

Supporting Information

**A new understanding towards reactivity of DNA peroxy
radical**

Shuang Zhao, Ru-bo Zhang * and Ze-sheng Li

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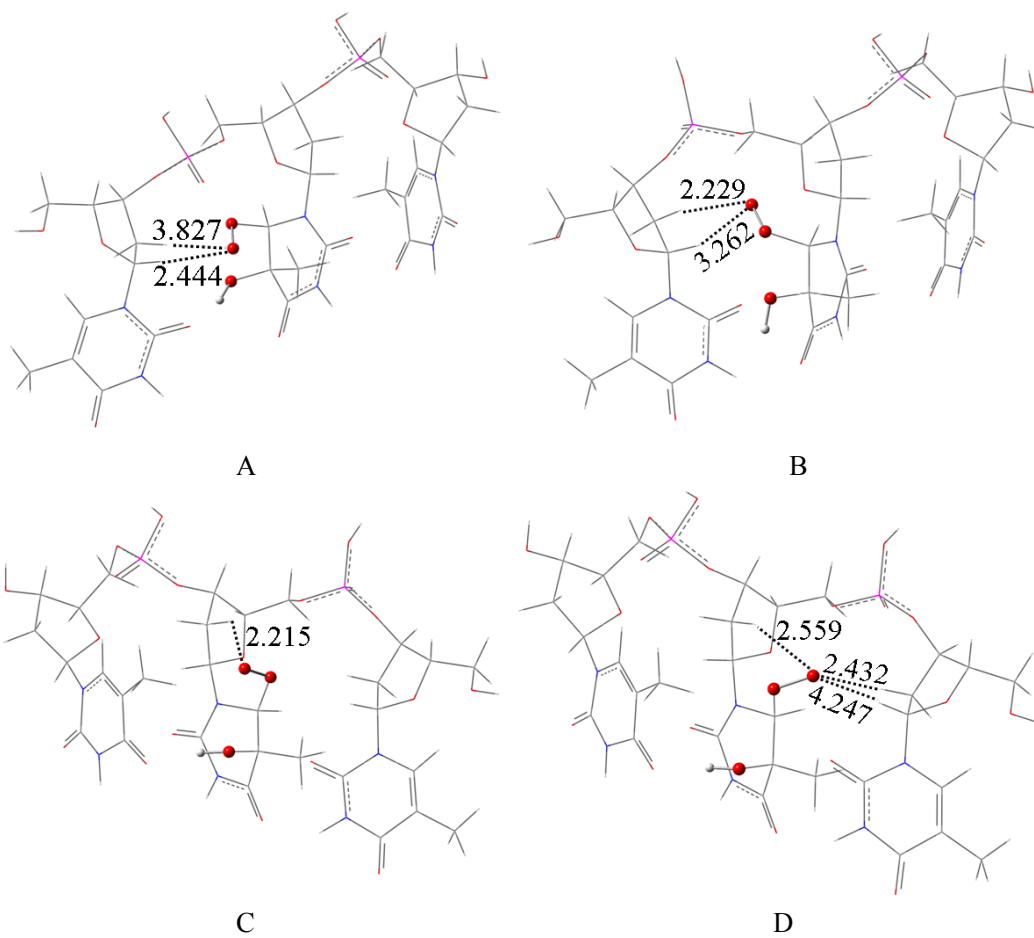
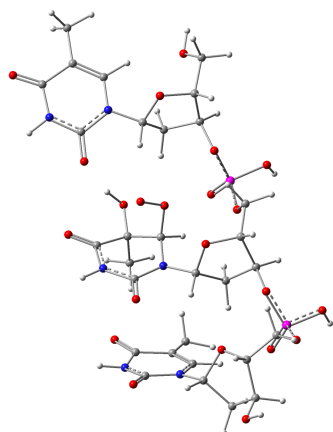
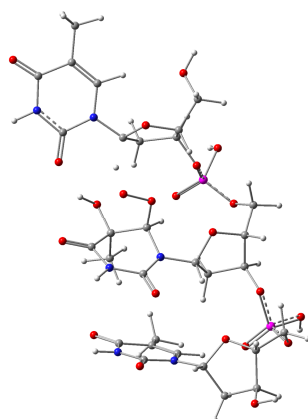


