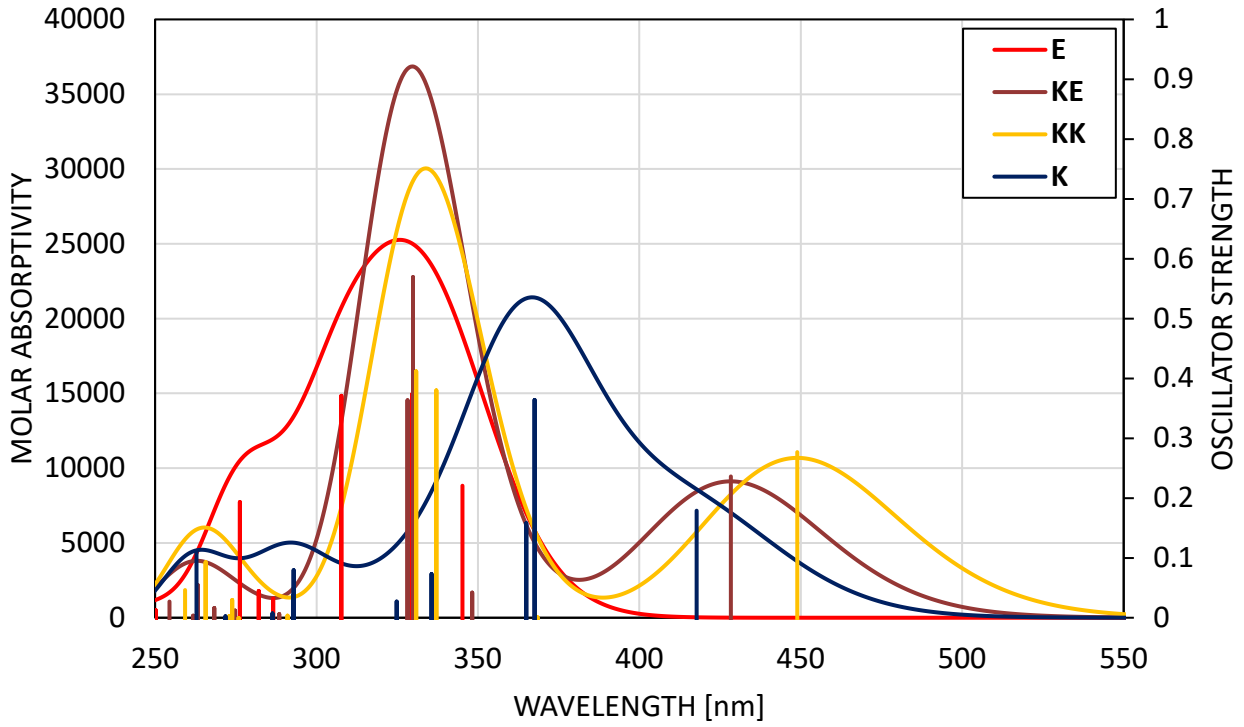
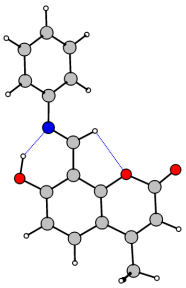
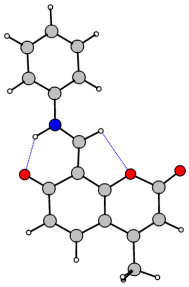
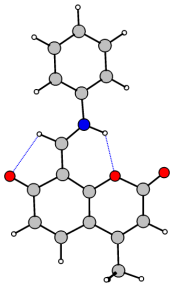
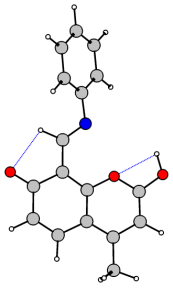


Figure S1. Predicted absorption spectra of the tautomers of **6** in acetonitrile.

Table S1. Relative energies of the tautomers of **6** and their spectral parameters in toluene and in acetonitrile (in brackets) in the ground state.

