

Structural, Electronic, and Photophysical Properties of Thieno-Expanded Tricyclic Purine

Analogs: A Theoretical Study

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TABLE S1: Changes in Bond Lengths of ttA and ttG after Excitation (Å).

ttA				ttG			
Bond	S ₀	S ₁	S ₁ -S ₀	Bond	S ₀	S ₁	S ₁ -S ₀
n1-c2	1.323	1.352	0.029	n1-c2	1.358	1.375	0.017
c2-n3	1.309	1.289	-0.020	c2-n3	1.283	1.289	0.006
n3-c4	1.333	1.365	0.032	c2-n2	1.362	1.363	0.001
c4-c5	1.389	1.440	0.051	n3-c4	1.366	1.347	-0.019
c5-c6	1.398	1.395	-0.003	c4-c5	1.371	1.475	0.104
c6-n6	1.355	1.365	0.010	c5-c6	1.434	1.423	-0.011
n1-c6	1.323	1.322	-0.001	c6-o6	1.192	1.199	0.007
c4-c3t	1.429	1.374	-0.055	n1-c6	1.403	1.416	0.013
c2t-c3t	1.354	1.433	0.079	c4-c3t	1.422	1.382	-0.040
c2t-S1t	1.742	1.759	0.017	c2t-c3t	1.358	1.385	0.027
s1t-c5	1.767	1.798	0.031	c2t-S1t	1.733	1.789	0.056
c2t-n7	1.356	1.326	-0.03	s1t-c5	1.755	1.734	-0.021
n7-c8	1.297	1.31	0.013	c2t-n7	1.359	1.335	-0.024
c8-n9	1.351	1.372	0.021	n7-c8	1.296	1.306	0.010
c3t-n9	1.37	1.369	-0.001	c8-n9	1.352	1.357	0.005
				c3t-n9	1.373	1.376	0.003

TABLE S2: Changes in Bond Lengths of ttX and ttHX after Excitation (Å).

ttX				ttHX			
Bond	S ₀	S ₁	S ₁ -S ₀	Bond	S ₀	S ₁	S ₁ -S ₀
n1-c2	1.372	1.372	0.000	n1-c2	1.354	1.369	0.015
c2-n3	1.374	1.376	0.002	c2-n3	1.27	1.282	0.012
c2-o2	1.188	1.188	0.000	n3-c4	1.374	1.349	-0.025
n3-c4	1.374	1.375	0.001	c4-c5	1.37	1.475	0.105
c4-c5	1.358	1.454	0.096	c5-c6	1.44	1.427	-0.013
c5-c6	1.449	1.43	-0.019	c6-o6	1.191	1.198	0.007
c6-o6	1.188	1.198	0.010	n1-c6	1.397	1.405	0.008
n1-c6	1.394	1.402	0.008	c4-c3t	1.421	1.38	-0.041
c4-c3t	1.419	1.366	-0.053	c2t-c3t	1.359	1.392	0.033
c2t-c3t	1.361	1.408	0.047	c2t-S1t	1.733	1.787	0.054
c2t-S1t	1.726	1.786	0.060	s1t-c5	1.749	1.741	-0.008
s1t-c5	1.75	1.745	-0.005	c2t-n7	1.359	1.333	-0.026
c2t-n7	1.358	1.328	-0.030	n7-c8	1.295	1.309	0.014
n7-c8	1.293	1.307	0.014	c8-n9	1.353	1.355	0.002
c8-n9	1.355	1.363	0.008	c3t-n9	1.372	1.375	0.003
c3t-n9	1.378	1.382	0.004				

