Electronic Supplementary Information for:

Don't help them to bury the light. The interplay between intersystem crossing and hydrogen transfer in photoexcited curcumin revealed by state-hopping dynamics

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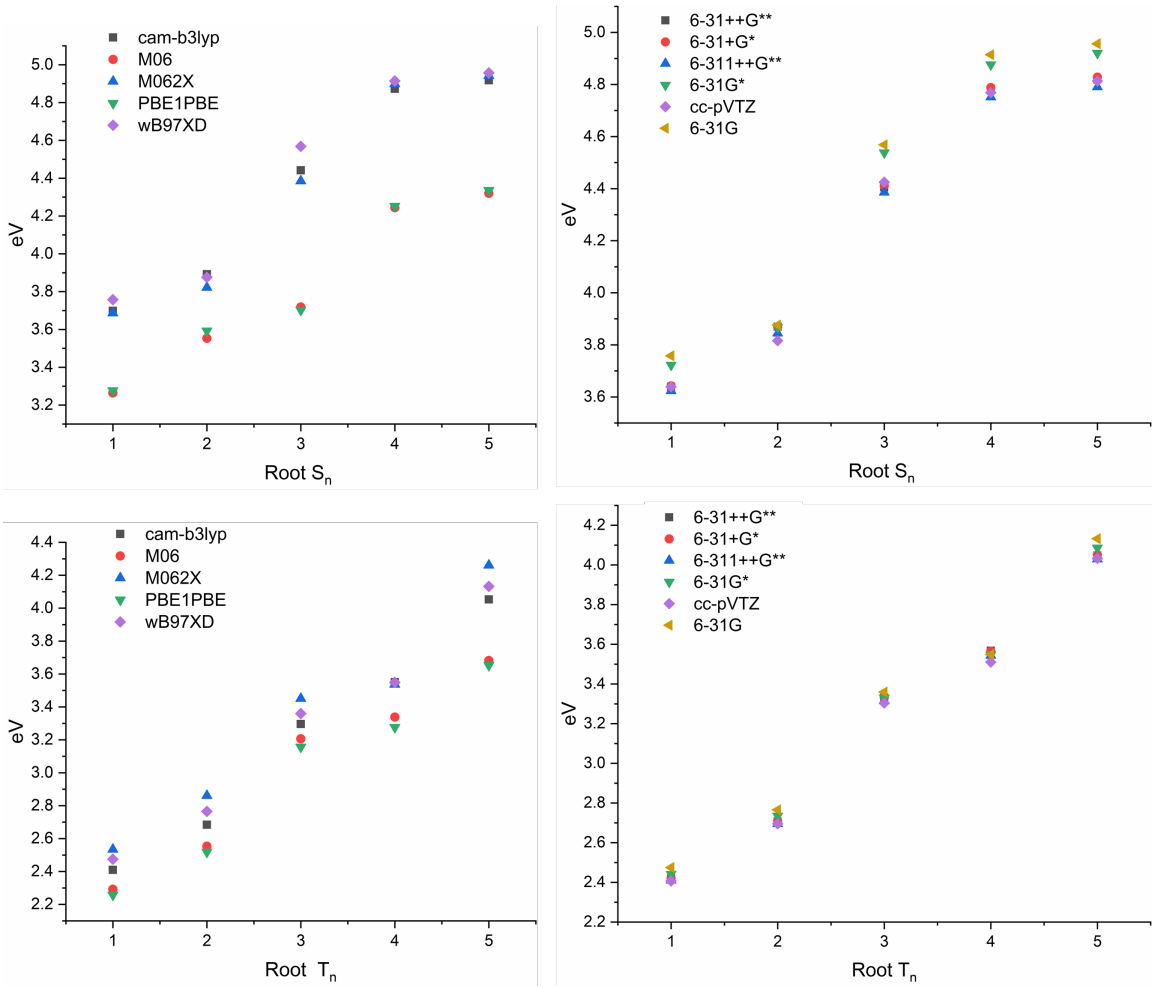

Figure S1. Energy levels of the excited singlet (top row) and triplet (bottom row) calculated with different functionals using the 6-31G and basis sets using the ωB97XD at the Franck-Condon geometry.

