Supporting information

of

Comparative study of the cyclobutane dimer formations of uracil and 6-azauracil in excited state and through conical intersections S_0/S_1

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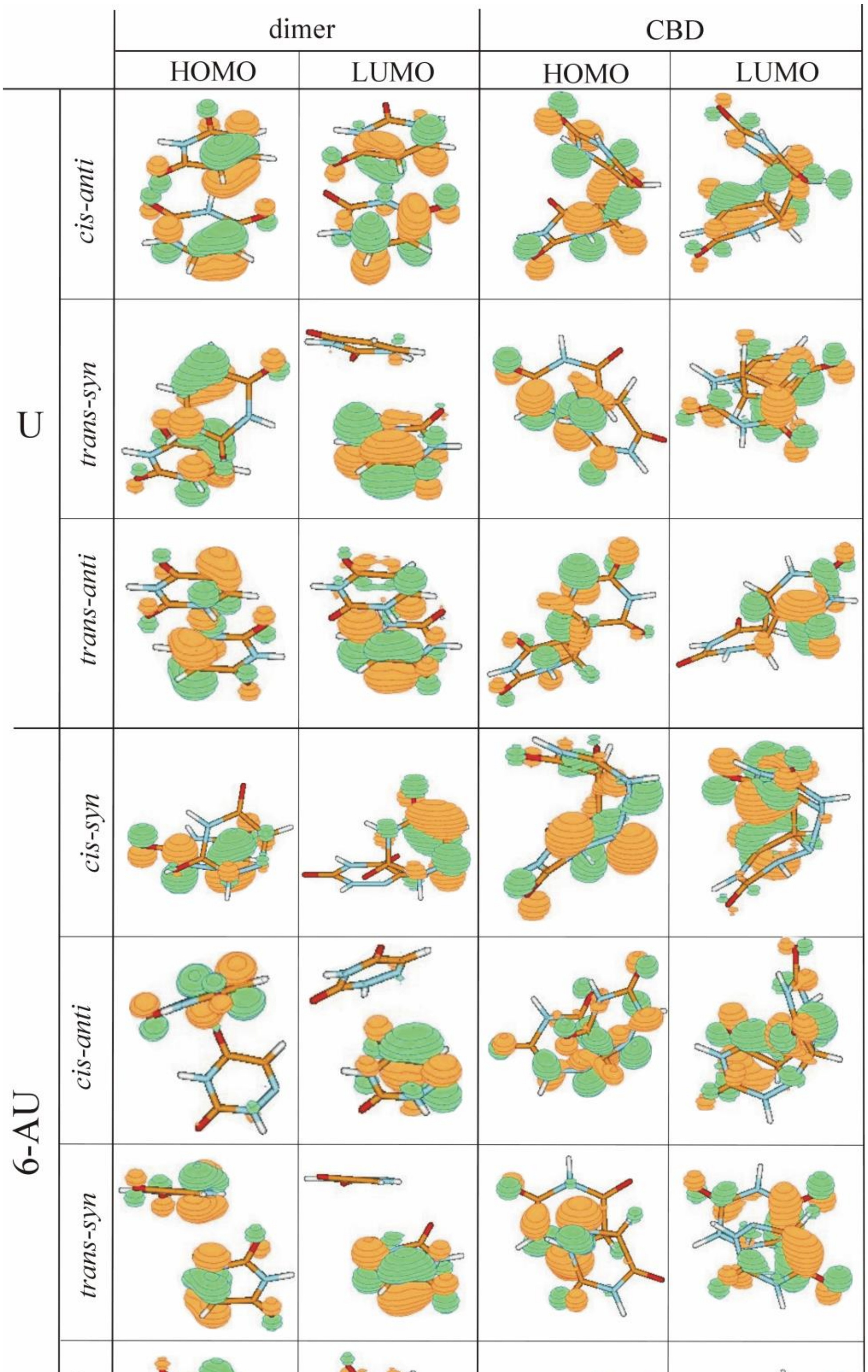

Fig. S1. HOMO and LUMO molecular orbitals of the CBDs and the SDs included in the active space (2,2)

Table S1. Freezed distances in dimers during the CASSCF optimizations

		cis-syn	*trans-syn*	*cis-anti*	*trans-anti*
freezed bond(s)	U	-	C_2-C_{13}=3.95 Å	C_1-C_{13}=3.9 Å C_2-C_{14}=3.9 Å	C_1-C_{13}=3.9 Å C_2-C_{14}=3.84 Å
	6-AU	N_2-N_{12}=3.8 Å C_1-C_{13}=3.9 Å	N_2-N_{12}=3.8 Å	C_1-N_{12}=3.9 Å	C_1-N_{12}=3.8 Å