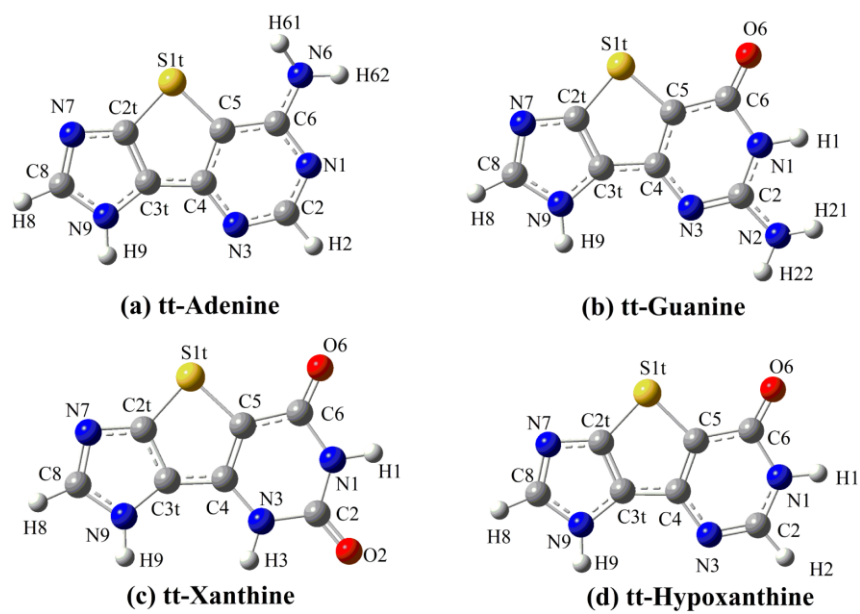


Figure S1. The B3LYP/6-311++G(d,p) optimized structures of thieno-expanded tricyclic nucleobase analogs: (a) tt-Adenine, (b) tt-Guanine, (c) tt-Xanthine, and (d) tt-Hypoxanthine.

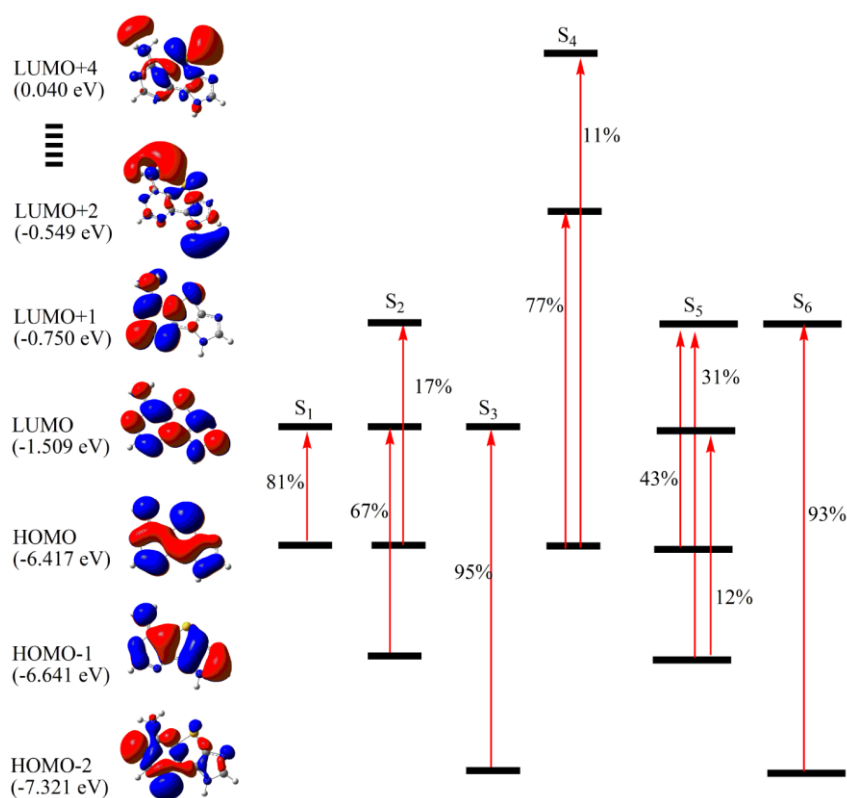


Figure S2. Molecular orbitals involved in the six lowest electronic singlet transitions of tTA calculated at the TD-B3LYP/6-311++G(d,p) level. Arrows indicate main contributions of the six lowest electronic singlet transitions and contributions larger than 10% are given. Orbital energies are given in parentheses.

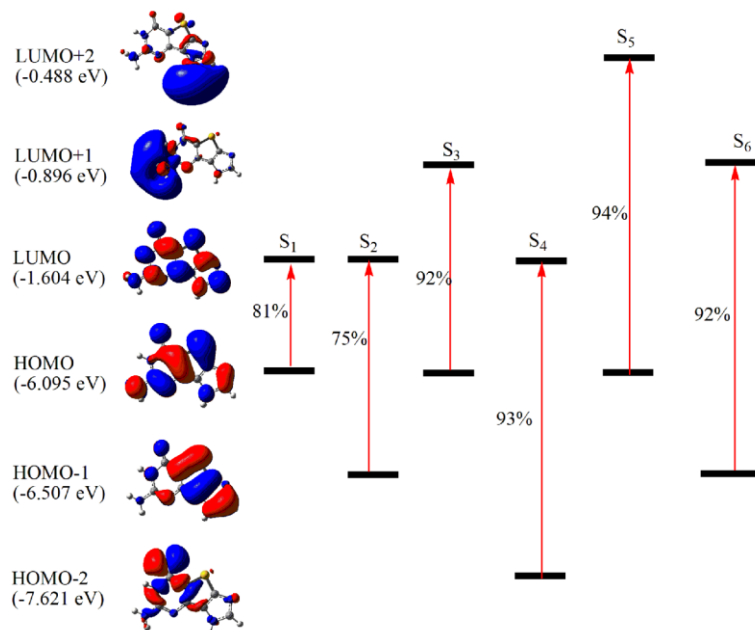


Figure S3. Molecular orbitals involved in the six lowest electronic singlet transitions of ttG calculated at the TD-B3LYP/6-311++G(d,p) level. Arrows indicate main contributions of the six lowest electronic singlet transitions and contributions larger than 10% are given. Orbital energies are given in parentheses.