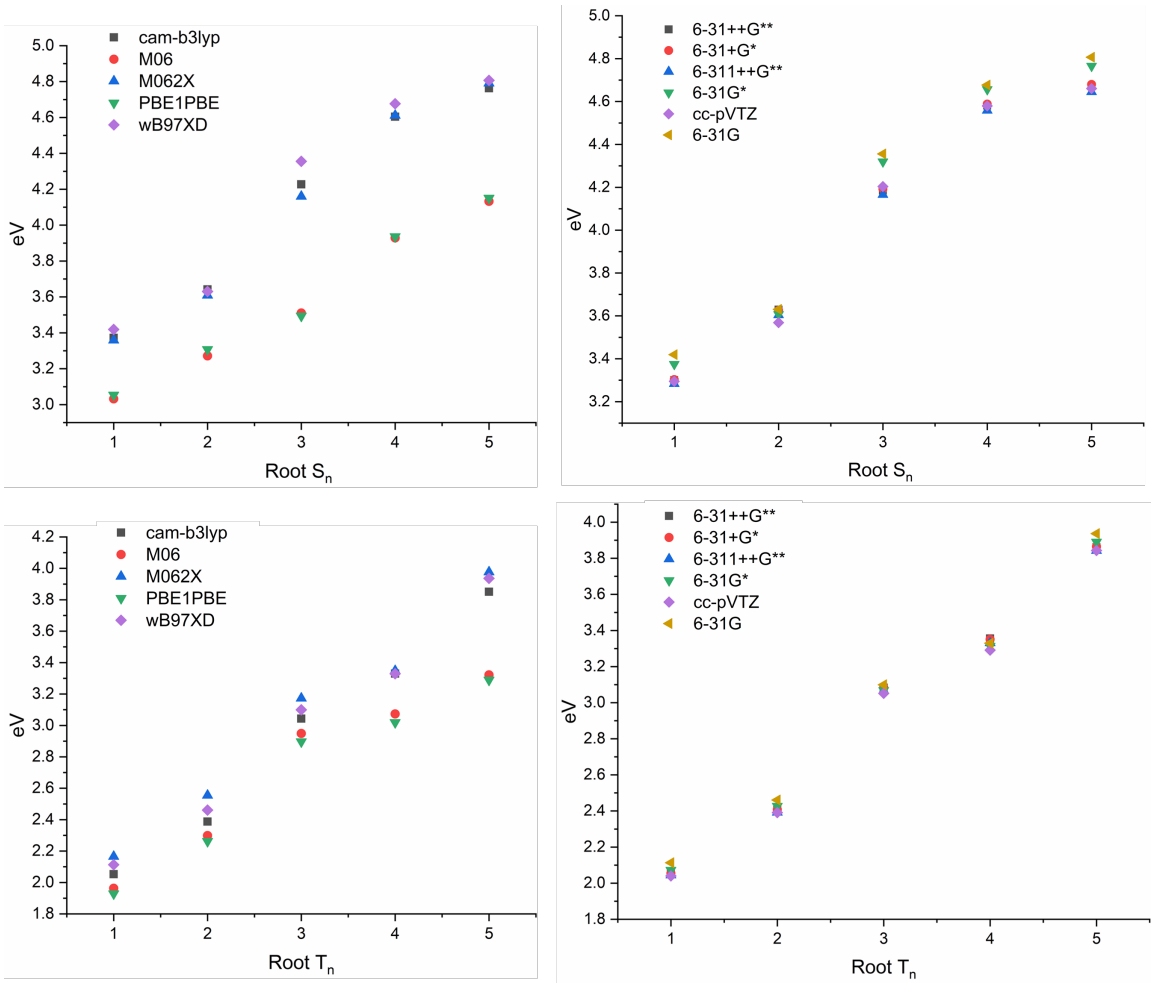

Figure S2. Energy levels of the excited singlet (top row) and triplet (bottom row) calculated with different functionals using the 6-31G and basis sets using the ωB97XD at the S_1 equilibrium geometry.

