.81921700
C	-1.67134200	-0.81118100	-0.15952000
C	-2.72479700	0.09334000	0.47516300
H	-2.24443100	1.01489200	0.82975000
H	0.19448900	2.02240100	0.39995500
H	2.28653900	1.57758400	-0.07333900
H	-0.91064000	-1.56799900	1.71701900
O	-3.74031300	0.35803700	-0.47318100
O	-1.23544800	-0.22770400	-1.37349400
H	-3.25217200	0.51959100	-1.29376000
H	-0.58599800	0.47374900	-1.18628900
O	1.66832300	2.66081000	-0.60447600
O	0.36438000	2.27699600	-0.57124800
H	-2.15225100	-1.75318500	-0.45196700
H	-3.18934100	-0.40024700	1.33658900

2. Cartesian coordinates of TS2 for double hydrogen abstraction from (C6,O6) pair of site of AA in absence of Fe-SOD

C	-1.87948600	-1.14411600	-0.20234400
C	-2.23228300	0.22217500	0.16884400
C	-1.29001400	1.03544000	-0.30191800
C	-0.20778700	0.21510800	-0.94134000
O	-0.73543600	-1.12429100	-0.90009100
O	-3.35870700	0.51154900	0.87192100
O	-1.18414200	2.37328100	-0.21245900
O	-2.53038100	-2.13030700	0.04637000
C	1.12301000	0.28726000	-0.15958300
C	1.91992100	1.56404500	-0.50823500
H	1.26227200	2.44491100	-0.46837300
H	-1.84483700	2.69857600	0.41071100
H	-3.75671500	-0.33623700	1.11503300
H	-0.05306500	0.47760800	-1.99310000
O	2.96931300	1.70848900	0.41785800
O	1.01824900	0.05626000	1.12883900
H	2.69874500	1.15686000	1.17231500
H	1.98209700	-1.46299800	1.20591900
O	2.42604300	-1.87909100	-0.57747400
O	2.76808200	-1.87679100	0.77341400
H	1.78418000	-0.66330300	-0.64540300
H	2.34298700	1.49231300	-1.51667100

3. Cartesian coordinates of TS3 for double hydrogen abstraction from (C5,C6) pair of site of AA in absence of Fe-SOD

C	2.13193400	-1.07868900	0.37899600
C	2.24555400	0.20447400	-0.21764300
C	0.97903100	0.66187400	-0.52482200
C	0.07464900	-0.33477300	-0.13981000
O	0.77762900	-1.38196200	0.41052000
O	3.43809500	0.84382600	-0.41301600
O	0.64683400	1.86533300	-1.07871500
O	3.00628300	-1.83098600	0.79905500
C	-1.36367900	-0.38671600	-0.13304400
H	-1.80620900	0.29025400	0.84171200
C	-1.96480300	-1.78742500	-0.18506900
H	-1.70156700	-2.34790300	0.71622900
H	-1.55993100	-2.33888400	-1.05219500
H	1.46015800	2.38432700	-1.10928300
H	4.09762200	0.24624600	-0.03030200
H	-0.78019300	2.36296700	0.42797100
O	-3.37126500	-1.69981300	-0.27000300
O	-1.94235800	0.42031800	-1.16039600
H	-3.50869500	-0.92229600	-0.83135000
H	-2.33992900	1.13806900	-0.62040700
O	-2.31681100	1.53684400	1.19356200
O	-1.04807900	2.18578200	1.34223900

4. Cartesian coordinates of TS4 for double hydrogen abstraction from (O6,O7) pair of site of AA in absence of Fe-SOD

C	2.40058700	-0.72213400	-0.48445700
C	2.23755000	0.59377200	0.12991900
C	1.13469100	0.56642200	0.87928200
C	0.47504600	-0.78353600	0.75645800
O	1.40617500	-1.52870200	-0.08878900
O	3.13243400	1.58878800	-0.11550200
O	0.54795500	1.51543800	1.62806300
O	3.31631200	-1.03869500	-1.21562600
C	-0.88164300	-0.70480500	0.13896000
C	-1.91862100	-1.25506600	0.79926300
H	-1.70396300	-1.79403000	1.72416600
H	0.95642000	2.36273000	1.41121900
H	3.74165800	1.20829300	-0.76821900
H	0.43604200	-1.30281800	1.71979100
O	-3.21377100	-1.24393100	0.46569800
O	-0.90974000	-0.04996500	-1.03781300
H	-3.53598400	-0.33120700	-0.11239100
H	-1.81345400	0.60416800	-1.13224600
O	-2.76702100	1.49928200	-1.07599400
O	-3.85814000	0.89340200	-0.57989400

5. Cartesian coordinates of TS5 for double hydrogen abstraction from (C6,C7) pair of site of AA in absence of Fe-SOD

C	-2.43944900	0.92926700	-0.26875000
C	-2.02710300	-0.52928200	-0.08844800
C	-0.80118800	-1.06959700	-0.19857500
C	0.37576000	-0.38398200	-0.66276000
O	-1.54855800	1.78276400	-0.46000700
O	-3.04347100	-1.33931000	0.33090400
O	-0.60869400	-2.38935400	0.20305400
O	-3.67416400	1.07814800	-0.15890400
C	1.64587200	-0.69064300	-0.31629000
C	2.75945000	0.19878700	-0.64027600
H	2.40420300	1.30446400	-0.02762100
H	-1.44530000	-2.69802300	0.57569000
H	-3.81064500	-0.72826800	0.33446700
H	0.21296000	0.51238800	-1.24621900
O	4.01730300	-0.23703500	-0.25537600
O	2.00158400	-1.71498900	0.51083000
H	3.89890000	-0.85622500	0.47628700
H	1.20480100	-2.22075500	0.73567100
O	1.82274100	2.34751100	0.38694100
O	0.74666400	1.90510200	1.11334200
H	-0.02877200	1.93214600	0.50174000
H	2.77656800	0.56428600	-1.66569900

6. Cartesian coordinates of TS6 for double hydrogen abstraction from (C7,O7) pair of site of AA in absence of Fe-SOD

C	2.45474700	-0.62569300	-0.16257300
C	1.99383200	0.75249300	-0.07028600
C	0.79201600	0.76998000	0.52682100
C	0.46959200	-0.65410200	0.94086300
O	1.53685400	-1.44466600	0.39134600
O	2.75138700	1.75938700	-0.56708800
O	0.05154300	1.82600800	0.83733200
O	3.48771500	-1.00523500	-0.66199200
C	-0.88989500	-1.22056400	0.53346100
C	-1.27713200	-0.90687500	-0.91969300
H	-0.45759600	-1.15389200	-1.62062900
H	-0.90869600	1.68843500	0.60266200
H	0.53233800	-0.72586800	2.03198500
O	-2.48005100	-1.32299000	-1.27696200
O	-1.81073400	-0.69254100	1.46515100
H	-3.35095600	0.10856100	-0.91855900
H	-2.55348600	-0.27534600	0.99512700
O	-2.17240900	1.55867300	-0.53749000
O	-3.35154400	0.86504900	-0.26534600
H	-0.83765400	-2.31139700	0.65478500
H	-1.31547400	0.28244900	-0.95190000
H	3.53048600	1.34612900	-0.96464000

