Supplementary Information

Table S1 and Figures S1 and S2

Table S1 Structural parameters for the ground and excited state optimized geometry of SA at RHF/6-31+G(d,p) [6-31G(d,p)] and CIS/6-31+G(d,p) [6-31G(d,p)] levels of theory along with the X-ray crystallographic data

Bonds[(a)]	X-ray Crystallographic Data	Enol form			Cis-keto form	
		Ground state (RHF) C_1	Excited State (CIS)		Ground state (RHF) C_1	Excited state (CIS) C_S
			C_1	C_S		
O11 – H22	0.89	0.955 [0.954]	0.945 [0.944]	0.963 [0.964]	1.875 [1.868]	1.874 [1.857]
N2 – H22	1.81	1.898 [1.889]	2.945 [2.084]	1.807 [1.788]	1.006 [1.005]	1.007 [1.007]
O11 – N2	2.598	2.717 [2.712]	2.836 [2.826]	2.654 [2.643]	2.659 [2.656]	2.682 [2.673]
Dipole moments[(b)]	-----	2.613 [2.609]	5.077 [5.017]	2.729 [2.663]	4.311 [4.085]	4.782 [4.618]

(a) in Å

(b) in Debye

Figure S1

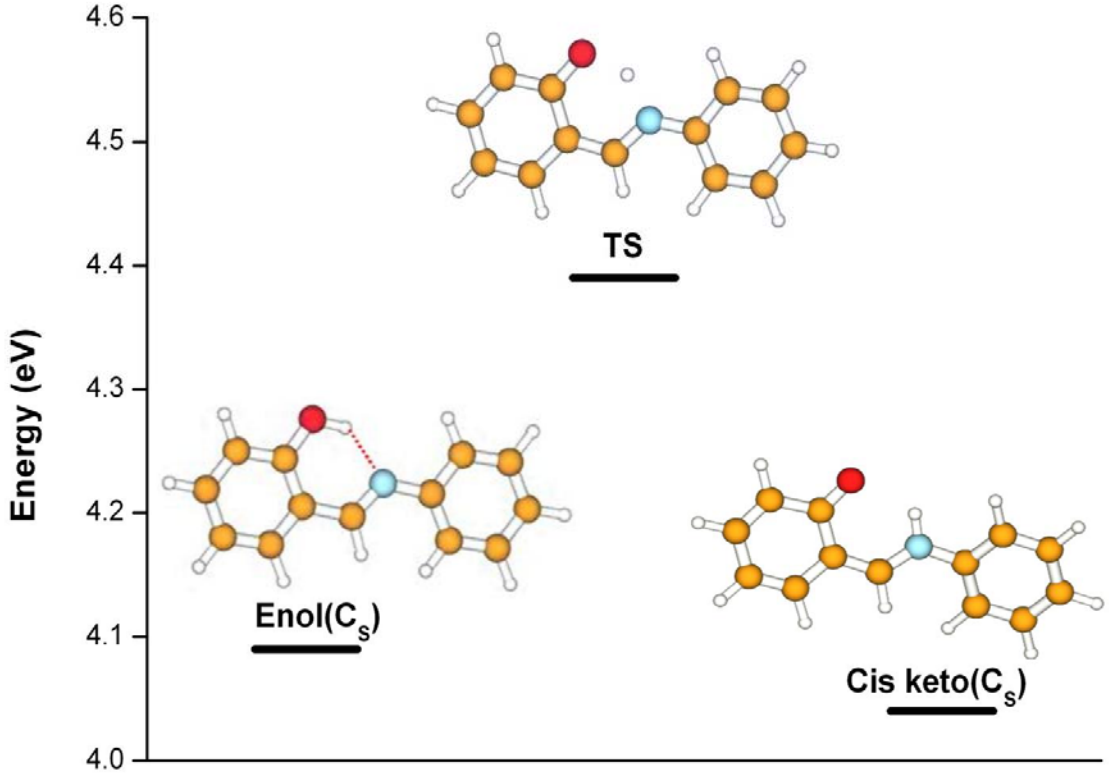
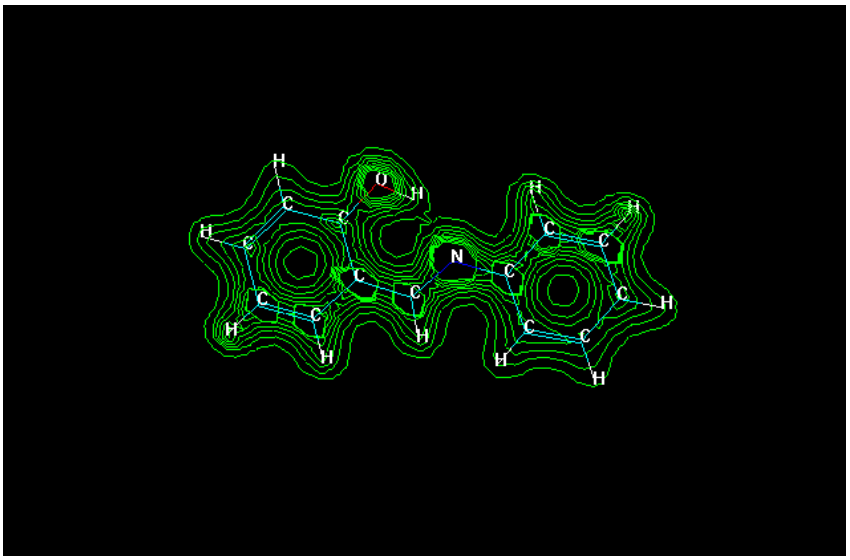


Figure S2

(a)



(b)

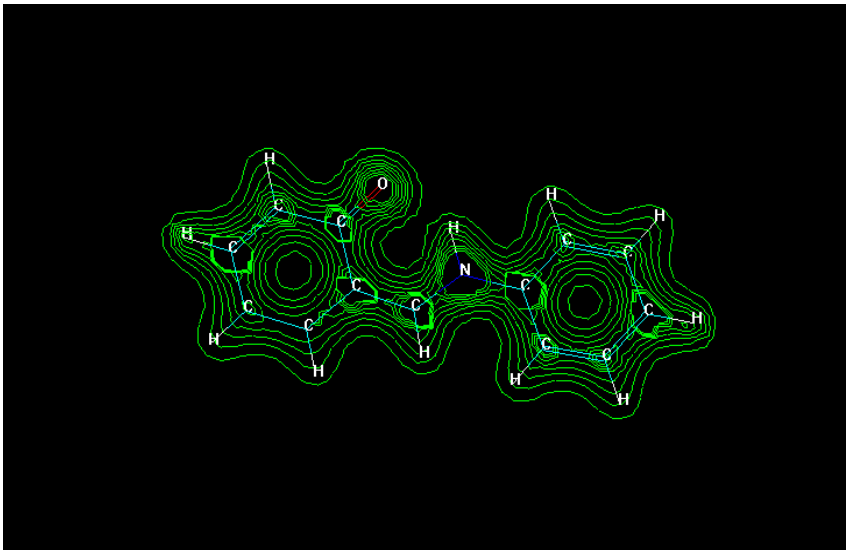


Figure captions

Figure S1: The energy (in eV) disposition of the transition state (TS), the enol (C_S) and the cis-keto (C_S) forms of the SA molecule in the S_1 state taking the energy of the optimized ground state of the enol (C_1) form as the reference level.

Figure S2: Total electronic charge density contour maps of (a) enol (C_S) and (b) cis-keto (C_S) forms of SA molecule. (Total charge density contour value : 0.05).