Ab-initio calculations on $^1O_2$ quenching mechanism by *trans*-resveratrol

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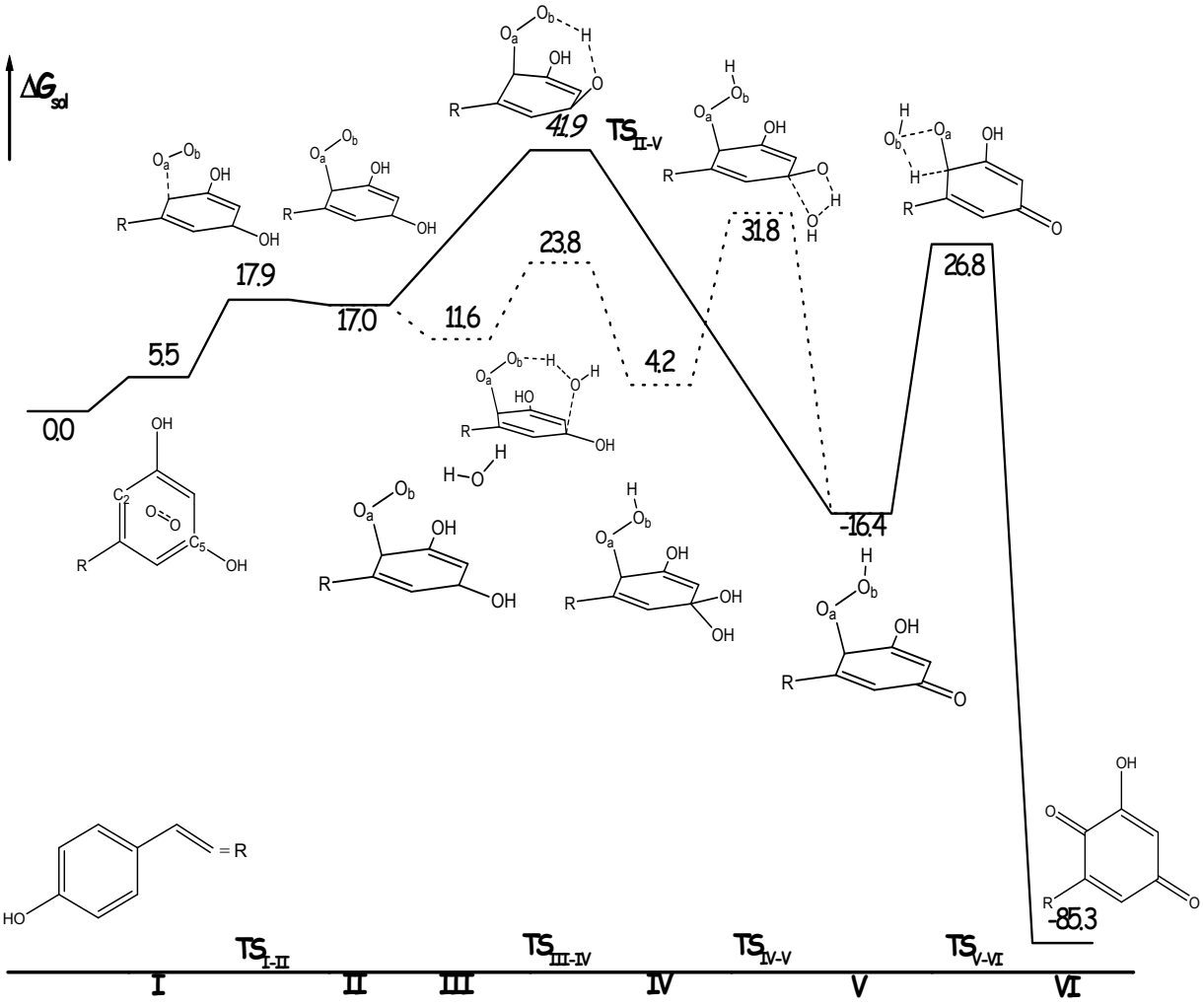
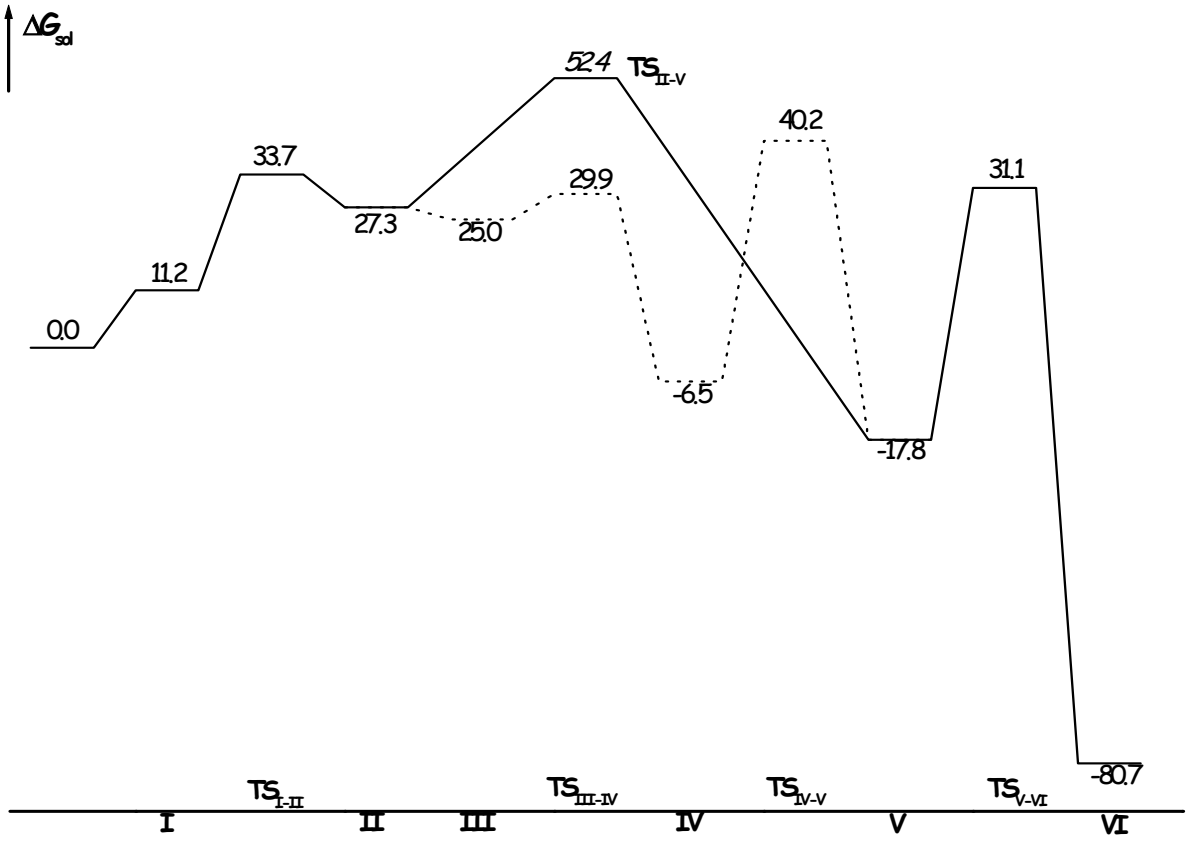
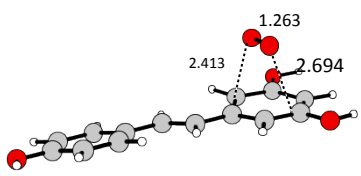
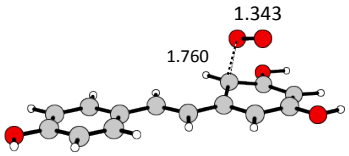
Supplementary Information