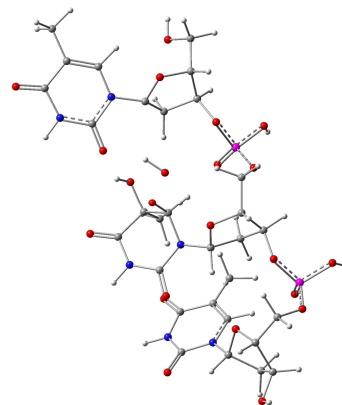
Fig. S1 The optimized models A - D using the M06-2X/6-31G(d,p) method.



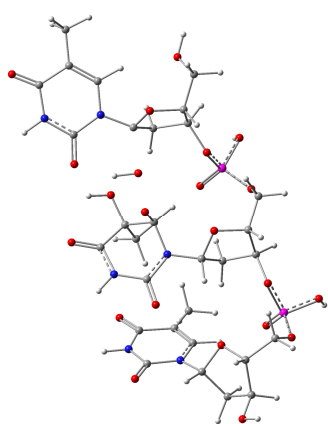
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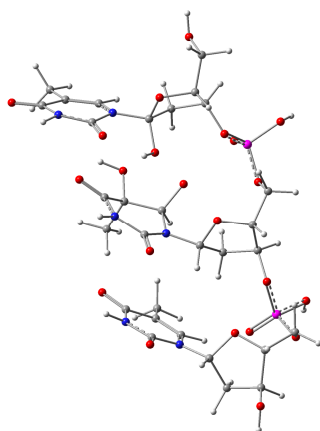
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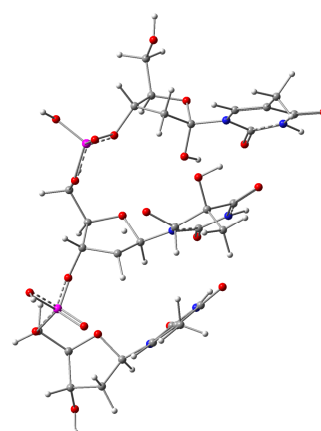
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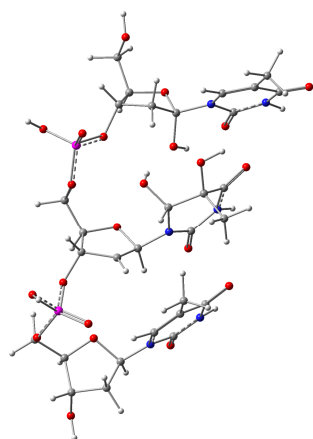
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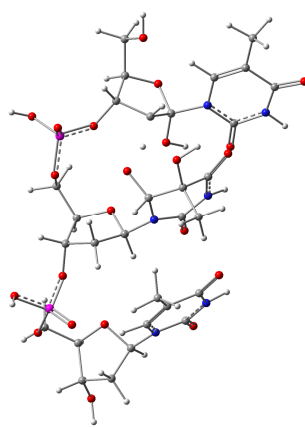
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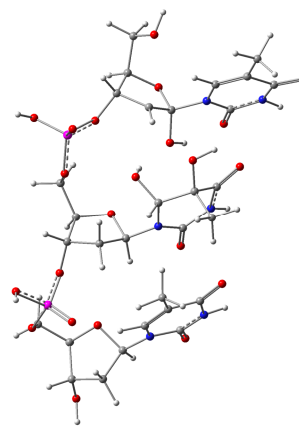
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A-I3