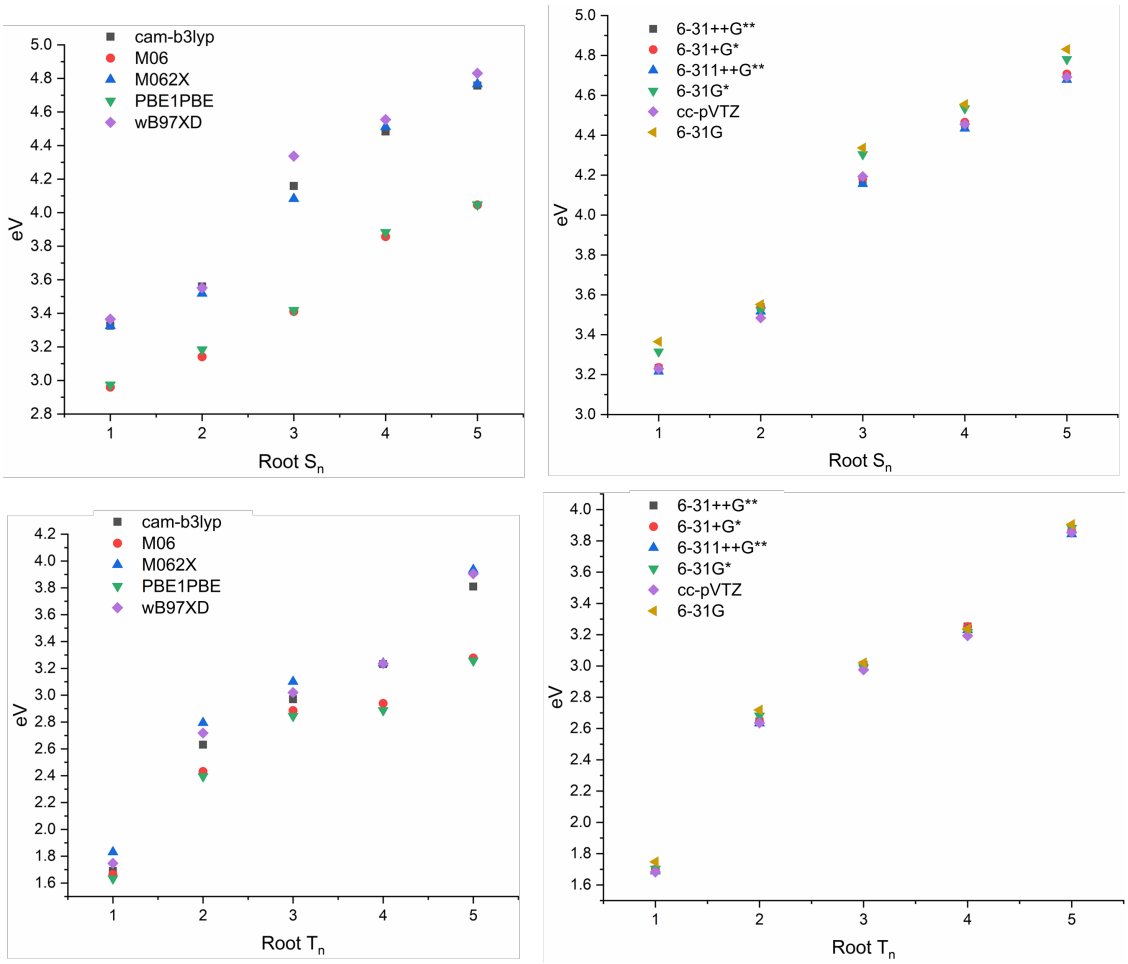

Figure S3. Energy levels of the excited singlet (top row) and triplet (bottom row) calculated with different functionals using the 6-31G and basis sets using the ωB97XD at the T_1 equilibrium geometry.