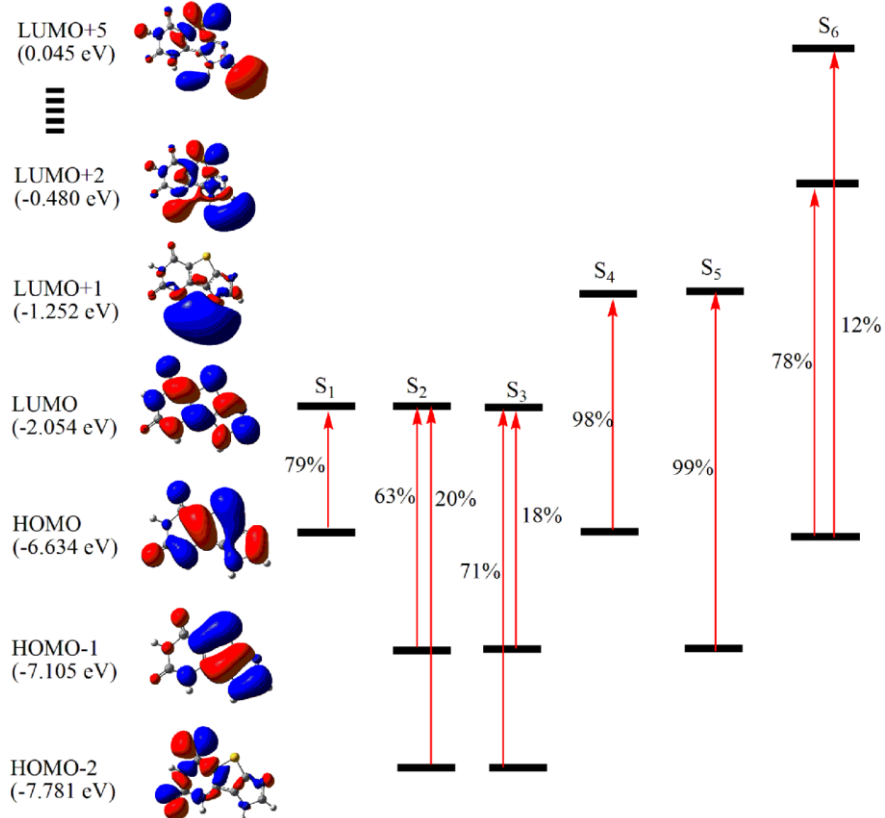


Figure S4. Molecular orbitals involved in the six lowest electronic singlet transitions of ttX calculated at the TD-B3LYP/6-311++G(d,p) level. Arrows indicate main contributions of the six lowest electronic singlet transitions and contributions larger than 10% are given. Orbital energies are given in parentheses.