7. Cartesian coordinates of PC1 for double hydrogen abstraction from (O3,O4) pair of site of AA in absence of Fe-SOD

C	0.68814900	2.21421600	-0.00952800
C	1.35369700	0.87253200	-0.10253600
C	0.32452400	-0.05937200	-0.44372900
C	-0.95786400	0.73442000	-0.64050700
O	-0.65496000	2.08132400	-0.27724700
O	2.57290600	0.69406600	0.13748000
O	0.31797600	-1.31179000	-0.51363900
O	1.16184900	3.28468800	0.26238200
C	-2.11320300	0.16759200	0.18853400
C	-2.91656400	-0.85907100	-0.60733900
H	-2.21958900	-1.62033000	-0.99197200
H	1.90327200	-2.23148900	-0.58455100
H	3.14533300	-0.97955400	0.53503100
H	-1.24895800	0.72835700	-1.70164100
O	-3.91476100	-1.42733900	0.21097400
O	-1.68582800	-0.44055700	1.39817000
H	-3.48198800	-1.52830100	1.07154600
H	-0.98023200	-1.06227300	1.15160200
O	3.20486200	-1.93888300	0.72665600
O	2.84649200	-2.48431800	-0.54638400
H	-2.76842300	0.99447400	0.48431800
H	-3.41014300	-0.38031200	-1.46083800

8. Cartesian coordinates of PC2 for double hydrogen abstraction from (C6,O6) pair of site of AA in absence of Fe-SOD

C	-1.87186500	-1.16003700	-0.20397800
C	-2.24350000	0.20079400	0.16771300
C	-1.31946200	1.02677700	-0.31349700
C	-0.21341300	0.22943200	-0.93791600
O	-0.72326300	-1.12858800	-0.89740400
O	-3.36876300	0.47874100	0.87876700
O	-1.21181500	2.36353400	-0.21406600
O	-2.51183300	-2.15400400	0.04633400
C	1.05329000	0.39047000	-0.12930400
C	1.90547600	1.59674500	-0.51047100
H	1.30205200	2.52097200	-0.50670100
H	-1.86887000	2.68526000	0.41458000
H	-3.75532700	-0.37264400	1.12703000
H	-0.05068300	0.49749600	-1.98673800
O	2.95646800	1.73531500	0.41773500
O	1.01025700	0.06897600	1.12386000
H	2.69763600	1.16701200	1.16276800
H	2.04010100	-1.41271000	1.19175200
O	2.46379300	-1.90111400	-0.59354700
O	2.80722200	-1.87168300	0.79011400
H	2.06880300	-1.00305900	-0.73394900
H	2.32660600	1.48316800	-1.51836400

9. Cartesian coordinates of PC3 for double hydrogen abstraction from (C5,C6) pair of site of AA in absence of Fe-SOD

C	-1.99258100	-1.25395600	-0.35519300
C	-2.12886900	0.02550200	0.19994200
C	-0.88130200	0.46177200	0.63254600
C	0.05716700	-0.54155500	0.32183600
O	-0.62959700	-1.57988100	-0.28039700
O	-3.32568000	0.68627300	0.33625800
O	-0.55609300	1.72595700	1.11017600
O	-2.82959400	-2.02957900	-0.82527500
C	1.42696900	-0.60162600	0.45814500
H	1.42177200	1.14951800	-1.24752600
C	2.27239900	-1.77992200	0.15831500
H	1.72857500	-2.48427800	-0.46938600
H	2.56673500	-2.29576600	1.08827100
H	-1.23789900	2.00588100	1.72903400
H	-3.99343600	0.09341800	-0.03333700
H	-0.15102900	2.61241300	-0.49210800
O	3.47039000	-1.40848600	-0.53491000
O	2.11314500	0.35427700	1.21574700
H	3.76037600	-0.58501900	-0.12449400
H	1.81318800	1.23582000	0.95725600
O	1.57833200	2.06536800	-0.95696200
O	0.37522400	2.73691000	-1.30229300

10. Cartesian coordinates of PC4 for double hydrogen abstraction from (O6,O7) pair of site of AA in absence of Fe-SOD

C	-2.29306900	0.11568400	-1.04579300
C	-2.36203300	-0.40868100	0.31613400
C	-1.42189800	0.19968600	1.04170300
C	-0.62344900	1.11029200	0.15380900
O	-1.32496500	1.04500900	-1.11556700
O	-3.28150700	-1.35199100	0.65429600
O	-1.07253700	0.06324400	2.33308300
O	-3.01911400	-0.21018400	-1.96040900
C	0.80995500	0.60847700	-0.01138600
C	1.83790700	1.56829400	0.24509100
H	1.46661700	2.57440900	0.53133800
H	-1.52889000	-0.71082600	2.68558200
H	-3.72417800	-1.56962900	-0.18131000
H	-0.65624200	2.15136000	0.49156100
O	3.07266100	1.37921700	0.17944100
O	0.95199900	-0.59755700	-0.34531300
H	3.84068000	-0.10699600	-0.44398400
H	2.45737300	-1.53243600	-0.07339600
O	3.37044200	-1.83126100	0.12436500
O	4.11054100	-0.99252600	-0.77078800

11. Cartesian coordinates of PC5 for double hydrogen abstraction from (C6,C7) pair of site of AA in absence of Fe-SOD

C	-2.53377000	0.52799600	-0.39736100
C	-1.83048600	-0.77584600	-0.06250400
C	-0.49043300	-1.08666400	-0.03993900
C	0.56227100	-0.24918600	-0.41790300
O	-1.84841200	1.51924300	-0.71736900
O	-2.68268800	-1.76333700	0.32687800
O	-0.15823900	-2.35990800	0.41618100
O	-3.77591500	0.41974400	-0.29628000
C	1.94245300	-0.51522200	-0.25537500
C	2.91406600	0.38811700	-0.57049100
H	0.89249100	1.44794100	1.22135600
H	-0.97181100	-2.78626600	0.71479900
H	-3.55721700	-1.31674300	0.25970700
H	0.28657900	0.69763500	-0.86204600
O	4.23171500	0.10273300	-0.38960600
O	2.41935800	-1.70099000	0.26503300
H	4.28192400	-0.79108300	-0.02361400
H	1.66877200	-2.27598000	0.47546000
O	0.50031400	2.30633600	1.44423600
O	0.30015600	2.89731400	0.16701400
H	-0.58096000	2.54587700	-0.09441400
H	2.70530900	1.37437400	-0.95851300

12. Cartesian coordinates of PC6 for double hydrogen abstraction from (C7,O7) pair of site of AA in absence of Fe-SOD

C	2.55878600	-0.80553600	0.08425600
C	2.33227900	0.57491600	-0.32602700
C	1.18010100	0.98722200	0.21744400
C	0.63441100	-0.13499400	1.06511100
O	1.54412700	-1.21940300	0.87756400
O	3.21244300	1.20004200	-1.14783800
O	0.54785200	2.15083500	0.11379500
O	3.50169400	-1.49432600	-0.22334700
C	-0.81528700	-0.46995000	0.71564700
C	-1.04514400	-0.82094700	-0.70120900
H	-0.28416500	-0.56429200	-1.44482000
H	-0.36631700	2.00232300	0.44770900
H	0.66976500	0.14992000	2.12154900
O	-2.16541400	-1.37076500	-1.07766800
O	-1.47326300	0.78193500	1.17430200
H	-3.42260600	-0.97670200	0.00462200
H	-2.42143800	0.69573700	0.96764600
O	-4.03401600	0.55898700	-0.90488200
O	-3.96291700	-0.19718400	0.31194600
H	-1.18827300	-1.26652000	1.37466800
H	-3.31033400	0.14944700	-1.42268600
H	3.88844200	0.54484500	-1.37099500