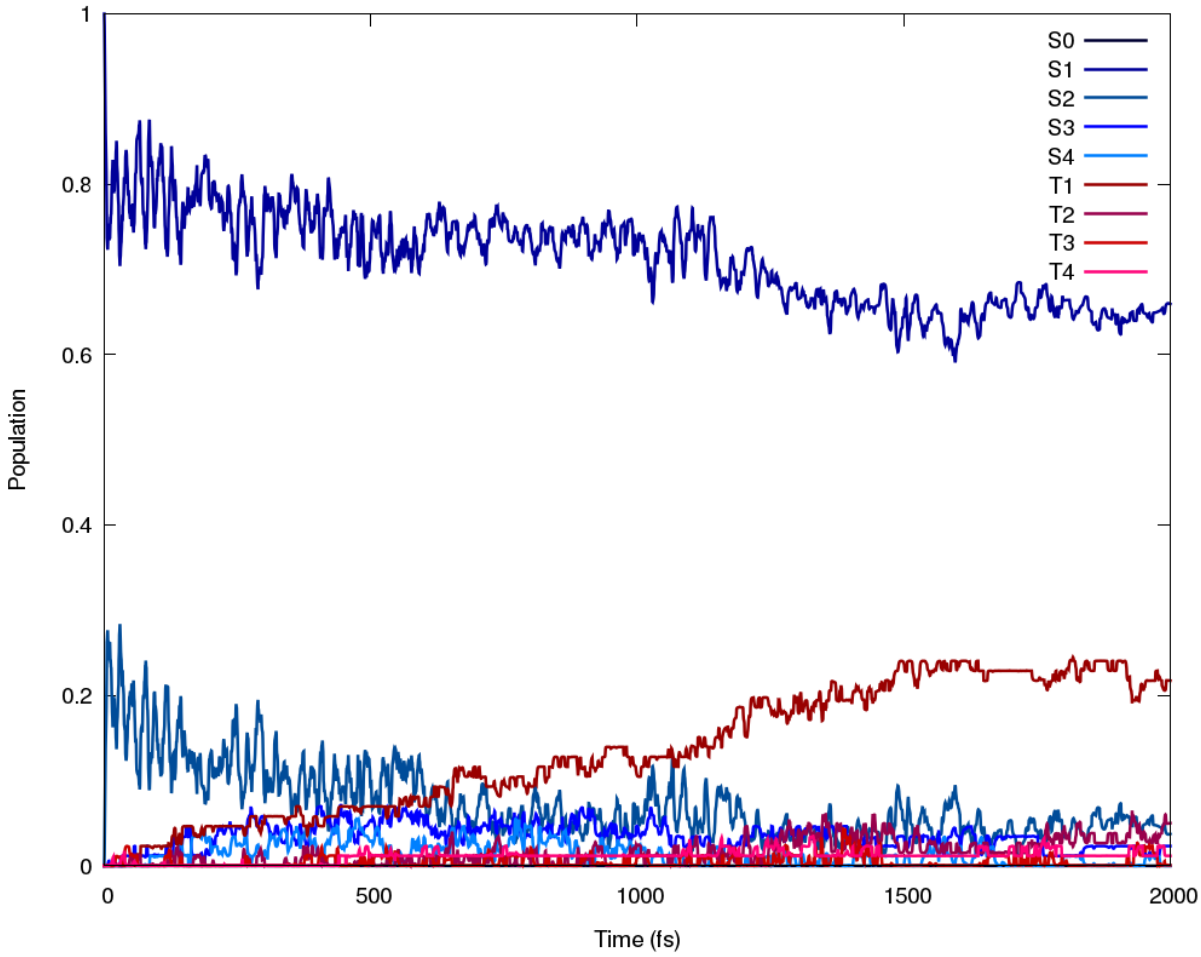

Figure S4. Evolution of the population of the states during the SH dynamic obtained from the multiconfiguration quantum amplitudes, triplet states are represented in red tones, convoluted for the ensemble of the trajectories, and for all the involved states.

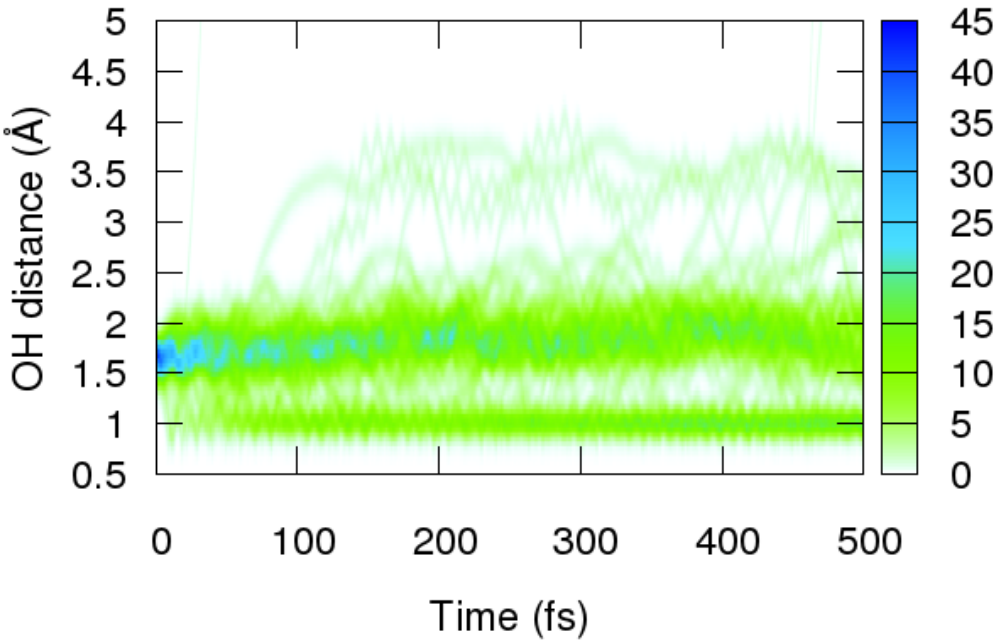

Figure S5. Evolution of the OH distance d for the ensemble of the trajectories during the first 500 fs of the SH dynamics.

