Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Theoretical Study of the proton transfer wires influence on the one- and two-photon absorption properties of Green Fluorescent Protein chromophore

(Supplementary Information)

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STABLE 1: Selected Optimized Structural Parameters (Bond Length (Å), angle(°)) of Cro A, Complex A and Complex I at the ground and excited state, respectively. Superscipt * notes as the first excited-state of that conformer.

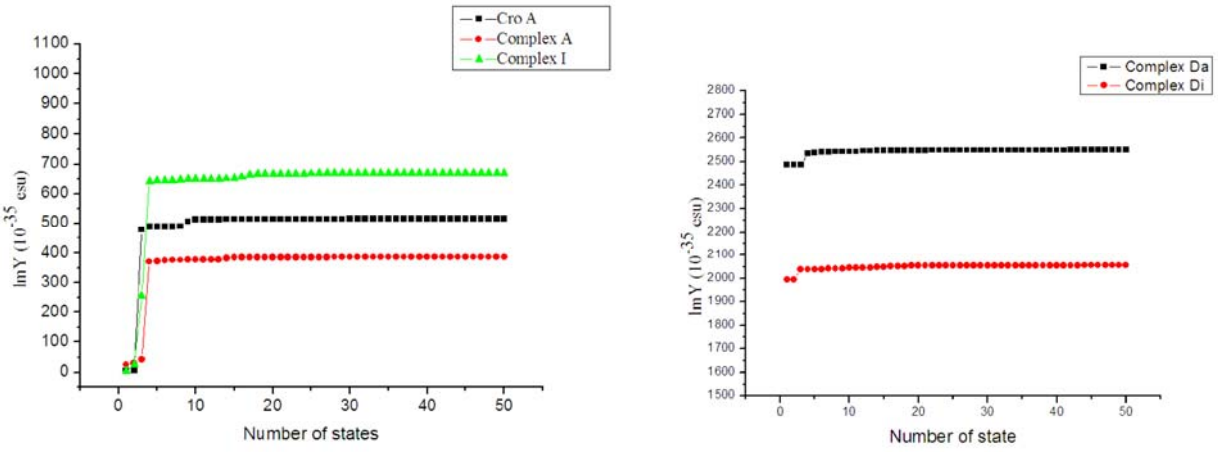
Parameters	Cro A	Complex A	Complex A*	Complex I	Complex I*
C1-O14	1.3573	1.3500	1.3431	1.2895	1.2853
C1-C2	1.4024	1.4055	1.4109	1.4354	1.4371
C2-C3	1.3864	1.3844	1.3786	1.3750	1.3761
C3-C4	1.4119	1.4123	1.4364	1.4220	1.4364
C4-C5	1.4126	1.4129	1.4370	1.4217	1.4363
C5-C6	1.3853	1.3856	1.3742	1.3784	1.3726
C1-C6	1.4003	1.4032	1.4148	1.4334	1.4429
C4-C7	1.4469	1.4463	1.4071	1.4289	1.4191
C7-C8	1.3588	1.3597	1.4275	1.3718	1.4192
∠C4-C7-C8-N12	-0.2346	-3.1359	-21.2130	-1.8576	-6.3401

Stable 2 Dipole Moments (Debye) at Ground and First Excitation States for Studied Conformers at B3LYP/6-311++G** Level

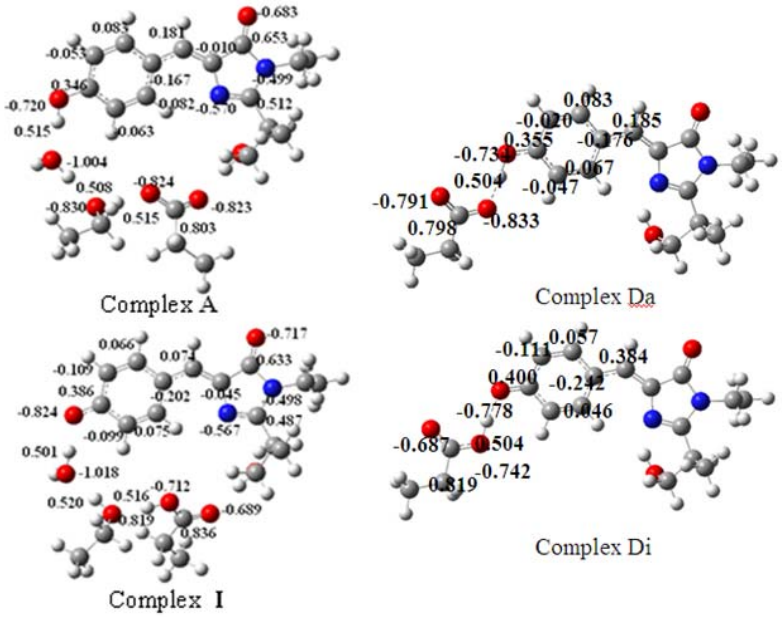
conformer	Ground state dipole moment			First excited state dipole moment			S0-S1 transition moments		
	X	Y	Z	X	Y	Z	X	Y	Z
Cro A	-0.1991	7.6458	1.0539	2.0662	1.1851	-0.0825	-7.9621	-1.4364	0.3424
Complex A	2.4613	-0.7405	8.0034	-3.0883	0.8274	-0.1661	-6.9451	4.0038	-0.5991
Complex I	-2.7947	-12.7435	3.4852	-4.7078	2.3418	-0.2874	-8.2455	4.4298	-0.5793
Complex Da	22.3256	6.2764	-0.2246	-5.0323	-0.8808	0.4805	-8.5375	-2.0525	0.6349
Complex Di	15.1529	9.9551	-2.2843	-3.8889	-0.6303	0.1723	-9.7151	-1.6804	0.3772

Stable 3 Dipole and Transition Moments (Debye) of Relevant Excitations for each Studied Conformer at B3LYP/6-311++G** Level. n Denotes the final transition excited-state.

conformer	Transition states	S0-Sn transition moments			S1-Sn transition moments		
		X	Y	Z	X	Y	Z
Cro A	S3	2.1506	0.2926	-0.0729	-9.3890	-1.4714	0.3284
Complex A	S4	-1.4831	0.8510	-0.2227	-7.6350	4.9392	-0.5943
Complex I	S4	-0.3869	0.1279	-0.1459	-5.6692	3.3234	-0.4176
Complex Da	S4	0.9844	0.2061	-0.0386	8.5635	2.3804	-0.6659
Complex Di	S3	-1.1151	-0.2483	-0.0465	-8.0582	-1.6877	0.3149



Sfigure 1. The relationship of the imaginary part of the third-order optical susceptibility and the number of state.



Sfigure 2. NBO charges of studied conformers (hydrogens summed on the corresponding heavy atoms).