13. Cartesian coordinates of TS2 for double hydrogen abstraction from (C6,O6) pair of site of AA in presence of Fe-SOD

C	-5.22169100	0.80421600	-1.11292500
C	-3.90702700	1.07907800	-1.71859900
C	-3.00276400	0.27281600	-1.15667200
C	-3.70214200	-0.65767800	-0.21361900
O	-5.05482800	-0.21804500	-0.19071700
O	-3.69367000	2.04903200	-2.61443500
O	-1.65812800	0.24556800	-1.27978500
O	-6.26197300	1.34041500	-1.32504700
C	-3.29266700	-0.54752300	1.25557800
H	-1.68970500	-1.70195500	1.14575700
C	-3.97605100	-1.48782300	2.23576200
H	-5.00652600	-1.64737700	1.90690200
H	-3.96558600	-1.04709500	3.23743900
H	-1.40326400	0.99528500	-1.84641300
H	-4.53414300	2.49320900	-2.83277500
H	-3.68690900	-1.70874900	-0.53682700
O	-3.30159500	-2.72393600	2.14817100
O	-2.54511300	0.36834600	1.65993000
H	-2.50592600	-2.72477400	2.70441400
H	-1.37576500	0.22778000	1.44019600
C	2.54352600	-4.03408200	-0.50853700
N	1.35098600	-3.85674400	-1.17267800
C	2.89125300	-2.80124600	-0.04140900
H	0.81232800	-4.58387500	-1.62892200
C	1.00447500	-2.56457900	-1.08970700
N	1.91639200	-1.88720700	-0.40799000
H	3.76016700	-2.51514500	0.53316600
H	0.11549900	-2.12819600	-1.51460700
C	5.90235300	0.74709400	-0.01169400
N	5.71247500	0.01247900	-1.15763300
C	4.66741800	0.87097300	0.55435900
H	6.43432000	-0.25225400	-1.81902600
C	4.41173400	-0.30114100	-1.26089900
N	3.74239300	0.20762900	-0.23253300
H	4.38336700	1.38631100	1.46009600
H	3.99310700	-0.89596500	-2.06055500
C	1.95119900	4.22675200	0.48320500
N	1.06105300	3.88551000	1.47506400
C	2.35346800	3.04796900	-0.07122600
H	0.58058500	4.52902500	2.09394000
C	0.94191900	2.55217500	1.49154700
N	1.71548800	1.99663100	0.57128700
H	3.06292600	2.88555100	-0.86942500
H	0.30814400	2.00459800	2.16873600
Fe	1.79986900	0.03588200	0.16016800
H	2.21495600	5.25063900	0.26667800
H	6.87293400	1.10775500	0.29272400
H	3.02351500	-4.99699200	-0.42536100
O	-0.72916900	-1.62846700	0.94124400
O	-0.26454500	-0.35301300	1.35812400

14. Cartesian coordinates of TS3 for double hydrogen abstraction from (C5,C6) pair of site of AA in presence of Fe-SOD

C	-3.87340700	-1.00064000	-0.04078100
C	-4.61888500	0.28041000	-0.15552600
C	-3.78368200	1.27071800	0.24961800
C	-2.56286300	0.62931100	0.66322400
O	-2.61715700	-0.68854800	0.52887100
O	-5.84021200	0.38968200	-0.62948900
O	-3.89571200	2.60137800	0.27977300
O	-4.17844700	-2.09863000	-0.35541400
C	-1.38577900	1.28638500	1.24547400
H	-0.79015500	1.57247400	0.31323300
C	-0.46188300	0.34231300	2.02466400
H	-0.77119200	-0.69932900	1.94678700
H	-0.46467800	0.64932000	3.07297200
H	-4.80248700	2.88754600	0.07106800
H	-6.24412500	-0.48108300	-0.80628100
H	-1.70739300	1.29784800	-2.16831500
O	0.88131800	0.38248900	1.51553300
O	-1.70263800	2.39086800	2.04786300
H	1.30488400	1.21783400	1.77915600
H	-2.04701400	3.12026600	1.50882800
O	-1.39751700	0.65055400	-1.51139800
O	-0.12045000	1.18843200	-1.18958100
C	-0.68038100	-3.64605700	0.23183500
N	-1.24980000	-3.29691700	-0.96824500
C	0.18554600	-2.63551200	0.52908700
H	-1.93875900	-3.83631100	-1.47644800
C	-0.73832000	-2.11490700	-1.35596000
N	0.13325100	-1.67586700	-0.46305700
H	0.85385000	-2.54319600	1.37266600
H	-1.03070100	-1.59852300	-2.25671700
C	4.46749600	-2.15117400	1.26207900
N	4.72256500	-2.28487100	-0.07847800
C	3.31971800	-1.41594400	1.34392100
H	5.50370600	-2.78098900	-0.48902600
C	3.75315700	-1.64656200	-0.76101800
N	2.88136100	-1.10526600	0.07183100
H	2.78295400	-1.09262800	2.22299500
H	3.72347400	-1.59602600	-1.84008800
C	4.11554800	3.09945100	-0.19075200
N	3.20006200	3.64034300	-1.05966500
C	3.62480100	1.86979700	0.13628400
H	3.26875000	4.54699400	-1.50458400
C	2.20091500	2.75827900	-1.23441800
N	2.42395000	1.66487600	-0.51933700
H	4.05852900	1.12014100	0.78145500
H	1.33782800	2.92696500	-1.86044500
Fe	1.25331700	0.00485600	-0.44582300
H	5.01111200	3.62264500	0.10486900
H	5.10722800	-2.57923100	2.01766400
H	-0.92713900	-4.56205900	0.74461200

15. Cartesian coordinates of TS5 for double hydrogen abstraction from (C6,C7) pair of site of AA in presence of Fe-SOD

C	-3.66575600	1.29914300	0.15167500
C	-3.72336700	0.55755900	-1.10675600
C	-3.75290800	-0.75277000	-0.82554600
C	-3.80659000	-0.91009600	0.67622600
O	-3.66465100	0.40022200	1.19511200
O	-3.68285300	1.12643900	-2.32275400
O	-3.79113000	-1.83768200	-1.59394700
O	-3.59399100	2.48610600	0.32108100
C	-2.77891400	-1.81264700	1.29029100
C	-1.81452300	-1.41939300	2.24674600
H	-2.08058200	-0.62296200	2.94276000
H	-3.94932100	-1.59621700	-2.52437300
H	-3.91553200	2.06947200	-2.26440300
H	-4.78445300	-1.32052500	0.97628400
O	-1.11515300	-2.53040500	2.74362200
O	-2.79305500	-3.02777300	0.86083100
C	3.14488100	-3.63746900	-0.58018600
N	3.31363700	-3.26875800	-1.89287900
C	2.51683800	-2.58305500	0.02064000
H	3.74470300	-3.83118600	-2.61802600
C	2.80161900	-2.03549400	-2.06123100
N	2.31344200	-1.58404800	-0.91381900
H	2.19966700	-2.46479800	1.04663500
H	2.80701200	-1.51013500	-3.00661300
C	4.53590800	2.16378300	1.59922300
N	5.22191800	1.12598500	1.01475000
C	3.23995900	2.01762400	1.20032100
H	6.21499800	0.94614100	1.10477100
C	4.35804100	0.39065900	0.29638500
N	3.13767000	0.90593500	0.38314800
H	2.38214100	2.62541000	1.44313400
H	4.63777400	-0.49252400	-0.25894200
C	-0.01614200	4.13668200	-0.68012200
N	-0.98330700	3.50897600	0.06363400
C	0.94158700	3.18982600	-0.91406800
H	-1.86979400	3.89404900	0.37586000
C	-0.60985600	2.23477300	0.25950100
N	0.55803100	2.00364200	-0.31868800
H	1.87267900	3.28714000	-1.45430200
H	-1.17808400	1.52125800	0.83720300
Fe	1.46235000	0.21626900	-0.45404700
H	-0.09058500	5.17186100	-0.97566800
H	5.01756800	2.89224400	2.23309500
H	3.47903200	-4.59098200	-0.20069600
O	-0.42099600	-0.75053800	-0.59044900
O	0.18393100	-0.70510500	0.71826300
H	-0.26897000	-1.67243300	-0.87581300
H	-0.92435700	-0.87640600	1.48679600
H	-1.28949400	-2.66297400	3.68945400
H	-2.15673200	-3.55639800	1.40236600

