Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Revising the formation and electronic properties in the Flavylium Derivatives. A Theoretical Tandem Towards Optimized DSSCs

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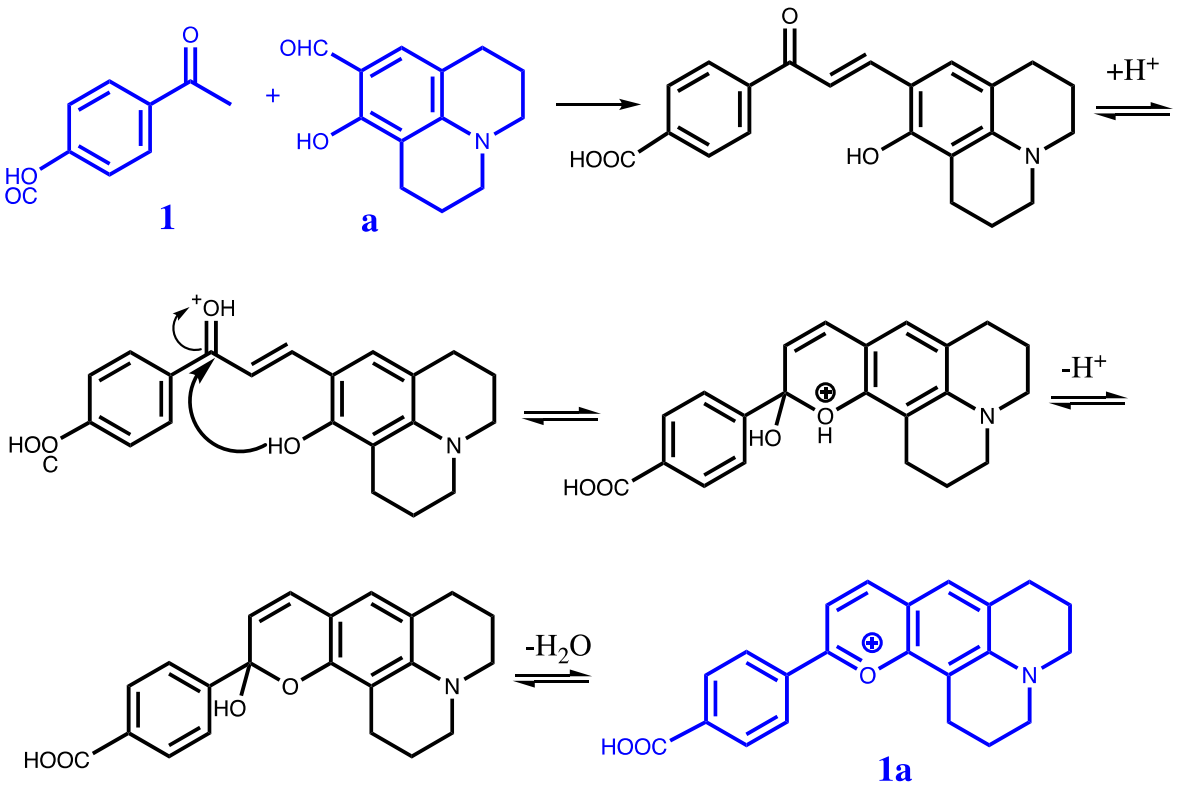
Supplementary Information



Scheme S1. The proposal mechanism of reaction for the flavylium ring-closure.

Table S1. Selected structural parameters of Flavylium derivatives.

Compounds	**1a**	**2a**	**3a**	**1b**	**2b**	**3b**	**[1,2]Exp.**
Distance (Å)							
O_{21}-C_{12}	1.34	1.34	1.34	1.34	1.35	1.34	1.34
O_{21}-C_{16}	1.37	1.37	1.36	1.37	1.37	1.37	1.37
C_{12}-C_1	1.463	1.458	1.455	1.439	1.434	1.429	1.45
C_{12}-C_1(ES)	1.419	1.418	1.44	1.40	1.40	1.42	
O_{21}-C_{12}**(ES)**	1.37	1.37	1.39	1.37	1.37	1.39	
O_{21}-C_{16}**(ES)**	1.34	1.35	1.37	1.35	1.35	1.37	
Dihedral Angle(Deg) **(ES)**			0.29, 93.5			0.13, 90.9	
Dihedral Angle(Deg)	9.47	16.32	11.36	1.192	0.854	1.06	