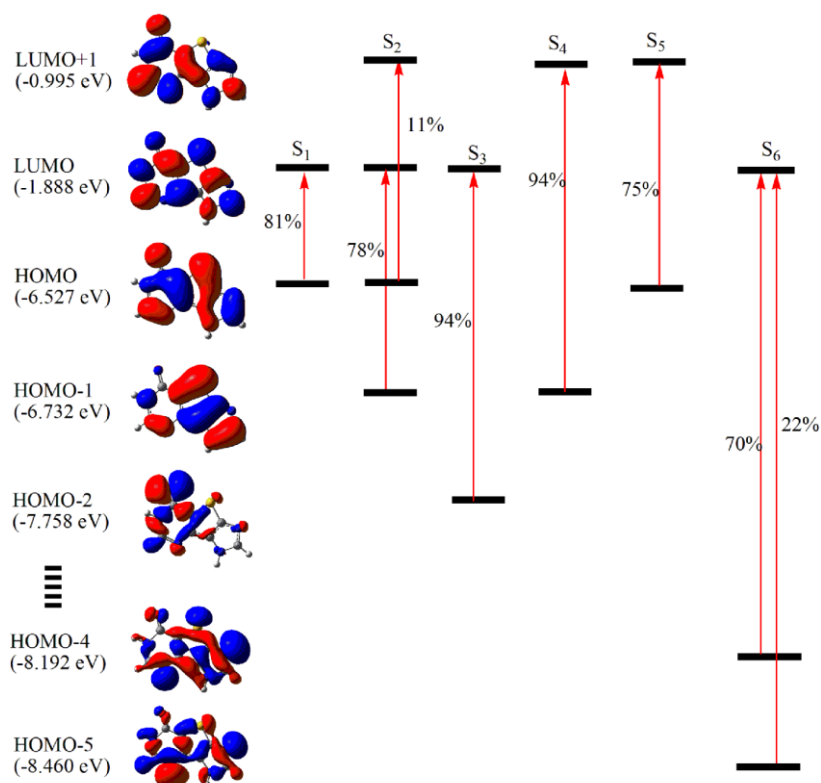


Figure S5. Molecular orbitals involved in the six lowest electronic singlet transitions of ttHX calculated at the TD-B3LYP/6-311++G(d,p) level. Arrows indicate main contributions of the six lowest electronic singlet transitions and contributions larger than 10% are given. Orbital energies are given in parentheses.

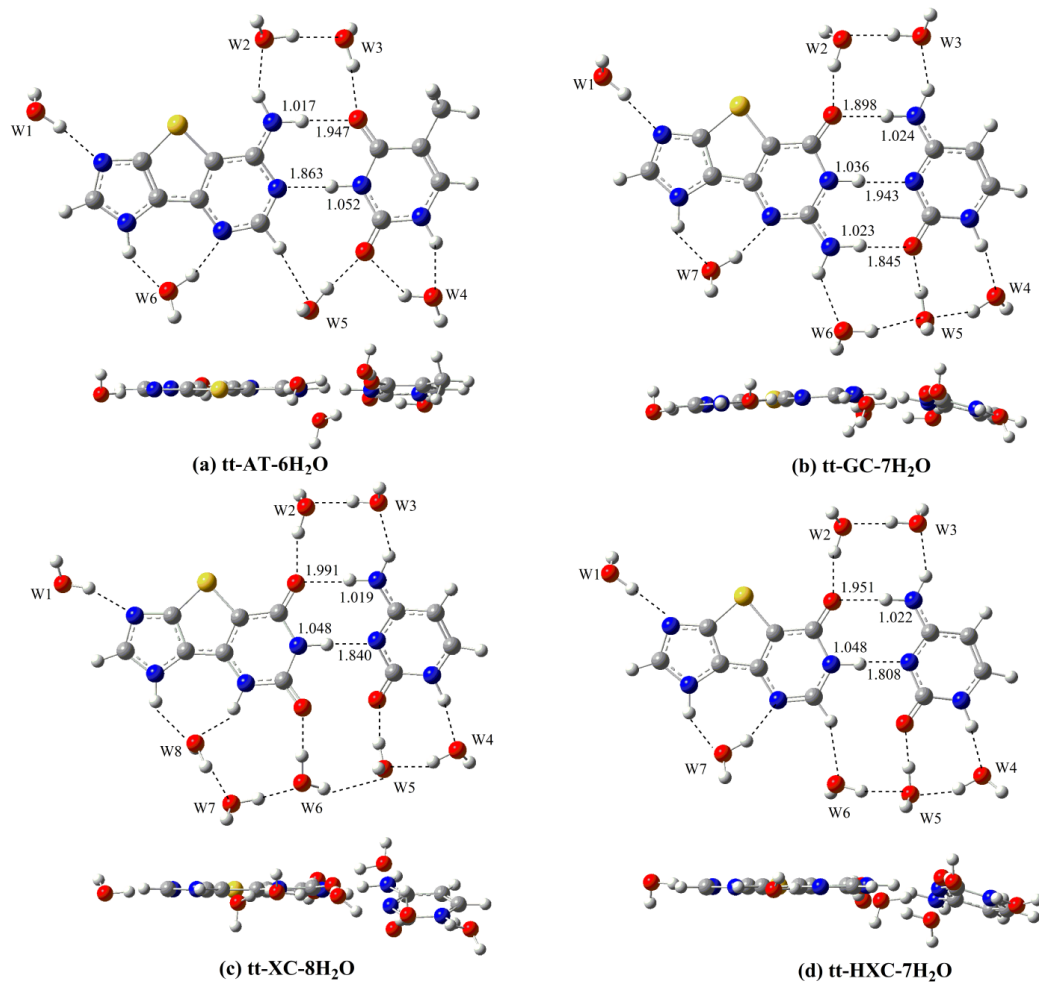


Figure S6. The B3LYP/6-31+G(d,p) optimized structures of hydrated base pairs (distances in Å).