16. Cartesian coordinates of TS6 for double hydrogen abstraction from (C7,O7) pair of site of AA in presence of Fe-SOD

C	3.68096800	-1.11599600	-0.52073500
C	4.88786400	-0.76937800	0.24620600
C	4.54666000	0.17551400	1.13431800
C	3.11995700	0.58871700	0.87937000
O	2.64217000	-0.37038400	-0.03030500
O	6.08832600	-1.33659900	0.06272500
O	5.23955800	0.87109400	2.04249000
O	3.54939100	-1.90056000	-1.41750800
C	3.17288500	2.01554500	0.18878600
C	1.92884200	2.87625500	0.32963500
H	1.94323900	3.56057600	1.19339000
H	6.15735900	0.55389200	2.11017900
H	6.02856400	-2.04055800	-0.60700800
H	2.50337600	0.57094200	1.78594900
O	0.97897500	2.92252700	-0.46310000
O	3.43403900	1.88994600	-1.17573800
H	0.64133500	1.81297300	-0.94903900
H	4.36473900	2.07290000	-1.37292800
C	-3.46237300	3.66784700	0.43685300
N	-3.04231100	3.82860800	-0.86112200
C	-3.16152400	2.37544600	0.76154000
H	-3.13324300	4.67295600	-1.41495800
C	-2.51142400	2.66983000	-1.28855700
N	-2.56906300	1.75985800	-0.32569700
H	-3.32124400	1.85268900	1.69399100
H	-2.10642300	2.52339700	-2.28077100
C	-4.88464500	-2.43047300	1.30616600
N	-5.57776600	-1.35190200	0.81029500
C	-3.56868500	-2.16081700	1.07346700
H	-6.58497000	-1.23763000	0.82063600
C	-4.70009800	-0.47250300	0.30423800
N	-3.45995000	-0.92887800	0.45193000
H	-2.70290500	-2.76252300	1.30094000
H	-4.98020400	0.46976300	-0.14490300
C	-0.30278000	-3.95569600	-1.13932800
N	0.35257200	-3.63630900	0.02336100
C	-1.10352900	-2.88544500	-1.41090400
H	1.03508300	-4.21537100	0.49729200
C	-0.02360800	-2.40295800	0.40750200
N	-0.93076500	-1.92547800	-0.43336900
H	-1.79358700	-2.75377500	-2.23183900
H	0.35913400	-1.91088700	1.29032400
Fe	-1.81992500	-0.12420400	-0.34397400
H	-0.15115600	-4.89032800	-1.65630300
H	-5.37712200	-3.26915600	1.77375200
H	-3.90939500	4.46936500	1.00497900
O	-0.07979900	0.51417900	0.58833700
O	0.01863400	0.73742800	-0.80446900
H	3.96707700	2.53959300	0.73855800
H	0.28796000	1.31280800	1.06250900

17. Cartesian coordinates of PC1 for double hydrogen abstraction from (O3,O4) pair of site of AA in presence of Fe-SOD

C	-4.46042300	0.62147300	-1.39171900
C	-2.99500000	0.28178600	-1.10699500
C	-3.02650500	-1.04864500	-0.33717600
C	-4.49620900	-1.28987400	-0.05232700
O	-5.19322800	-0.43974400	-0.97875000
O	-2.02626800	0.89668400	-1.45010500
O	-2.07115500	-1.68249200	0.01415800
O	-4.87216300	1.57142500	-1.95610600
C	-4.72822800	-0.78860100	1.37163900
H	-4.23139900	-1.47023900	2.07282000
C	-6.19463500	-0.64180100	1.74651900
H	-6.64673300	-1.62856900	1.88962700
H	-6.73415000	-0.09993300	0.96418500
H	-4.81410700	-2.31922900	-0.21486600
O	-6.14729800	0.09934200	2.94997600
O	-4.08210800	0.47541700	1.37692100
H	-7.02981100	0.33266500	3.25459800
H	-4.44883700	1.00050300	2.10415000
O	0.36865300	-0.34022500	-1.38117500
O	0.24650700	-0.26718200	0.03555900
C	2.27698800	4.20758500	-0.85683600
N	0.93658000	3.99995200	-0.64506200
C	2.85492200	2.97737700	-0.77639900
H	0.21951800	4.71244300	-0.64199200
C	0.73039800	2.68826900	-0.44924300
N	1.87818100	2.03094600	-0.52258800
H	3.89468100	2.71234200	-0.88550100
H	-0.23939600	2.25792100	-0.24981700
C	5.57995100	0.06639700	2.01797200
N	4.81463500	1.06266400	2.57501500
C	4.84465400	-0.42742800	0.98496800
H	5.06901300	1.62771300	3.37366000
C	3.66778200	1.15859100	1.88754800
N	3.64645000	0.26255700	0.91153800
H	5.08976000	-1.22036000	0.29771800
H	2.88767800	1.86938700	2.10968100
C	2.91472600	-4.09109100	-0.06526500
N	2.75966500	-3.97421100	-1.42570700
C	2.79002400	-2.82866200	0.42804900
H	2.80500000	-4.72991000	-2.09536900
C	2.54665300	-2.68311000	-1.72207200
N	2.56290100	-1.95244200	-0.61787700
H	2.85284800	-2.48967400	1.44943200
H	2.38474400	-2.31847600	-2.72459300
Fe	2.20936600	0.03289800	-0.45862300
H	3.09347800	-5.03809600	0.41585500
H	6.55502000	-0.19296800	2.39476300
H	2.68895100	5.18513900	-1.04414900
H	-0.33486200	0.27472600	-1.68692100
H	-0.30791200	-1.04640700	0.25786400