ΔG_sol
0.0
5.5
17.9
17.0
11.6
23.8
4.2
41.9
TS_II-V
31.8
-16.4
26.8
-85.3
TS_I-II
TS_III-IV
TS_IV-V
TS_V-VI
I
II
III
IV
V
VI

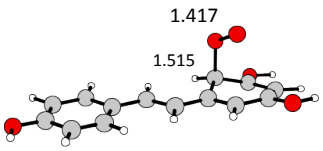

ΔG_sol
52.4
TS_II-V
40.2
33.7
29.9
31.1
27.3
25.0
11.2
0.0
-6.5
-17.8
-80.7
TS_I-II
TS_III-IV
TS_IV-V
TS_V-VI
I
II
III
IV
V
VI



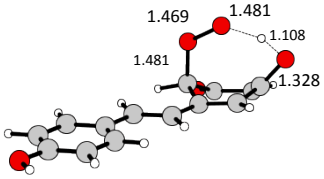
I



TS_{I-II}

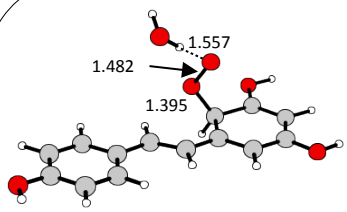


II

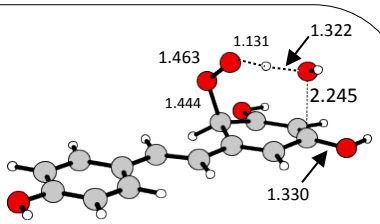


TS_{II-V}

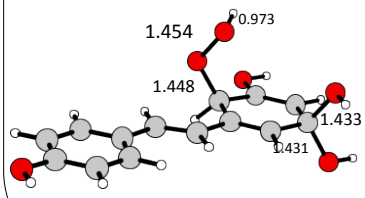
Pathway (a)



