Electronic Supplementary Information (ESI)

Exploring and elaborating the novel excited state dynamical behavior for bisflavonol system

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Table S1: The potential energy barriers (kcal/mol) of twisting dihedral angle Φ in octane, dichloromethane, acetone and acetonitrile solvents in S_0 and S_1 states.

	octane	dichloromethane	acetone	acetonitrile
S_0	4.38	3.78	3.64	3.58
S_1	12.94	14.92	15.80	15.95

Table S2: The primary bond lengths (Å) and bond angles δ (°) involved in dual hydrogen bonds of Anti-SPT and Syn-SPT structures in S_0 and S_1 states.

	Anti-SPT		Syn-SPT	
	S_0	S_1	S_0	S_1
O1$\cdots$H2	1.838	2.016	1.840	2.015
H2-O3	0.999	0.982	0.999	0.982
O4-H5	0.979	0.983	0.980	0.983
H5$\cdots$O6	1.989	1.956	1.989	1.961
δ(O1$\cdots$H2-O3)	123.6	117.4	123.6	117.4
δ(O4-H5$\cdots$O6)	119.3	120.4	119.2	120.1

Table S3: The primary bond lengths (Å) and bond angles δ (°) involved in dual hydrogen bonds of Anti-DPT and Syn-DPT structures in S_0 and S_1 states.

	Anti-DPT		Syn-DPT	
	S_0	S_1	S_0	S_1
O1$\cdots$H2	1.840	1.947	1.843	1.948
H2-O3	0.999	0.987	0.999	0.987
O4$\cdots$H5	1.840	1.947	1.843	1.948
H5-O6	0.999	0.987	0.999	0.987
δ(O1$\cdots$H2-O3)	123.6	119.8	123.4	119.8
δ(O4$\cdots$H5-O6)	123.6	119.8	123.4	119.8

Table S4: The potential energy barriers (kcal/mol) along with the I → II or III path in octane, dichloromethane, acetone and acetonitrile solvents in the S_1 states for both Anti and Syn systems.

	octane	dichloromethane	acetone	acetonitrile
Anti	5.54	5.92	6.00	6.03
Syn	5.59	5.98	6.05	6.08

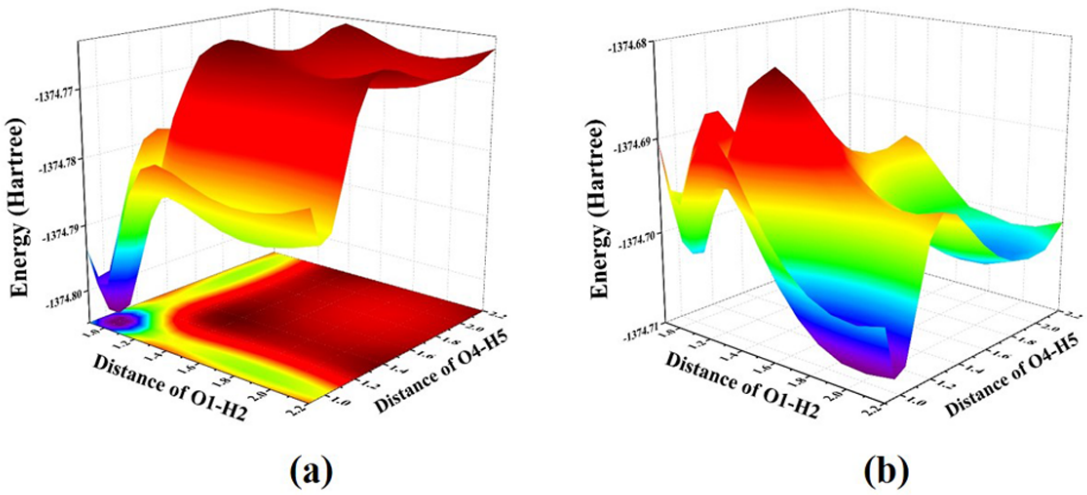

Figure S1: The constructed S_0-state (a) and S_1-state (b) PESs for Syn system as functions of both O1-H2 and O4-H5 bond distances from 0.9 Å to 2.2 Å in step of 0.1 Å based on DFT//TDDFT/Cam-B3LYP/TZVP level in toluene solvent. Herein, the S_0-state projective plane is also shown.

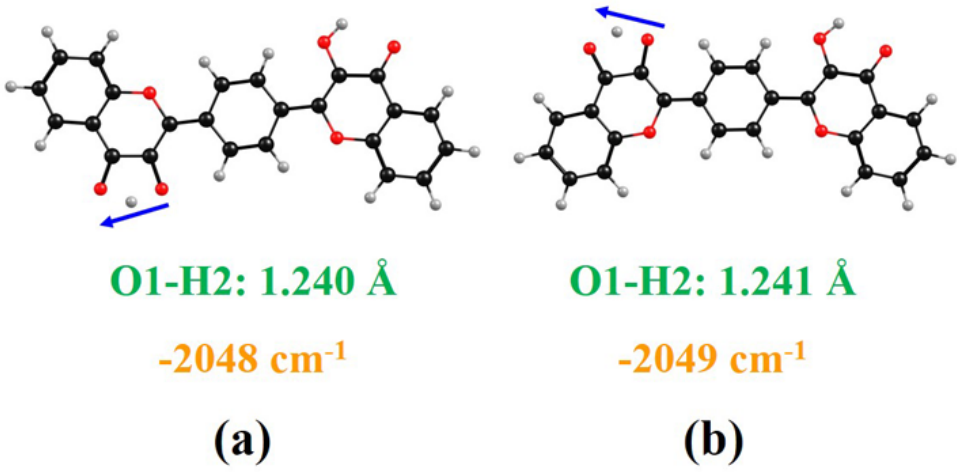

Figure S2: The S_1-state TS structures for Anti (a) and Syn (b) systems in toluene solvent. The TS for Anti system separates the S_1-state Anti and Anti-SPT forms, and TS for Syn system separates the S_1-state Syn and Syn-PT forms. Herein, the vibrational eigenvector of TS configuration points to the correct ESIPT direction. The corresponding O1-H2 bond distances and imaginary frequencies of the TS structures are listed for both Anti and Syn.

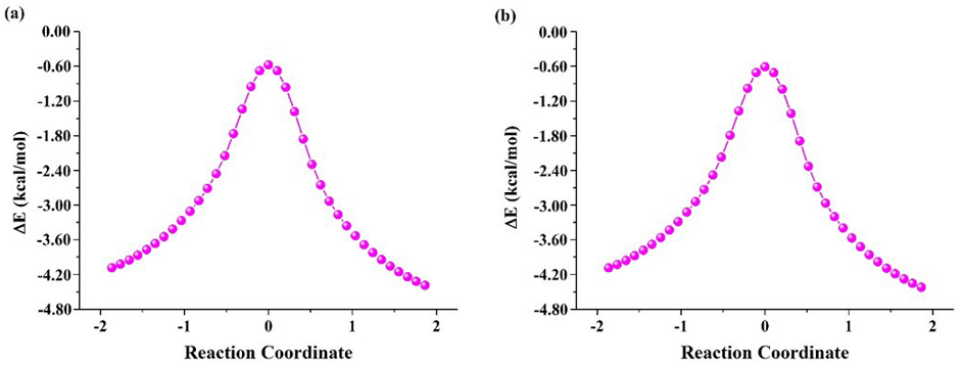

Figure S3: The energy profile along the excited state IRC for the ESIPT path (I $\rightarrow$ II) for Anti (a) and Syn (b) systems based on TDDFT/Cam-B3LYP/TZVP/IEFPCM (toluene solvent) level.