18. Cartesian coordinates of PC2 for double hydrogen abstraction from (C6,O6) pair of site of AA in presence of Fe-SOD

C	5.53308000	0.91502100	0.14084700
C	4.56218600	1.86604000	-0.43218600
C	3.33537200	1.41001100	-0.19073200
C	3.42934700	0.10492400	0.54787900
O	4.81912200	-0.10457800	0.73204100
O	4.89742700	2.99743700	-1.05380700
O	2.13440300	1.97398000	-0.47125800
O	6.71507500	0.97912000	0.12812800
C	2.82177000	-1.10515600	-0.16986600
C	3.65745000	-2.36239600	-0.14272500
H	4.08107300	-2.47479800	0.86378600
H	2.27829600	2.76641600	-1.00866100
H	5.85984200	3.10912700	-1.07459400
H	2.94833200	0.16358700	1.53514300
O	2.87778700	-3.46212600	-0.52214200
O	1.72272100	-1.05721400	-0.67129100
H	3.43647200	-4.13832200	-0.91936700
C	-3.94085000	3.75161300	0.81700300
N	-3.02109600	4.04691900	-0.15856700
C	-3.71276400	2.45175700	1.15462600
H	-2.92283700	4.93677800	-0.62789200
C	-2.27162400	2.95460300	-0.38526300
N	-2.66454100	1.96291300	0.39827600
H	-4.22671600	1.84519800	1.88345600
H	-1.48274800	2.90358600	-1.11989500
C	-5.37454900	-2.03473800	-0.60383600
N	-5.57883200	-0.83641400	-1.24579900
C	-4.16409800	-1.92330200	0.00580300
H	-6.38695600	-0.59366600	-1.80242000
C	-4.52590400	-0.04099800	-1.01559900
N	-3.63640500	-0.66944100	-0.25894600
H	-3.64113900	-2.64578900	0.60955100
H	-4.43361300	0.96118400	-1.40220100
C	-0.18058500	-3.59125700	-0.33090000
N	0.33350200	-3.37459500	0.92007200
C	-1.08213500	-2.59418300	-0.53536500
H	1.07177200	-3.92050400	1.34143900
C	-0.23244800	-2.27208900	1.43348200
N	-1.10468900	-1.76736600	0.57510200
H	-1.70502600	-2.40663800	-1.39522900
H	0.00261600	-1.87404300	2.40841100
Fe	-1.93195000	0.07369100	0.47779800
H	0.14543000	-4.40668900	-0.95258000
H	-6.09208600	-2.83729400	-0.63658400
H	-4.65247500	4.47451700	1.17983500
O	-0.29876000	0.62105000	-0.61753600
O	0.02521600	0.80746900	0.75744600
H	4.51443600	-2.18818000	-0.80729300
H	0.41110000	-0.02500800	-0.88697000
H	0.45993100	1.68027500	0.76668000

19. Cartesian coordinates of PC3 for double hydrogen abstraction from (C5,C6) pair of site of AA in presence of Fe-SOD

C	-3.91945300	-0.77809300	0.07393900
C	-4.32225700	0.56726600	-0.36224400
C	-3.41731400	1.43809400	0.13143800
C	-2.44690900	0.68359000	0.90859600
O	-2.79973000	-0.65246000	0.87424600
O	-5.37017500	0.82067200	-1.14994600
O	-3.27558900	2.77379800	0.01235400
O	-4.39987200	-1.83635400	-0.22057400
C	-1.35305600	1.11840100	1.55548300
H	-1.20687300	0.75456600	-1.36181600
C	-0.44521700	0.21584100	2.32360400
H	-0.84178300	-0.79783500	2.34710200
H	-0.32315300	0.58530600	3.34542400
H	-4.07406000	3.17429900	-0.37454000
H	-5.91758300	0.02005500	-1.23887500
H	0.82027400	1.16244300	-2.79914400
O	0.86600300	0.14976700	1.70702400
O	-0.94811500	2.41474400	1.55477400
H	1.43999400	0.82821300	2.09642600
H	-1.64236200	2.99123500	1.18094500
O	0.42779200	0.42106800	-2.29370900
O	-0.29936200	1.11475900	-1.26862100
C	-1.20259600	-3.43148300	0.45060800
N	-1.76726300	-3.03388000	-0.73101100
C	-0.16984700	-2.56653000	0.67346600
H	-2.61605800	-3.41374200	-1.13548800
C	-1.10129300	-1.95887300	-1.18217500
N	-0.12156400	-1.63804600	-0.34613600
H	0.54260800	-2.54569900	1.48591100
H	-1.32616500	-1.47410400	-2.12336200
C	4.66153400	-2.03554600	0.73738100
N	4.06499100	-2.95147900	-0.09318900
C	3.80625700	-0.97404800	0.78290600
H	4.44144700	-3.85702000	-0.34596600
C	2.89505800	-2.44473800	-0.51920400
N	2.70413200	-1.23909800	-0.00510100
H	3.91856300	-0.04166500	1.31549400
H	2.21544400	-2.96927600	-1.17507100
C	3.93016300	3.03612400	-0.82376300
N	2.93934100	3.68373400	-0.12801900
C	3.50750600	1.74432300	-0.94618200
H	2.94439000	4.66143100	0.13701400
C	1.96125500	2.80378000	0.14867500
N	2.27623000	1.60818100	-0.33334400
H	4.00818600	0.90776900	-1.41112100
H	1.04857900	3.04670300	0.67892600
Fe	1.12004600	-0.04783000	-0.29488300
H	4.82491600	3.53820500	-1.15732600
H	5.61497200	-2.21541900	1.20848600
H	-1.57418900	-4.27437400	1.01199800

20. Cartesian coordinates of PC4 for double hydrogen abstraction from (O6,O7) pair of site of AA in presence of Fe-SOD

C	5.63947400	0.92673000	-0.40087100
C	5.71378700	0.30295300	0.93607300
C	5.07052700	-0.86162500	0.88375200
C	4.54890700	-1.05650000	-0.51811500
O	4.94424000	0.07964400	-1.23548300
O	6.31706500	0.87501300	1.98070200
O	4.78510800	-1.81266700	1.78834900
O	6.07989000	1.97496400	-0.73623400
C	3.03875000	-1.17366300	-0.48205100
C	2.44105700	-2.41530600	0.23710900
H	3.09004700	-3.27155900	0.46393900
H	5.23050400	-1.64709800	2.63094400
H	6.78514100	1.67590600	1.70167200
H	4.97144000	-1.96221700	-0.97594700
O	1.27137700	-2.41884400	0.52811200
O	2.28546900	-0.36573400	-0.94877100
H	0.13122200	-1.11076300	0.45415900
H	0.42475800	-0.09687300	-1.61046700
C	-0.69159400	4.05543800	-0.23953000
N	-1.00939000	4.00509200	-1.57501100
C	-1.06123100	2.84858200	0.27199200
H	-0.85922700	4.74326000	-2.24939100
C	-1.54807300	2.80439500	-1.84123100
N	-1.59890100	2.07291100	-0.73812400
H	-0.97374800	2.48145400	1.28193200
H	-1.88423900	2.50706900	-2.82289600
C	-5.05406100	0.58091700	2.55759700
N	-5.02947200	1.85073300	2.03191600
C	-4.15311600	-0.13490400	1.83229800
H	-5.58962000	2.63218100	2.34373600
C	-4.13757100	1.88402200	1.03240400
N	-3.58207700	0.68925700	0.87824800
H	-3.87500700	-1.17097400	1.92737000
H	-3.91516100	2.76579400	0.45293000
C	-4.27350900	-3.47243500	-0.94878800
N	-2.98682300	-3.91724400	-0.75318700
C	-4.21995800	-2.11904600	-0.80967200
H	-2.68242300	-4.88062400	-0.77154700
C	-2.20836300	-2.85477300	-0.49994200
N	-2.91615300	-1.74098600	-0.53710400
H	-5.02086900	-1.40027100	-0.88236800
H	-1.14645100	-2.93216300	-0.32534300
Fe	-2.23196100	0.16070500	-0.49082000
H	-5.08991500	-4.14112800	-1.16420600
H	-5.69000300	0.30964300	3.38340800
H	-0.23668400	4.92085700	0.21257400
O	-0.38734100	-0.54098500	-1.29679100
O	-0.34696400	-0.31737400	0.10730700