Dihedral Angle(Deg)(**ES**)	1.025	0.122	0.288	0.857	0.133	0.773	

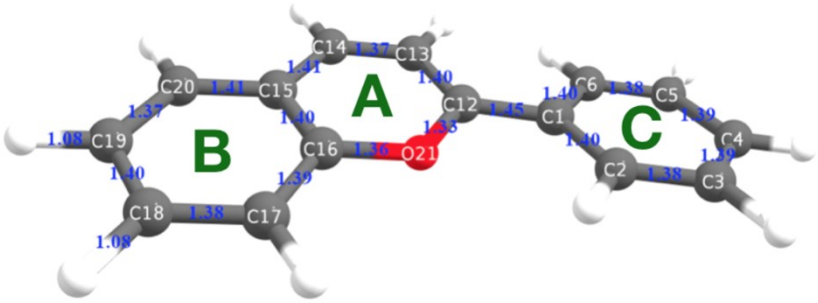


Figure S1: structural Representation of Flavylium ion backbone

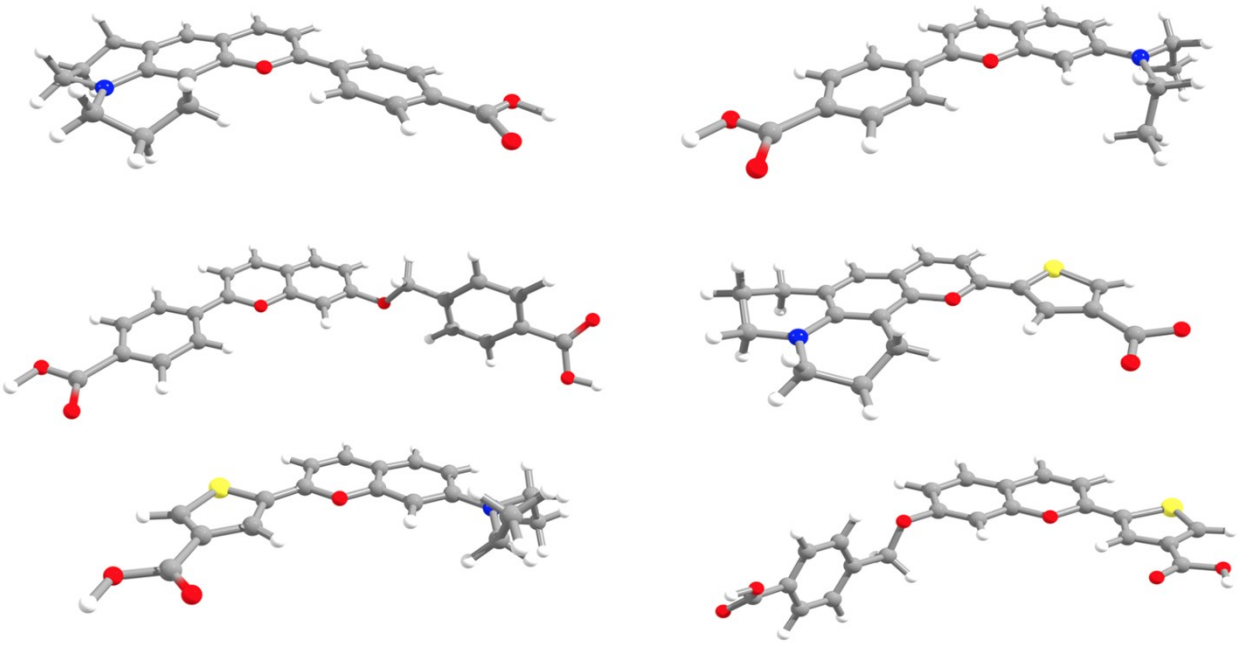


Figure S2. Excited state geometries of corresponding flavyliums