III



TS_{III-IV}



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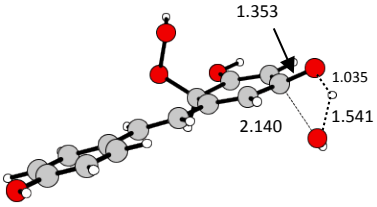
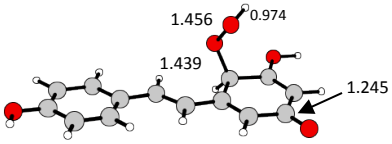
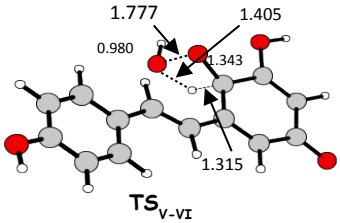


TS_{IV-V}

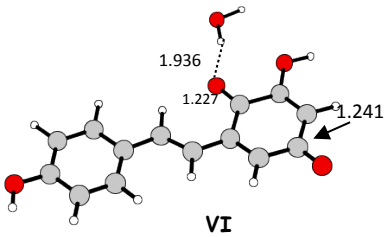
Pathway (b)



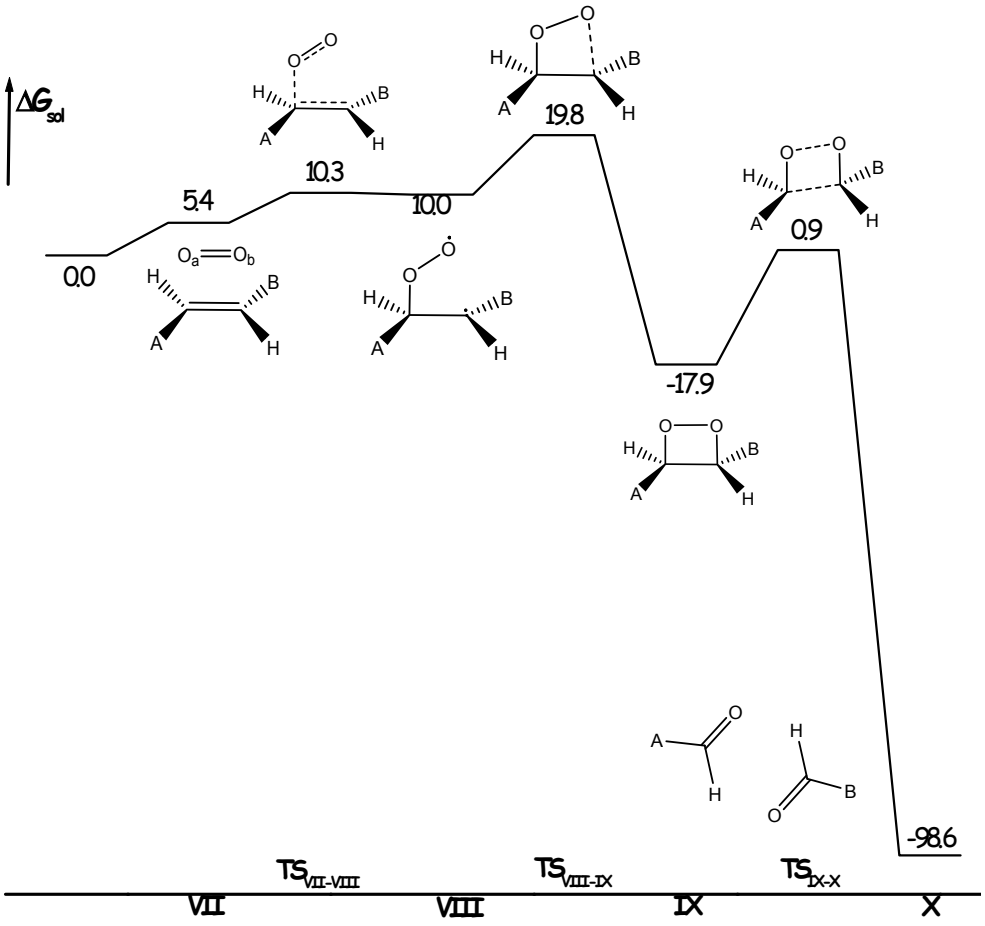
V

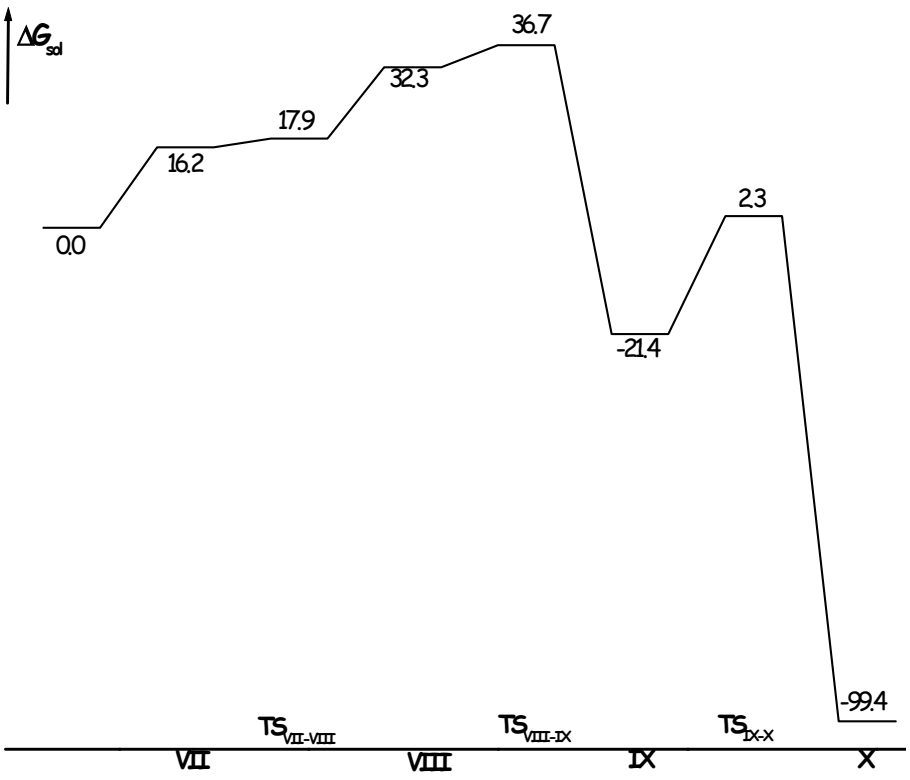


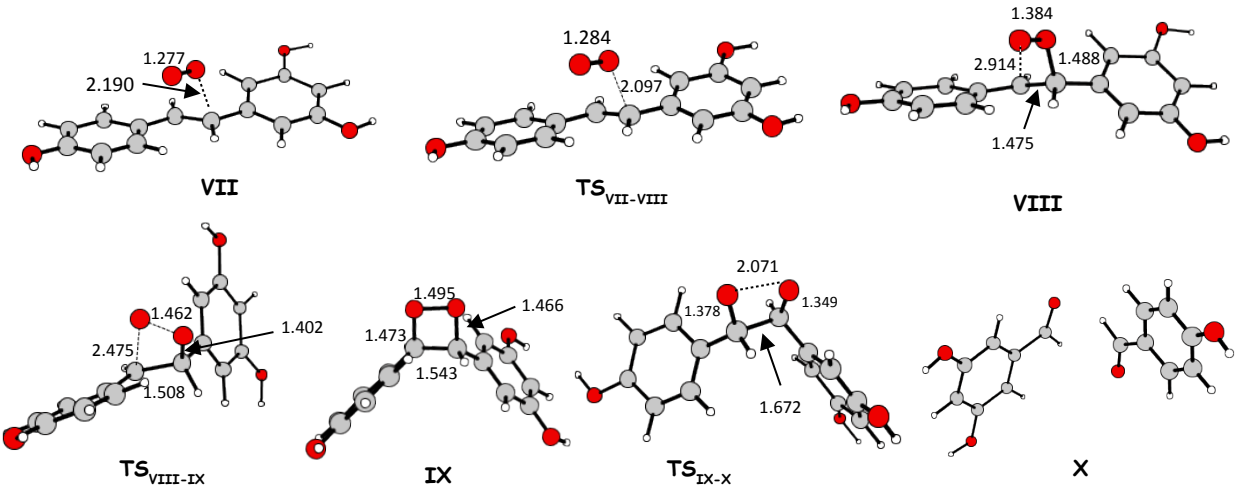
TS_{V-VI}



VI


ΔG sol
0.0
5.4
10.3
10.0
19.8
-17.9
0.9
-98.6
TS VII-VIII
TS VIII-IX
TS IX-X
VII
VIII
IX
X


ΔG_sol
0.0
16.2
17.9
32.3
36.7
-21.4
2.3
-99.4
TS_VII-VIII
TS_VIII-IX
TS_IX-X
VII
VIII
IX
X


1.277
2.190
VII
1.284
2.097
TS$_{VII-VIII}$
1.384
2.914
1.488
1.475
VIII
1.462
2.475
1.402
1.508
TS$_{VIII-IX}$
1.495
1.466
1.473
1.543
IX
2.071
1.378
1.349
1.672
TS$_{IX-X}$
X