21. Cartesian coordinates of PC5 for double hydrogen abstraction from (C6,C7) pair of site of AA in presence of Fe-SOD

C	-5.14348000	0.07132200	0.58286100
C	-4.23502600	0.67200000	-0.41872200
C	-3.39012700	-0.27357300	-0.82809200
C	-3.69178100	-1.56608900	-0.10426800
O	-4.77981800	-1.23501100	0.76212800
O	-4.31590200	1.97686800	-0.75304300
O	-2.35666800	-0.25011700	-1.71222900
O	-6.02807000	0.62495200	1.16180200
C	-2.52797000	-2.01924400	0.72816200
H	-0.65977700	-0.77772400	-1.26739900
C	-1.70979000	-3.01358900	0.38372700
H	0.28778300	-1.84329600	0.74430600
H	-1.83484300	-3.62886300	-0.49932700
H	-2.44188300	0.51111800	-2.31406700
H	-5.18140700	2.32156200	-0.45565900
H	-4.00755000	-2.34941300	-0.80190900
O	-0.55400000	-3.27012400	1.10220400
O	-2.23276400	-1.25368600	1.82430400
H	-0.75380600	-3.23587900	2.05578800
H	-3.04849200	-1.09146500	2.33262300
C	4.42653100	-2.95352200	0.12019200
N	4.15754400	-3.07678100	-1.22104000
C	3.72745800	-1.85679500	0.53461200
H	4.52533000	-3.79338100	-1.83689700
C	3.32349500	-2.08842200	-1.58583300
N	3.04321700	-1.32021600	-0.54164700
H	3.66499400	-1.42145600	1.52175700
H	2.94454200	-1.96299900	-2.59047400
C	3.84173400	3.02960300	1.81866900
N	4.86875800	2.32833100	1.23218600
C	2.69541300	2.42373100	1.39701200
H	5.85746400	2.52788400	1.33486100
C	4.34810600	1.33613300	0.49491400
N	3.02094600	1.36148600	0.57216400
H	1.67059000	2.66992700	1.62837800
H	4.93880200	0.63027700	-0.07154600
C	-0.73793700	3.51385000	-1.22998100
N	-1.52591000	2.78582900	-0.37254200
C	0.44265500	2.83113300	-1.31277400
H	-2.49730700	2.98035900	-0.14112700
C	-0.83485500	1.70857000	0.03910300
N	0.36836500	1.69989200	-0.52340600
H	1.33115200	3.08292600	-1.87417700
H	-1.22230700	0.96314200	0.72406800
Fe	1.74531400	0.22259100	-0.44157900
H	-1.07363400	4.43189800	-1.68799700
H	4.01484600	3.87330600	2.46902700
H	5.07109200	-3.64010000	0.64764300
O	0.24819600	-1.10913200	-1.03663200
O	0.30643000	-0.90570300	0.37967600

22. Cartesian coordinates of PC6 for double hydrogen abstraction from (C7,O7) pair of site of AA in presence of Fe-SOD

C	3.22259800	0.33603200	-1.29719400
C	4.33554200	0.93517700	-0.55366500
C	4.81601000	0.01092900	0.28453100
C	4.06055500	-1.26809500	0.09229600
O	3.11605200	-0.97911500	-0.93373400
O	4.70027800	2.22780400	-0.63807300
O	5.74748500	0.04993000	1.23173500
O	2.48575300	0.85145900	-2.08628100
C	3.28297200	-1.69820700	1.35376300
C	2.50076600	-2.94115400	0.97197800
H	3.03356500	-3.90165400	1.06154200
H	6.24200300	0.88235300	1.21684600
H	4.61688800	2.55249300	-1.54427800
H	4.72446100	-2.07254300	-0.24072600
O	1.38296200	-2.89099800	0.52902000
O	2.38647000	-0.68225500	1.76541200
H	0.59705800	-0.44758300	1.52058600
H	2.86204800	-0.01988800	2.28090700
C	-3.67357700	-3.33542500	-1.37706300
N	-2.60097500	-3.87420200	-0.70971200
C	-3.52229100	-1.98607100	-1.28144800
H	-2.41159300	-4.85939800	-0.59049600
C	-1.83957800	-2.87326600	-0.23854100
N	-2.37076200	-1.70604600	-0.56822300
H	-4.15553100	-1.20675200	-1.67487500
H	-0.93408800	-3.02322800	0.33022300
C	-5.31114500	1.95479900	0.63104700
N	-5.39853300	0.78449900	1.34588300
C	-4.07944600	1.93976800	0.05183000
H	-6.18792800	0.48889700	1.90351000
C	-4.25675900	0.09847400	1.18667000
N	-3.42542700	0.77340800	0.40825300
H	-3.62399200	2.67747000	-0.58869200
H	-4.06380200	-0.86528200	1.63110900
C	-0.38043400	4.11684100	0.42634400
N	0.38424400	3.74022600	-0.65302400
C	-1.15219100	3.03637800	0.72292800
H	1.05984000	4.31694200	-1.13336900
C	0.07436300	2.47612800	-0.98009300
N	-0.86393100	2.01597000	-0.16575400
H	-1.88630000	2.92173800	1.50360200
H	0.55884200	1.92545600	-1.77279100
Fe	-1.63661900	0.15564100	-0.24747800
H	-0.30642800	5.09360200	0.87408700
H	-6.11351000	2.67241700	0.59678700
H	-4.42561800	-3.94382700	-1.85058600
O	0.32590100	-0.51881400	-0.35935800
O	-0.18170500	-0.66473100	0.96074900
H	3.99847000	-1.94207100	2.14579200
H	0.72551500	-1.39288600	-0.55278900

23. Cartesian coordinates of TS1 for double hydrogen abstraction from (O3,O4) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	0.14259100	1.98097900	-0.16123900
C	1.17045200	0.90132900	-0.11258500
C	0.53941300	-0.28739800	-0.50706000
C	-0.89507300	0.02808800	-0.82518700
O	-1.03910300	1.42999400	-0.58613200
O	2.38022400	1.14402200	0.22699700
O	0.96542000	-1.48511700	-0.59797900
O	0.25785100	3.12957700	0.11664600
C	-1.88315200	-0.73338600	0.05845700
C	-3.32225400	-0.56806300	-0.41213400
H	-3.44257300	-0.97592400	-1.41798800
H	2.08581600	-1.66929700	-0.56157800
H	2.94942800	0.24476400	0.58961100
H	-1.09787700	-0.17182400	-1.88286600
O	-4.19683200	-1.28276600	0.42560100
O	-1.75951700	-0.31762900	1.40433600
H	-3.93779400	-1.11349900	1.33981200
H	-1.88767000	0.63983700	1.44774000
H	-1.61405600	-1.79289700	0.04502000
H	-3.57943800	0.50079200	-0.44193200
O	3.58148600	-0.75361000	0.99186100
O	3.31360700	-1.89639500	-0.50107000
H	4.52628400	-0.59453700	0.85108000
H	3.46092800	-2.74131000	-0.05248300