Structure	α [°] See Scheme 2	μ [D]	Relative energetics [kcal/mol] (M06-2X/TZVP)		UV-Vis* (B3LYP/6-311+G(2d,p))		^{1}H NMR (M06-2X/TZVP) [ppm]
			ΔE	ΔG	λ_{max} [nm]	*f*	
 **E**	0 (0)	3.3 (4.1)	0.0	0.0	348 (345)	0.24 (0.22)	15.0 (15.2)
TS(E-KE)	1 (1)	2.1 (2.5)	4.7 (4.1)	3.0 (2.2)			
 **KE**	1 (0)	1.8 (1.9)	2.8 (1.76)	3.5 (2.4)	439 (428)	0.24 (0.24)	15.4 (15.0)
TS(KE-KK)	90 (90)	6.2 (6.4)	32 (26)	33 (27)			
 **KK**	180 (179)	1.3 (1.7)	7.3 (6.0)	8.0 (6.7)	459 (449)	0.31 (0.28)	11.0 (11.1)
	N/A	N/A	N/A	N/A			

 **K**	176 (174)	8.5 (10.9)	32 (30)	32 (29)	434 (418)	0.17 (0.18)	6.67 (7.11)

* S_0-S_1 transition, the entire spectra are presented in Figures 1 and S1.

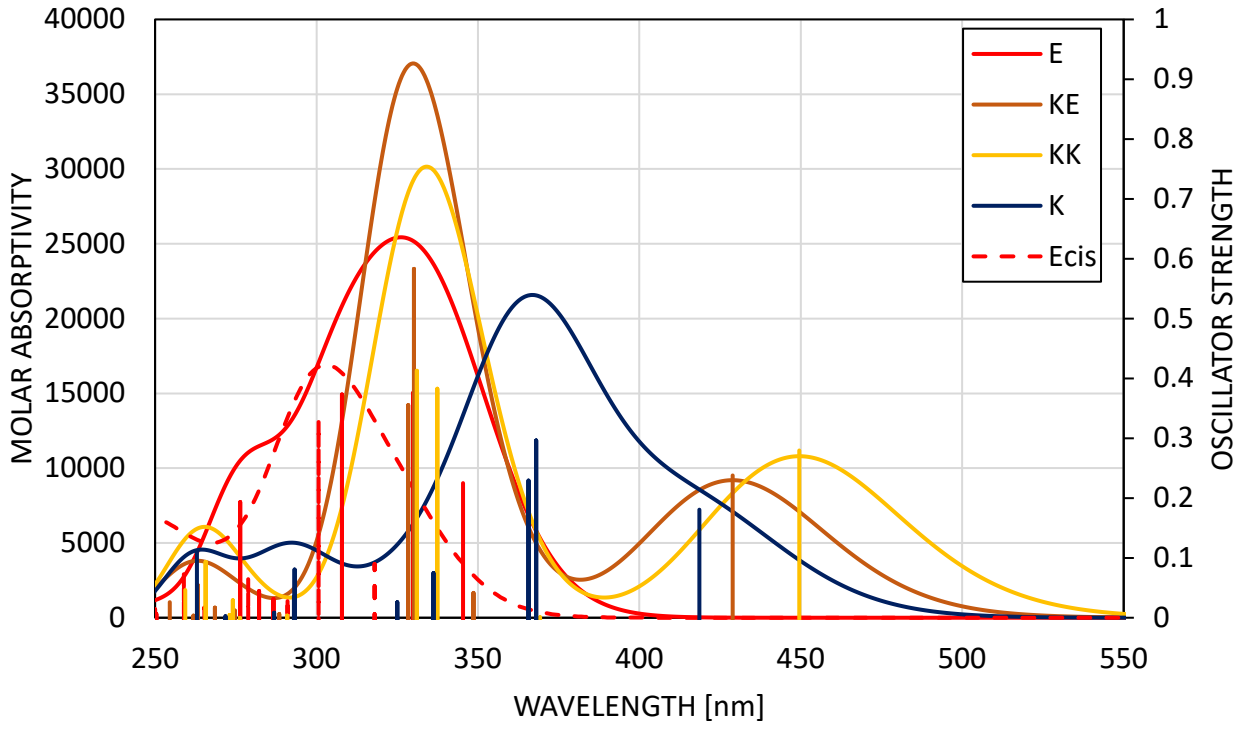


Figure S2. Predicted absorption spectra of the tautomers and isomers of **6** in ethanol.