molecules

MDPI

Supplementary Materials

Effect of Water Microsolvation on Excited-State Proton Transfer of 3-Hydroxyflavone Enclosed in γ-Cyclodextrin

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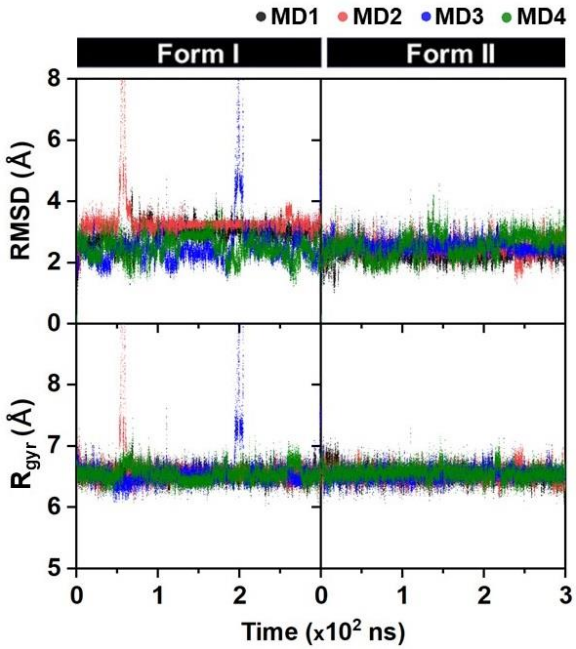

Figure S1. RMSD plots for all atoms and R_{gyr} of the two orientations of C-ring insertion (Form I), and P-ring insertion (Form II) inclusion complexes for four different MD runs of each system.

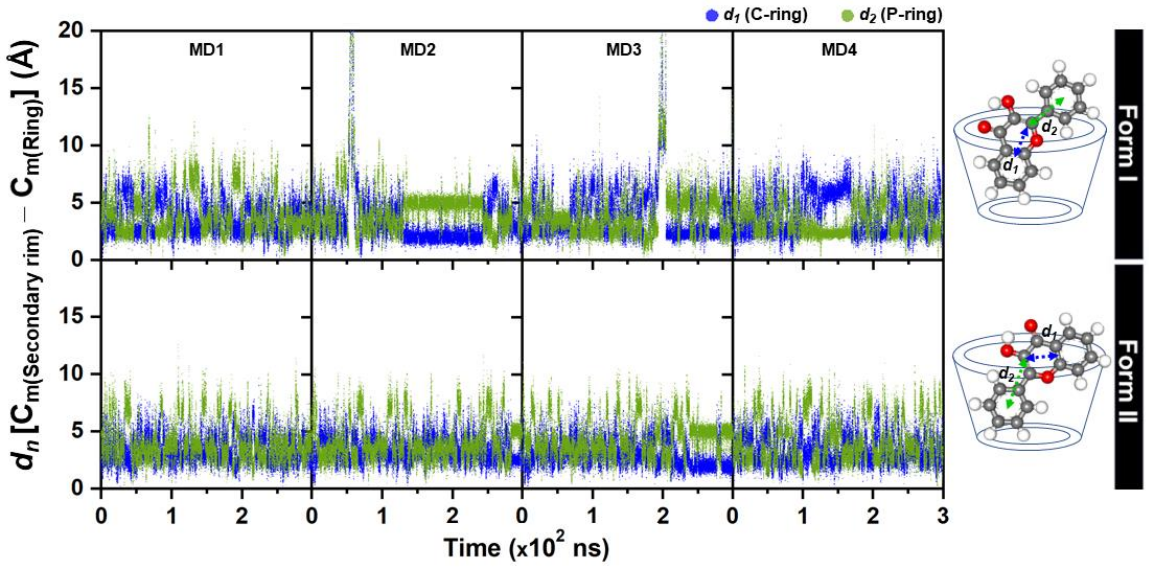

Figure S2. The plots of distance measured from the C_m of each 3HF ring to the C_m of the secondary rim of γ-CD (all 7 O2 atoms) for the four MD simulations MD1-MD4 with different initial structures of complexes in Form I and Form II.

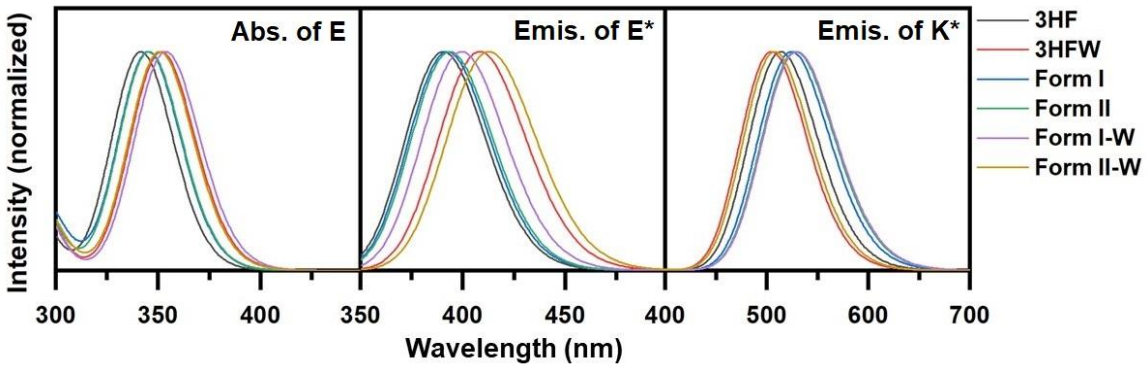

Figure S3. The simulated absorption spectra of E, and the simulated emission spectra of E* and K* for all studied compounds computed at TD-PBE0/def2-SVP level of theory.

Table S1. Electron density ρ(r), the Lagrangian kinetic energy G(r), potential energy density V(r), the Hamiltonian kinetic energy density H(r), the Laplacian of the electron density $\nabla^2\rho$(r), the electron delocalization index (DI), and hydrogen-bonded energy (E_{HB}) at selected BCPs in the S_1 state (a.u.) for all compounds.

Cluster	BCPs	ρ(r)	G(r)	V(r)	H(r)	$\nabla^2\rho$(r)	DI	E_{HB}
3HF	**O2···H1**	0.0516	0.0418	-0.0448	-0.0031	0.1549	0.6756	0.0224
3HFW	**Ow···H1**	0.1007	0.0764	-0.1298	-0.0534	0.0918	0.0054	0.0649
	O2···Hw	0.0633	0.0538	-0.0634	-0.0096	0.1769	0.1481	0.0317
Form I	**O2···H1**	0.0414	0.0342	-0.0350	-0.0009	0.1330	0.0826	0.0175
Form II	**O2···H1**	0.0249	0.0218	-0.0221	-0.0003	0.0860	0.0346	0.0111
Form I-W	**Ow···H1**	0.0575	0.0435	-0.0505	-0.0070	0.1461	0.0000	0.0253
	O2···Hw	0.0636	0.0553	-0.0646	-0.0093	0.1837	0.0159	0.0323
Form II-W	**Ow···H1**	0.1052	0.0785	-0.1391	-0.0606	0.0717	0.0077	0.0696
	O2···Hw	0.0618	0.0528	-0.0612	-0.0084	0.1774	0.0000	0.0306