	S_0	S_1	S_2	S_3	S_4	T_1	T_2	T_3	T_4
S_0	0	0	0	0	0	0	0	0	0
S_1	0	0	6	1	-9	0	-1	-8	-18
S_2	0	-6	0	7	-1	0	0	1	2
S_3	0	-1	-7	0	-10	0	0	0	0
S_4	0	9	1	10	0	0	0	0	0
T_1	0	0	0	0	0	0	23	-6	0
T_2	0	1	0	0	0	-23	0	26	1
T_3	0	8	-1	0	0	6	-26	0	14
T_4	0	18	-2	0	0	0	-1	-14	0

Table S1. Matrix summing the differences of the hops between the states obtained on the ensemble of the SH trajectories.

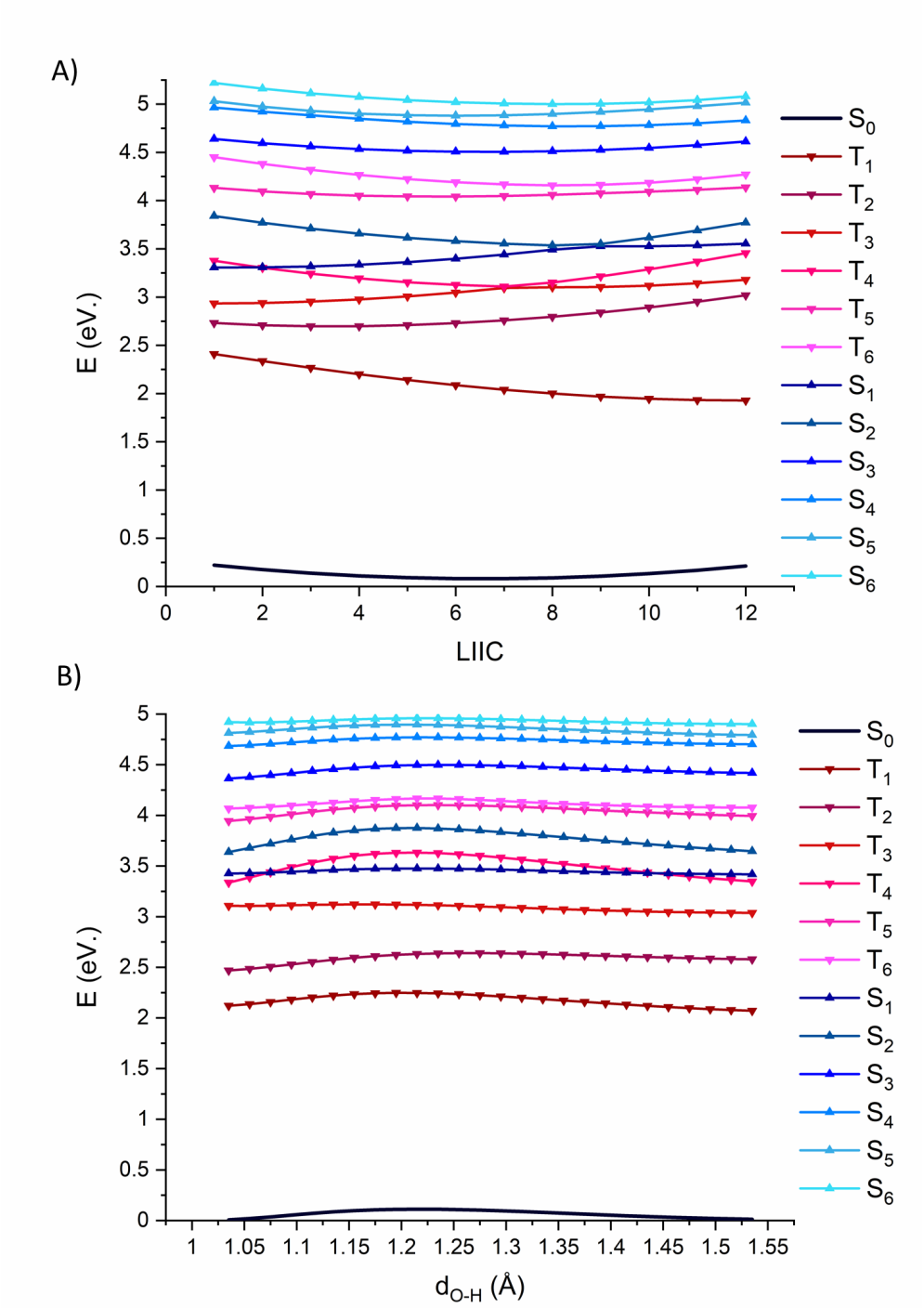

Figure S6. PES for the enol CURC along the LIIC connecting the equilibrium geometry of the first singlet and triplet with six states (A). PES of the different excited state along the Hydrogen transfer coordinate considering six states (B).