Electronic Supplementary Material for

The mechanism of oxidation in chromophore maturation of wild-type green fluorescent protein: a theoretical study

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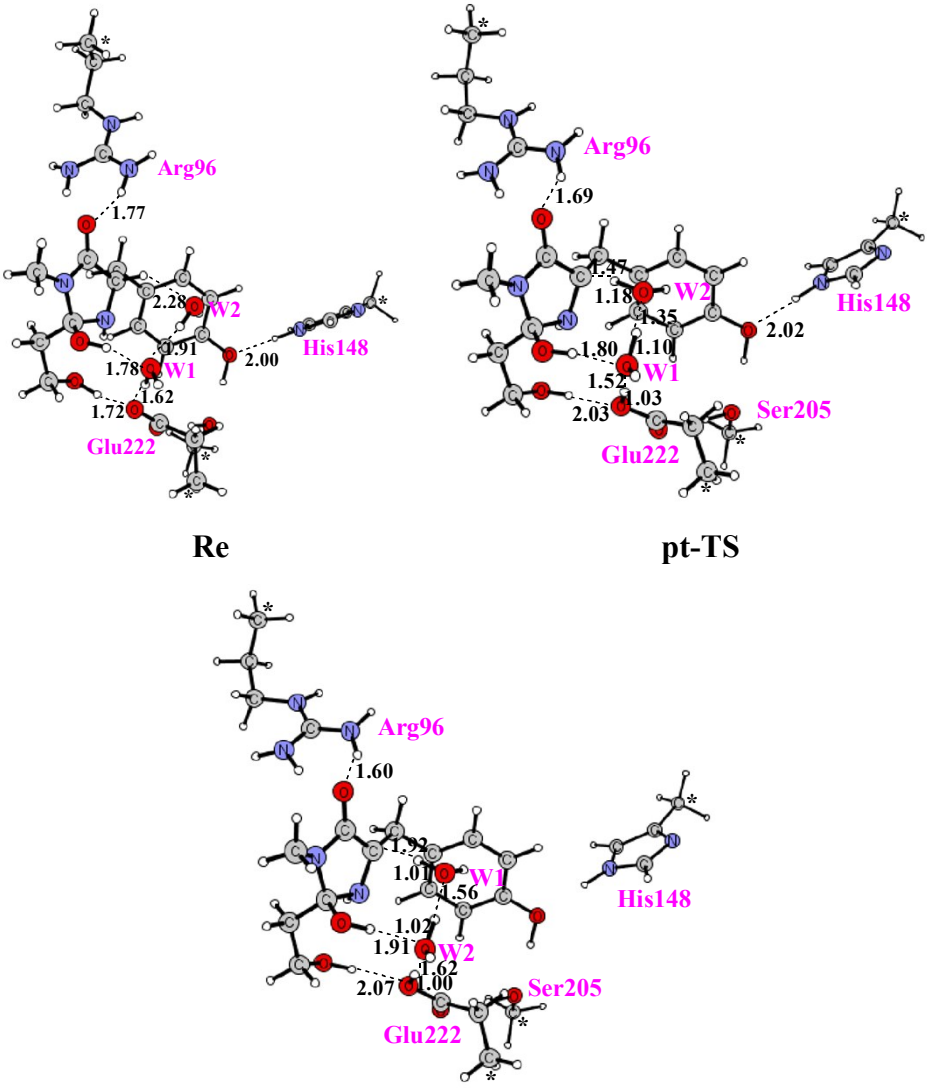


Figure S1. Optimized geometries of the reactant, transition state and product of the model system in the step of deprotonation of the Tyr66 α-carbon.