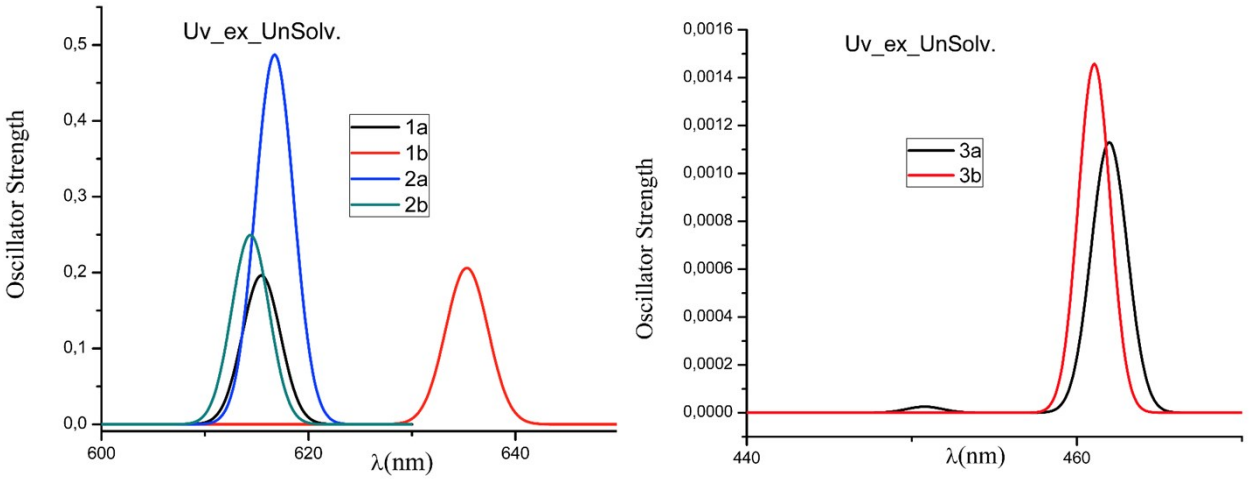


Figure S3. Uv-Vis absorptions bands of flavylium derivatives in current study for gas phase.

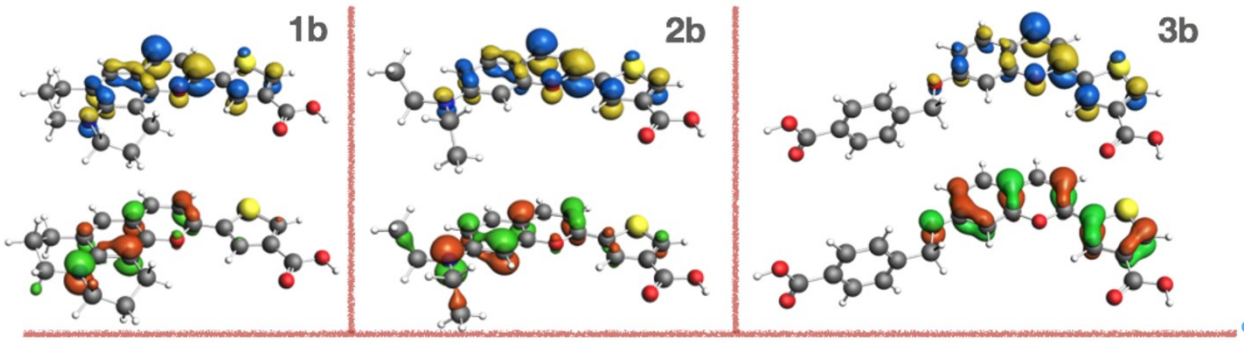


Figure S4. Molecular orbitals involved at the electronic transitions of pyrylium derivatives.