A-TS4



A-I4

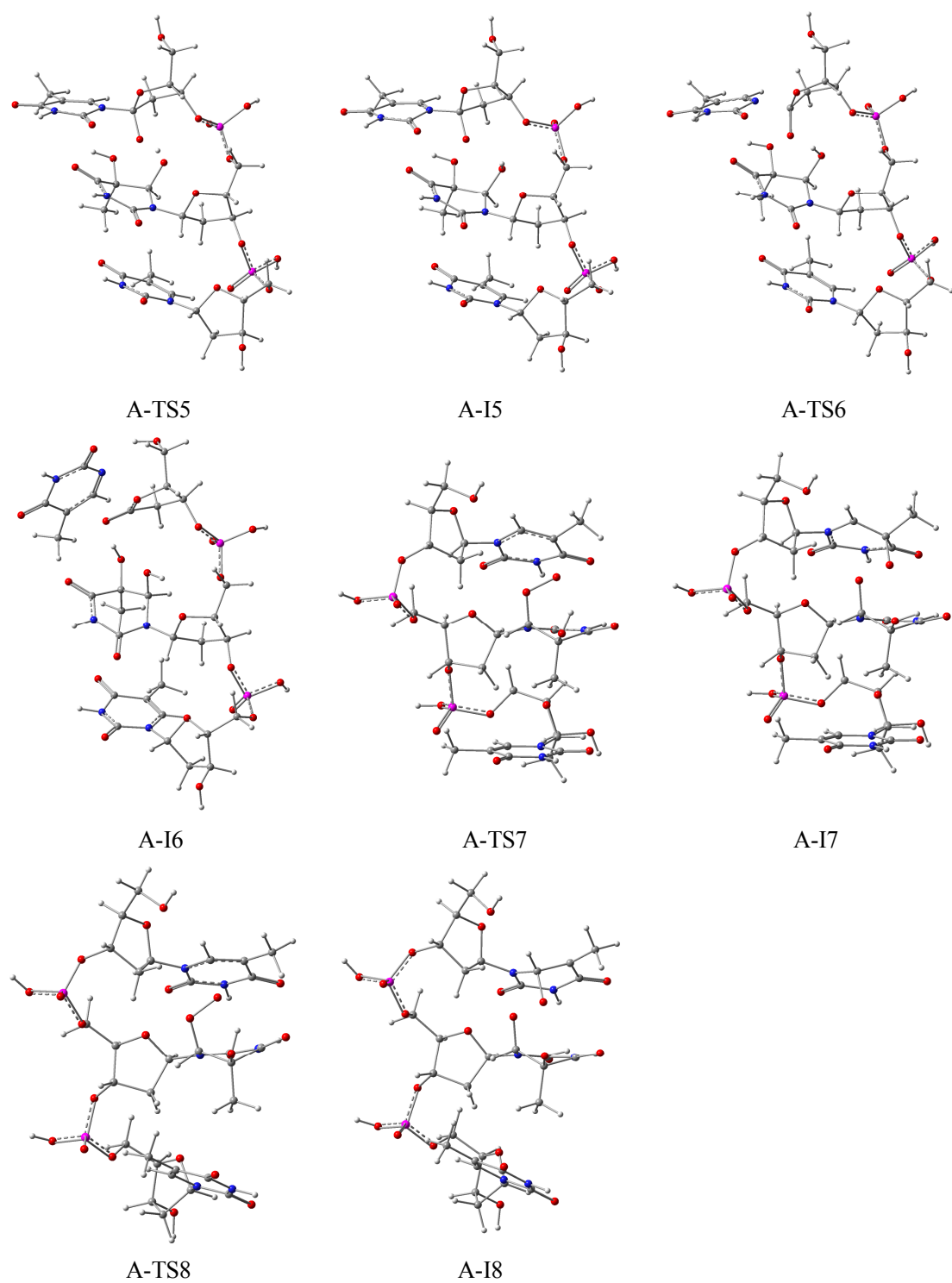


Fig. S2 The optimized structures of all the stationary points and the transition states which relevant to the thymine C6-peroxyl radical reactions at the M06-2X/6-31+G(d,p)// M06-2X/6-31G(d,p) method.