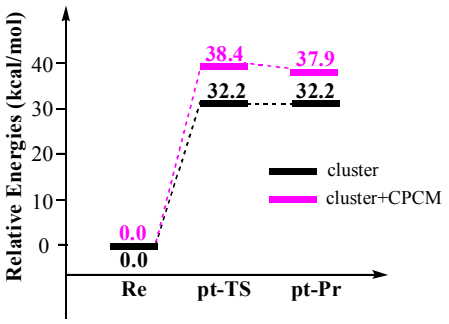
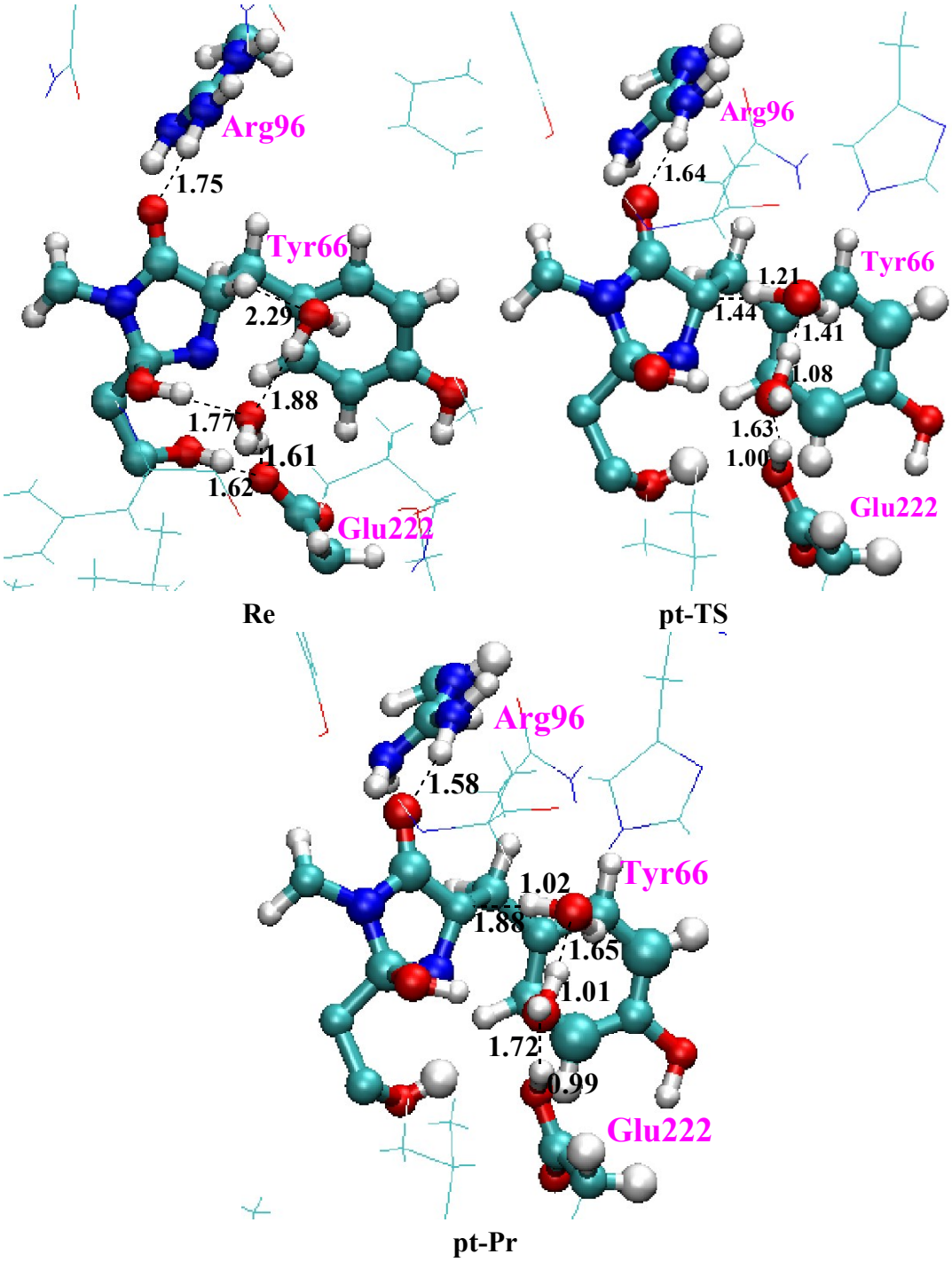


Figure S2. The potential energy profile of the model system in the step of deprotonation of the Tyr66 α-carbon. Digits in black are the energies of the B3LYP/6-311+G(2d,2p) level with zero-point correction, digits in red are the energies of cpcm (ε=4).