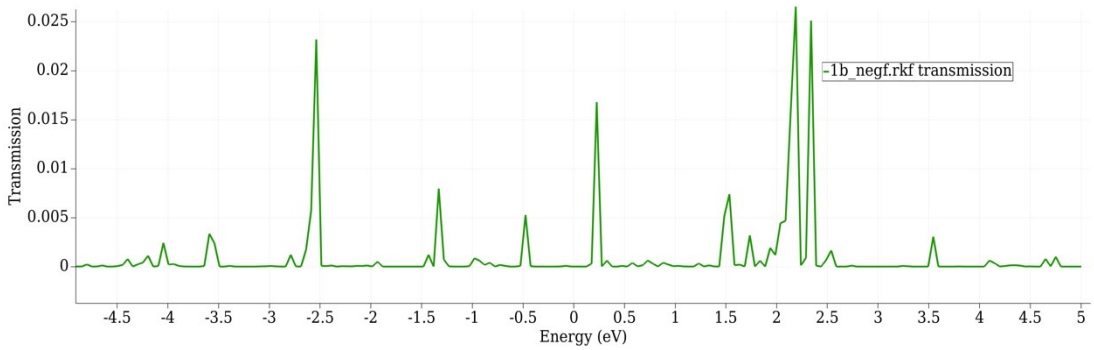


Figure S5. Transmission spectra thorough 1b-flavylium-TiO_2 junction.

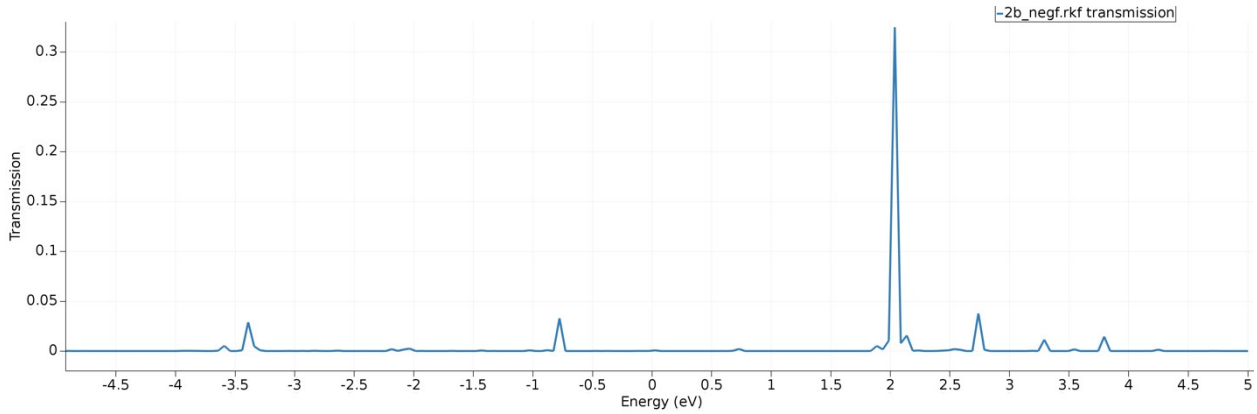


Figure S6. Transmission spectra thorough 2b-flavylium-TiO_2 junction.

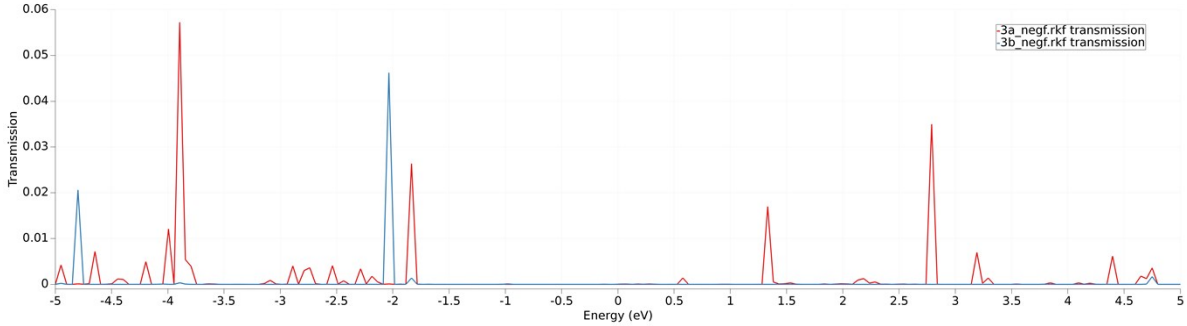


Figure S7. Transmission spectra thorough 3(a,b)-flavylium-TiO_2 junction.