Table S2. Twist angles of the cyclobutane rings in U and 6-AU

		cis-syn	*trans-syn*	*cis-anti*	*trans-anti*
U		($C_1C_2C_{13}C_{14}$)		($C_1C_2C_{14}C_{13}$)	
	SD	16.2 ° [ref. 51]	-77.5 °	21.9°	-0.03°
	CBD	20.8 ° [ref. 51]	-18.9 °	12.0°	17.6°
6-AU		($C_1C_2C_{12}C_{13}$)		($C_1C_2C_{13}C_{12}$)	
	SD	50.6°	-82.9°	7.1°	-1.9°
	CBD	21.7°	-25.6°	-18.3°	0.01°

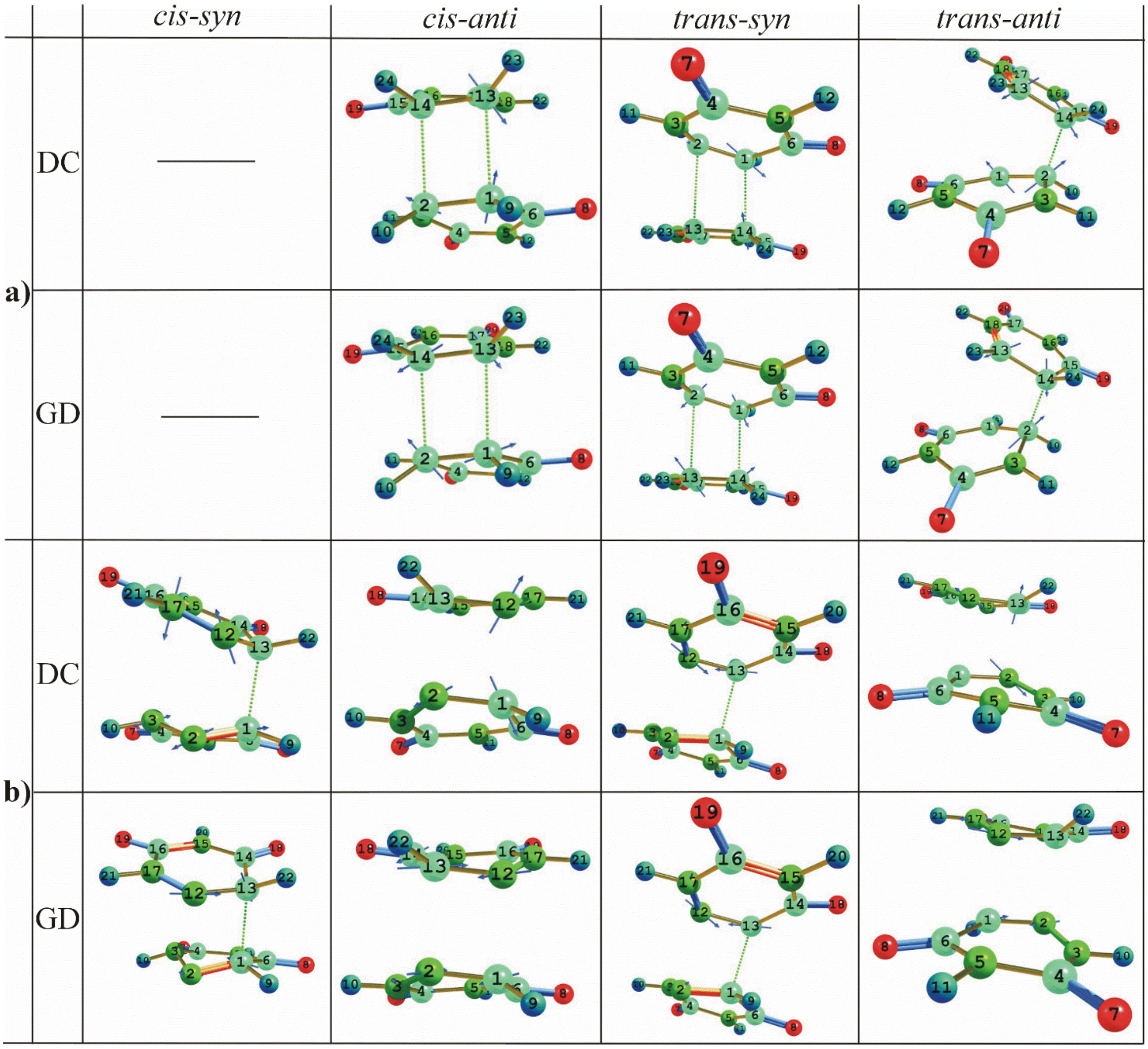

Fig. S2. Branching space vectors (Gradient Difference and Derivative Coupling) of the conical intersections S_0/S_1 of a) Uracil and b) 6-Azauracil