24. Cartesian coordinates of TS2 for double hydrogen abstraction from (C6,O6) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	2.08893200	-1.05826800	-0.25335600
C	2.08466500	0.38426100	0.02376100
C	0.99972700	0.66197900	0.73767500
C	0.19944400	-0.59041400	0.94380400
O	0.99824500	-1.60999400	0.32511200
O	3.05316800	1.21400200	-0.40611900
O	0.55620800	1.85023200	1.21618500
O	2.91892500	-1.66003000	-0.87034300
C	-1.18129400	-0.55541300	0.25567300
C	-1.97853600	-1.85538800	0.43348300
H	-2.21502600	-2.03890600	1.48320500
H	1.19112300	2.54603400	1.00132300
H	3.69712900	0.69724300	-0.91142700
H	0.09423800	-0.84474300	2.00313400
O	-3.18353300	-1.77262200	-0.27461400
O	-1.17879900	-0.11344500	-0.97928100
H	-2.96361600	-1.37493900	-1.12817800
H	-1.37893400	1.31223200	-1.30752300
H	-1.80494800	0.25943800	0.94399200
H	-1.35126400	-2.67903100	0.06409200
O	-2.08088600	1.71852400	0.41651900
O	-1.67241100	2.32979500	-1.20612300
H	-1.27643500	2.11062400	0.81599000
H	-2.55723500	2.43979000	-1.58154100

25. Cartesian coordinates of TS3 for double hydrogen abstraction from (C5,C6) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	-1.99288800	-0.87793400	-0.59204100
C	-2.12238300	0.37678200	0.16064300
C	-0.93476600	0.99438700	0.10869900
C	0.02402900	0.14469500	-0.59050100
O	-0.72586100	-0.97543800	-1.05720300
O	-3.26986400	0.75540300	0.75995200
O	-0.49124900	2.16241900	0.64116400
O	-2.86522000	-1.68265700	-0.78136700
C	1.09866000	-0.35085000	0.43382900
C	2.00217900	-1.37518800	-0.25247200
H	2.60262000	-0.95274000	-1.07061100
H	-1.21391800	2.63720700	1.06957800
H	-3.92974200	0.06432700	0.60169100
H	1.05602900	1.07314900	-1.20581700
O	2.95386200	-1.88258300	0.65449000
O	0.48170800	-1.10882500	1.46808300
H	2.45715200	-2.28359500	1.37770800
H	0.14049800	-0.53124200	2.15707400
H	1.90199500	0.85594600	0.44001000
H	1.39356700	-2.18130400	-0.68194800
O	2.40000800	1.77194000	0.12532200
O	1.91179300	1.56315400	-1.45507900
H	1.64729700	2.33531100	0.41290700
H	2.33410700	0.68428000	-1.55241100

26. Cartesian coordinates of TS4 for double hydrogen abstraction from (O6,O7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	-2.48002300	-0.88397600	-0.21167100
C	-2.43559300	0.47040900	0.33786800
C	-1.34165000	1.07817100	-0.12551500
C	-0.59500600	0.11636200	-1.01598700
O	-1.38279800	-1.06882500	-1.00178700
O	-3.38193000	0.95916900	1.16476200
O	-0.85495900	2.30222100	0.07305800
O	-3.31273200	-1.71943800	-0.01555100
C	0.80527200	-0.14216400	-0.51487000
C	1.04892200	-1.26244300	0.28465300
H	0.22577300	-1.95403400	0.44192300
H	-1.40886700	2.78548300	0.69950300
H	-4.04773900	0.27289300	1.31278900
O	2.17339600	-1.58391500	0.83242900
O	1.63688900	0.77930600	-0.86468500
H	2.90550100	-0.79099300	1.04870200
H	2.70832200	0.64645300	-0.73139700
O	4.01045300	0.52684700	-0.63970400
H	4.31402300	-0.36193900	-0.87119100
H	-0.52719700	0.49751700	-2.03919900
O	3.75864300	0.14213400	1.20946800
H	4.64295300	-0.05352900	1.54807600

27. Cartesian coordinates of TS5 for double hydrogen abstraction from (C6,C7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	-2.14264600	-0.88487600	-0.55592500
C	-2.30042300	0.43706600	0.07023800
C	-1.12116600	1.04838700	0.03129500
C	-0.09846600	0.12655300	-0.55456200
O	-0.86017300	-1.02192900	-0.95474800
O	-3.48119000	0.88307000	0.54178600
O	-0.74701800	2.28189900	0.44624000
O	-3.00768900	-1.69855900	-0.71236200
C	0.99095500	-0.26304600	0.44699200
C	1.96129700	-1.30145300	-0.15843500
H	2.66321700	-0.46442800	-0.98035600
H	-1.52397100	2.76420100	0.75718400
H	-4.14454900	0.19278700	0.39721500
H	0.35018500	0.55969900	-1.45799700
O	2.88277900	-1.70637800	0.83459200
O	0.41846700	-0.89444100	1.58467900
H	2.36286500	-1.95365400	1.60817200
H	0.11220400	-0.23435500	2.21468100
H	1.83271200	0.82009900	0.52151400
H	1.38734100	-2.15317400	-0.54424000
O	2.77489200	1.64830200	0.05193000
O	3.07685200	0.76588100	-1.27790800
H	2.31171000	2.42461500	-0.31854300
H	2.45562900	1.00567500	-1.98891700

28. Cartesian coordinates of TS6 for double hydrogen abstraction from (C7,O7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	1.42984800	1.06686100	-0.43755000
C	2.20732500	-0.08620700	0.00091400
C	1.47188500	-1.17888000	-0.21663000
C	0.16045800	-0.77893100	-0.82480500
O	0.27424700	0.63459200	-0.99782300
O	3.42289900	0.00850600	0.57764900
O	1.69208500	-2.46599800	0.05537900
O	1.70618100	2.23100100	-0.30946600
C	-1.01827000	-1.10494700	0.07880600
C	-2.39276300	-0.72740900	-0.47233000
H	-2.58607800	-1.18660600	-1.45060200
H	2.52622600	-2.57345600	0.53019800
H	3.66495000	0.94182800	0.65000700
H	0.00800400	-1.23741900	-1.80632400
O	-3.35506300	-0.83247700	0.45364200
O	-0.83866300	-0.48554800	1.33091400
H	-3.38495000	0.47870600	0.04847300
H	-1.69920400	-0.58471000	1.77554800
H	-1.03916000	-2.19854500	0.18988700
H	-0.33135200	2.81790700	0.43273900
O	-2.55946100	0.76802100	-0.71086000
O	-1.06157700	2.32128200	0.82310400
H	-1.88467400	1.35795600	-0.26482700
H	-0.66985300	1.60638900	1.34416300

29. Cartesian coordinates of PC1 for double hydrogen abstraction from (O3,O4) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	0.99942700	-0.97987300	-0.38946300
C	1.29971900	0.48898500	-0.73642100
C	0.16340200	1.28026200	-0.08892600
C	-0.74015000	0.24838400	0.57116800
O	-0.18095000	-1.04469600	0.24788600
O	2.21055400	0.87557400	-1.39685200
O	0.00202000	2.46031400	-0.10363600
O	1.65972800	-1.93317800	-0.66127600
C	-2.15924400	0.31195100	0.02452600
C	-3.13073900	-0.58668800	0.77504400
H	-3.17398500	-0.30403500	1.82894400
H	2.03195700	1.18214200	2.30306400
H	4.19598200	-0.09119900	-0.31104700
H	-0.70434000	0.36550600	1.65614900
O	-4.43063800	-0.44442700	0.25839500
O	-2.15844100	-0.00952600	-1.35697600
H	-4.38137200	-0.47584500	-0.70480200
H	-1.85433200	-0.92076200	-1.46263900
H	-2.50154400	1.34846500	0.08648200
H	-2.78810100	-1.63014800	0.71584800
O	4.02575500	-0.65452300	0.45158900
O	1.88715100	0.42311200	1.73160900
H	3.69774900	-1.48928800	0.09572500
H	2.76205600	0.05583600	1.49078800

