Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary information for

Regularly tuning the ESIPT reactions of 3-hydroxychromone-based derivatives by the functional group substitutions

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Table S1. Calculated transition properties of the studied molecules in DMSO by using TD-DFT/mPW1PW91/6-311++G(d) method.

Molecule	State	λ_{abs} (nm)	Contribution MO	*f*
BFHC	S1	382	(70.231%)H→L	0.8533
	S6	262	(60.321%)H-3→L	0.1599
BTHC	S1	382	(70.202%)H→L	0.7726
	S6	263	(61.559%)H-3→L	0.1569
BSeHC	S1	388	(70.058%)H→L	0.6396
	S2	358	(69.618%)H-1→L	0.2256
BDFHC	S1	410	(70.360%)H→L	0.9850
	S5	294	(67.414%)H→L+1	0.1861
BDTHC	S1	427	(70.227%)H→L	0.6208
	S2	368	(69.472%)H-1→L	0.4931
BDSeHC	S1	440	(70.103%)H→L	0.4953
	S2	379	(69.353%)H-1→L	0.6469

Table S2. Calculated fluorescence properties of the studied molecules at enol and keto forms in DMSO by using TD-DFT/mPW1PW91/6-311++G(d) method.

Molecule	Form	State	λ_{flu} (nm)	Contribution MO	*f*
BFHC	enol	S1	431	(70.419%)H→L	0.9436
	keto	S1	567	(71.288%)H→L	0.7199
BTHC	enol	S1	432	(70.369%)H→L	0.8875
	keto	S1	564	(71.210%)H→L	0.7095
BSeHC	enol	S1	438	(70.289%)H→L	0.8071
	keto	S1	567	(71.138%)H→L	0.6908
BDFHC	enol	S1	464	(70.488%)H→L	1.1117
	keto	S1	592	(71.293%)H→L	0.9297
BDTHC	enol	S1	482	(70.257%)H→L	0.8250
	keto	S1	601	(71.016%)H→L	0.8629
BDSeHC	enol	S1	494	(70.088%)H→L	0.7028
	keto	S1	614	(70.602%)H→L	0.7727

Table S3. Obtained HOMO, LUMO energies and energy gaps (Δ_{H-L}) of the studied molecules based on the optimized structures of the enol and keto forms at S_1 state (unit: eV).

	Enol			Keto		
Molecule	HOMO	LUMO	Δ_{H-L}	HOMO	LUMO	Δ_{H-L}
BFHC	-5.896	-2.848	3.048	-5.512	-3.222	2.291
BTHC	-5.897	-2.857	3.040	-5.526	-3.213	2.314
BSeHC	-5.878	-2.873	3.005	-5.526	-3.221	2.305
BDFHC	-5.691	-2.869	2.822	-5.406	-3.224	2.182
BDTHC	-5.658	-2.904	2.754	-5.412	-3.237	2.175
BDSeHC	-5.624	-2.920	2.704	-5.399	-3.248	2.151