Arg96
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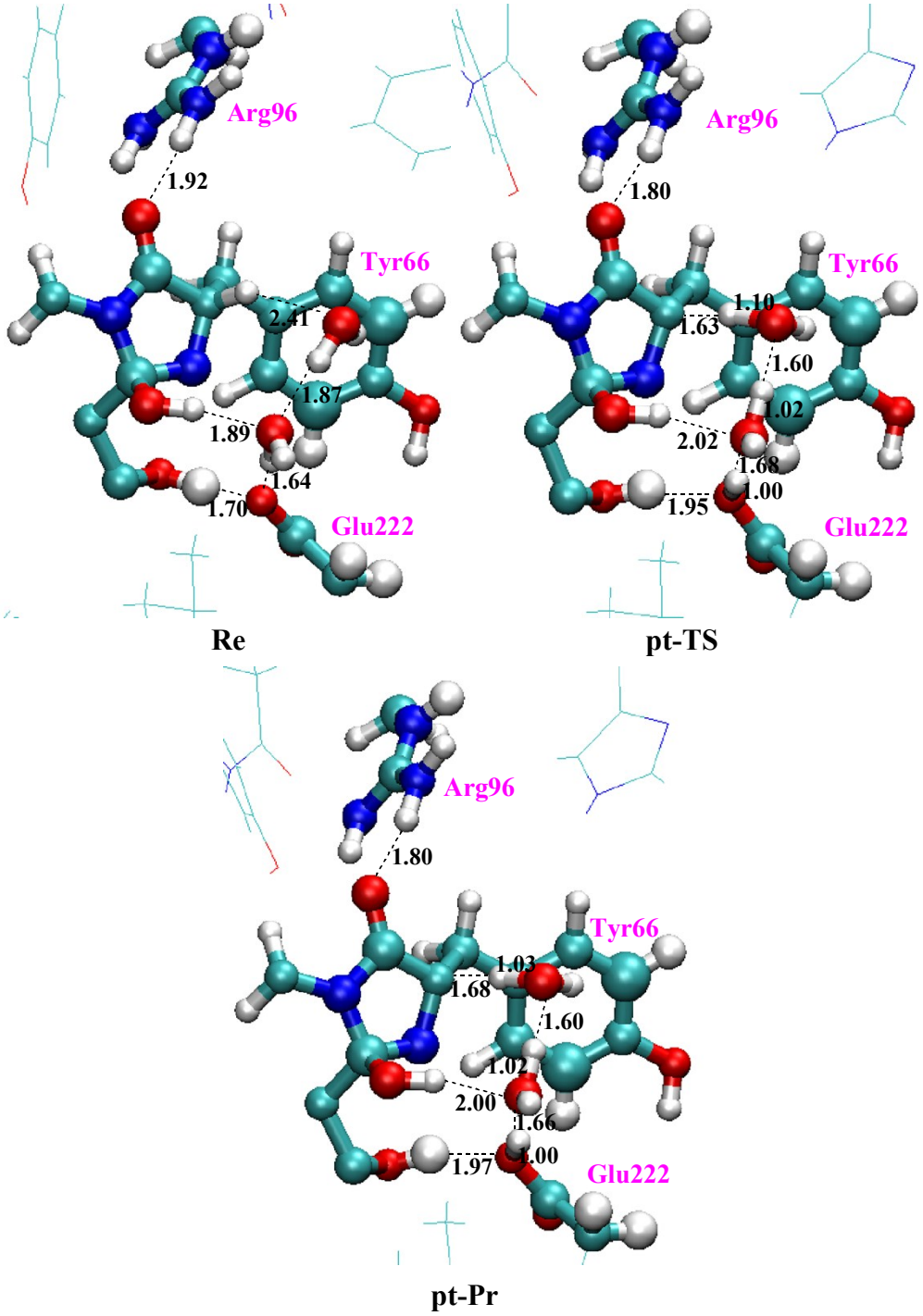
Tyr66
2.29
1.88
1.77
1.61
1.62
Glu222
Re
Arg96
1.64
Tyr66
1.21
1.44
1.41
1.08
1.63
1.00
Glu222
pt-TS
Arg96
1.58
Tyr66
1.02
1.88
1.65
1.01
1.72
0.99
Glu222
pt-Pr

(a)



(b)

Figure S3. Optimized geometries of the reactant, transition state and product of large protein system by ONIOM-ME (a) and ONIOM-EE (b) respectively in the step of deprotonation of the Tyr66 α-carbon. For the sake of clarity, some atoms are omitted.

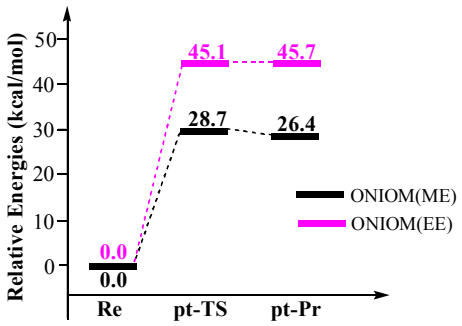


Figure S4. Potential energy profile of large protein system in the step of deprotonation of the Tyr66 α-carbon, energies of ONIOM(b3lyp/6-31G(d,p):Amber) corresponding to geometries optimized by mechanical embedding and electronic embedding respectively.