30. Cartesian coordinates of PC2 for double hydrogen abstraction from (C6,O6) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	2.32507200	-0.56313700	-0.32138500
C	1.63250400	0.64927400	0.12171700
C	0.62207400	0.29829600	0.92717400
C	0.53058700	-1.21346300	0.87875900
O	1.69597600	-1.64824200	0.21602900
O	2.05445100	1.87752900	-0.26013300
O	-0.27969000	0.98327500	1.61022200
O	3.30583400	-0.61930600	-1.00272600
C	-0.70404000	-1.53425200	0.03194100
C	-2.06837600	-1.35322100	0.67470400
H	-2.07023600	-0.48212500	1.33125900
H	-0.40169300	1.88071000	1.17593200
H	2.88014900	1.77067400	-0.75469200
H	0.47058200	-1.66586000	1.87278900
O	-3.04360900	-1.16337200	-0.32568800
O	-0.61854900	-1.84913300	-1.12326400
H	-2.78102200	-1.68478000	-1.09844800
H	0.19245900	2.97176500	-0.54717400
H	-2.95720500	0.62188600	-0.78438400
H	-2.28631100	-2.24207800	1.28245400
O	-2.77403800	1.56234900	-0.95449600
O	-0.60597000	2.93035800	-0.00830800
H	-3.61693300	2.01269400	-1.04637300
H	-1.33196000	2.52846000	-0.52191200

31. Cartesian coordinates of PC3 for double hydrogen abstraction from (C5,C6) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	1.59006000	1.43922000	0.29915500
C	2.51417700	0.35628100	-0.02898900
C	1.81010400	-0.78593400	-0.06402200
C	0.43200000	-0.47866000	0.25344500
O	0.33587400	0.89170200	0.46030400
O	3.82759400	0.53736000	-0.25476800
O	2.17800800	-2.05604100	-0.32410000
O	1.82382800	2.60572800	0.40655200
C	-0.62502100	-1.29429300	0.34708500
C	-2.01626200	-0.85648300	0.67801500
H	-2.05953200	0.18945800	0.97495400
H	3.12363100	-2.11410000	-0.50815000
H	4.03628600	1.47842000	-0.17245700
H	-2.14301200	0.66798100	-1.44406600
O	-2.85135600	-0.98804700	-0.46902200
O	-0.56356700	-2.62294200	0.09591500
H	-2.87897700	-1.91295000	-0.73991100
H	0.32544600	-2.90181300	-0.16637900
H	-4.38777500	0.60842400	0.13164600
H	-2.39481200	-1.47139600	1.50069500
O	-4.14420100	1.46110900	0.50535300
O	-1.99874600	1.61963300	-1.35683400
H	-3.52675000	1.84612500	-0.13450400
H	-1.18432500	1.74104600	-0.85716900

32. Cartesian coordinates of PC4 for double hydrogen abstraction from (O6,O7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	1.27442800	-1.63902100	-0.15171800
C	1.49496200	-0.21822500	0.08820100
C	0.57805800	0.22834900	0.96457000
C	-0.37104100	-0.91756000	1.23916800
O	0.17732800	-2.04314500	0.56965100
O	2.53658200	0.42837600	-0.48768300
O	0.35079200	1.38836300	1.53243800
O	1.91852300	-2.37119800	-0.84279200
C	-1.70543700	-0.56519400	0.59492900
C	-1.97070800	-1.17870300	-0.79704400
H	-2.10900600	-2.27004300	-0.85779300
H	0.79399300	2.11338300	0.99360100
H	3.05665600	-0.21785100	-0.98712700
O	-2.05188200	-0.47463400	-1.76582800
O	-2.49614100	0.19133800	1.07956600
H	-1.56654500	1.45165900	-1.53326500
H	1.99650700	2.48063700	-0.70421600
O	1.27080100	2.95199700	-0.27916700
H	0.47104300	2.83099000	-0.82307400
H	-0.49319600	-1.12039600	2.30482800
O	-1.22470900	2.19981000	-1.02602100
H	-1.80138800	2.30649300	-0.26291300

33. Cartesian coordinates of PC5 for double hydrogen abstraction from (C6,C7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	2.66465300	-0.60489700	0.31579000
C	2.21032900	0.76964400	0.03934400
C	0.91832000	0.84095200	0.33000300
C	0.43659000	-0.52276800	0.75243000
O	1.60931800	-1.34140200	0.71407500
O	3.04832100	1.72997900	-0.38924100
O	0.02606800	1.84291600	0.26963700
O	3.77380900	-1.02392600	0.18632400
C	-0.63879100	-1.03203000	-0.15173000
C	-1.85876900	-1.40415600	0.27122300
H	-4.04493900	0.17252800	1.13852100
H	0.43940500	2.64548900	-0.08087000
H	3.93489700	1.34915000	-0.47203100
H	0.06141500	-0.50745000	1.77331900
O	-2.84875600	-1.78461400	-0.55200500
O	-0.42064000	-1.11834300	-1.50586100
H	-2.56215100	-1.74251800	-1.46710800
H	0.16563200	-0.41409100	-1.81421100
H	-1.94439100	0.87523000	-1.16126900
H	-2.13236700	-1.45499100	1.32831000
O	-2.44277100	1.60328000	-1.54663500
O	-4.04652800	1.03741200	1.56311400
H	-2.43659500	2.27650100	-0.84982500
H	-3.46547200	0.95726800	2.34754300

34. Cartesian coordinates of PC6 for double hydrogen abstraction from (C7,O7) pair of site of AA by H_2O_2 in absence of Fe-SOD

C	0.89791300	1.21006800	-0.44097500
C	2.05010400	0.47972700	0.06839800
C	1.83000400	-0.81970700	-0.14079600
C	0.49771300	-0.99410400	-0.79725500
O	0.01341300	0.34152400	-0.97410700
O	3.11096400	1.07338900	0.65229600
O	2.54714700	-1.90336900	0.16094700
O	0.72777800	2.40495200	-0.41078800
C	-0.48484100	-1.77499700	0.09838500
C	-1.76729800	-2.01642500	-0.68220800
H	-1.62728900	-2.52449000	-1.65880600
H	3.32590600	-1.65958100	0.67774900
H	2.92974700	2.01897800	0.74061500
H	0.59283800	-1.45846400	-1.78410300
O	-2.86162300	-1.70898800	-0.30584000
O	-0.64622300	-1.18340200	1.32906200
H	-3.22804800	0.21381900	0.76460000
H	-1.30861300	-0.44918200	1.29447200
H	-0.02863900	-2.76692000	0.24065100
H	-1.06685500	2.94611700	-0.48085300
O	-2.51796400	0.71597100	1.17636200
O	-2.01397300	2.98175100	-0.27379200
H	-2.39759300	1.54114300	0.66994900
H	-2.20917000	3.85659600	0.06931400