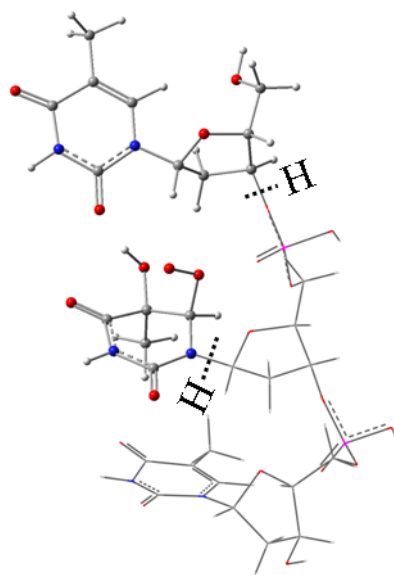
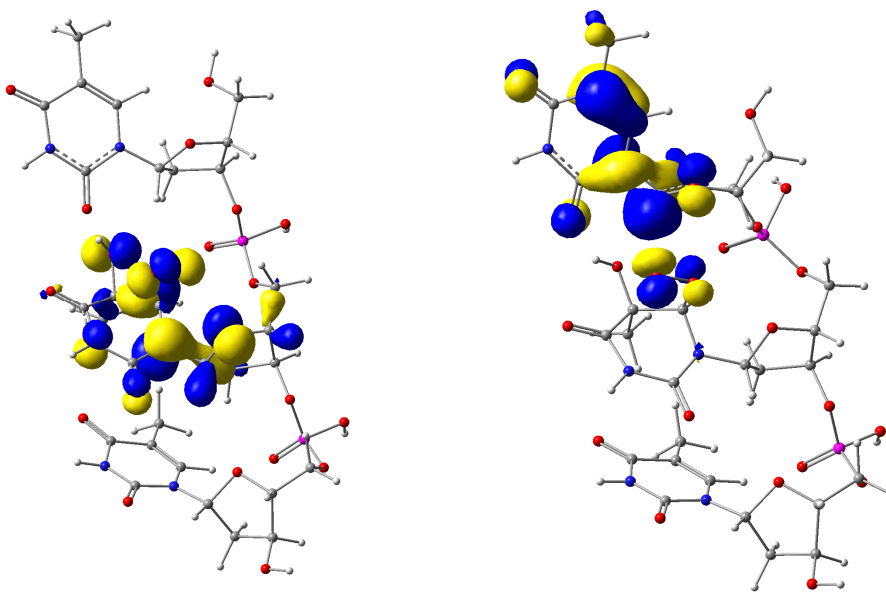


Fig. S3 The regions diagram of the modified (dT)₃ model with ONIOM method, in which the reactive region is described by the Ball & Bond type and the remaining atoms are described by the wireframe as the low region.



A

A-TS1

Fig. S4 The single occupancy molecular orbitals (SOMOs) of the reactant and H1'-abstraction transition state.

Table S1 The $\langle S^2 \rangle$ values of each structures.

structures	$\langle S^2 \rangle$	structures	$\langle S^2 \rangle$	structures	$\langle S^2 \rangle$	structures	$\langle S^2 \rangle$
A	0.7540	A-TS3	0.7594	A-TS5	0.7593	A-TS7	0.7745
A-TS1	0.7595	A-I3	0.7550	A-I5	0.7539	A-I7	0.7561
A-I1	0.7539	A-TS4	0.7598	A-TS6	0.7784	A-TS8	0.7846
A-TS2	0.7874	A-I4	0.7549	A-I6	0.7733	A-I8	0.7596
A-I2	0.7539						

Table S2 The activation Gibbs free energies of H1' abstraction with different methods in the gas and in water solution.

Methods	ΔG^\ddagger (kcal/mol)	
	In the gas	In water solution
M06-2X/6-31+G(d,p)	22.6	21.0
B3LYP/6-31+G(d,p)	20.9	19.2
B3LYP/DZP++	20.0	18.3
ONIOM(MP2/6-31+G(d, p):M06-2X/6-31+G(d,p))	23.2	21.2
ONIOM(MP2/6-311++G(d, p):M06-2X/6-31+G(d,p))	23.1	21.0

The coordinates of all the stationary points and the transition states which relevant to the thymine C6-peroxyl radical reactions at the M06-2X/6-31+G(d,p)//M06-2X/6-31G(d,p) method in water solution.

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A-I7:

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