Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supporting information

for

Novel push-pull quinoxalinone-based chromophores with high sensitivity of emission and absorption to small structural modifications

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Table S1. Electronic energies (in Hartrees/eV) of ground state (S_0) and the first three electronically excited singlet states (S_1, S_2 and S_3) of molecule **1** calculated with the use of long-range corrected *ω*B97XD functional [100] and def2-TZVP basis set [95, 96].

Energy[a]								
State			LR-PCM/**SS-PCM**[b]					
	Gas		**Dioxane**[c]		**DCM**[d]		**CH_3CN**[e]	
	Hartree	**ΔE,** eV	Hartree	**ΔE,** eV	Hartree	**ΔE,** eV	Hartree	**ΔE,** eV
	On the optimized ground state (S_0) geometry							
S_0	-1092.923826	0.00	-1092.929455	0.00	-1092.935578	0.00	-1092.937674	0.00
S_1	-1092.781448	3.87	-1092.792476	3.73	-1092.799495	3.70	-1092.801309	3.71
S_2	-1092.779456	3.93	-1092.788426	3.84	-1092.795151	3.82	-1092.797186	3.82
S_3	-1092.775781	4.03	-1092.780268	4.06	-1092.784872	4.10	-1092.78641	4.12
	On the optimized geometry of the first excited singlet state (S_1)							
S_0	-1092.911731	0.00	-1092.916281	0.00	-1092.921023	0.00	-1092.922526	0.00
S_1	-1092.793661	4.03	-1092.80619	3.00	-1092.818377	2.79	-1092.822184	2.73
			-1092.801829	**3.11**	**-1092.810582**	**3.01**	**-1092.813535**	**2.97**
S_2	-1092.779004	3.61	-1092.78691	3.52	-1092.794963	3.43	-1092.797487	3.40
S_3	-1092.763617	4.03	-1092.766998	4.06	-1092.77056	4.09	-1092.771659	4.11
	On the optimized geometry of the second excited singlet state (S_2)							
S_0	-1092.911481	0.00	-1092.916675	0.00	-1092.924927	0.00	-1092.92688	0.00
S_1	-1092.779236	3.60	-1092.791243	3.41	-1092.808782	3.16	-1092.812507	3.11
S_2	-1092.793051	3.22	-1092.80159	3.13	-1092.808267	3.17	-1092.811092	3.15
			-1092.811378	**2.87**	**-1092.843546**	**2.21**	**-1092.856739**	**1.91**
S_3	-1092.772055	3.79	-1092.776145	3.82	-1092.781101	3.91	-1092.782716	3.92

a – Energies of S_n states (n = 1, 2, 3) are obtained from the TD-DFT calculations of the $S_0 \rightarrow S_n$ transitions; b – for the solvents considered both linear-response (LR) and state-specific (SS) [109] PCM calculations were used; the results of SS-PCM calculations including solvent relaxation upon excitation are given in bold; c – PCM calculations using 1,4-dioxane as a solvent model; d – PCM calculations using dichloromethane as a solvent model; e – PCM calculations using acetonitrile as a solvent model. Values in *eV* represent the difference between S_n and S_0 energies (where *n* = 1,2,3).

Table S2. Experimental solvatochromic shifts for every solvent used relative to those in 1,4-dioxane.

Compound	**1**	**2**	**3**	**4**	**5**	**6**
Solvatochromic shift[a]						
	1,4-dioxane ($\varepsilon = 2.25$)					
$\Delta\lambda_{abs}$, nm	0	0	0	0	0	0
eV	0.00	0.00	0.00	0.00	0.00	0.00
	Ethyl Acetate ($\varepsilon = 6.02$)					
$\Delta\lambda_{abs}$, nm	0	3	3	4	-4	2
eV	0.00	0.02	0.02	0.02	-0.03	0.01
	CH_2Cl_2 ($\varepsilon = 8.93$)					
$\Delta\lambda_{abs}$, nm	8	4	6	7	11	7
eV	0.08	0.03	0.05	0.04	0.07	0.04
	Acetone ($\varepsilon = 20.7$)					
$\Delta\lambda_{abs}$, nm	5	-1	0	-2	7	4
eV	0.05	-0.01	0.00	-0.01	0.04	0.02
	CH_3CN ($\varepsilon = 37.5$)					
$\Delta\lambda_{abs}$, nm	5	-3	0	-4	9	5
eV	0.05	0.00	0.02	0.00	0.03	0.04
	DMSO ($\varepsilon = 46.7$)					
$\Delta\lambda_{abs}$, nm	13	12	10	9	11	8
eV	0.12	0.07	0.08	0.05	0.07	0.05

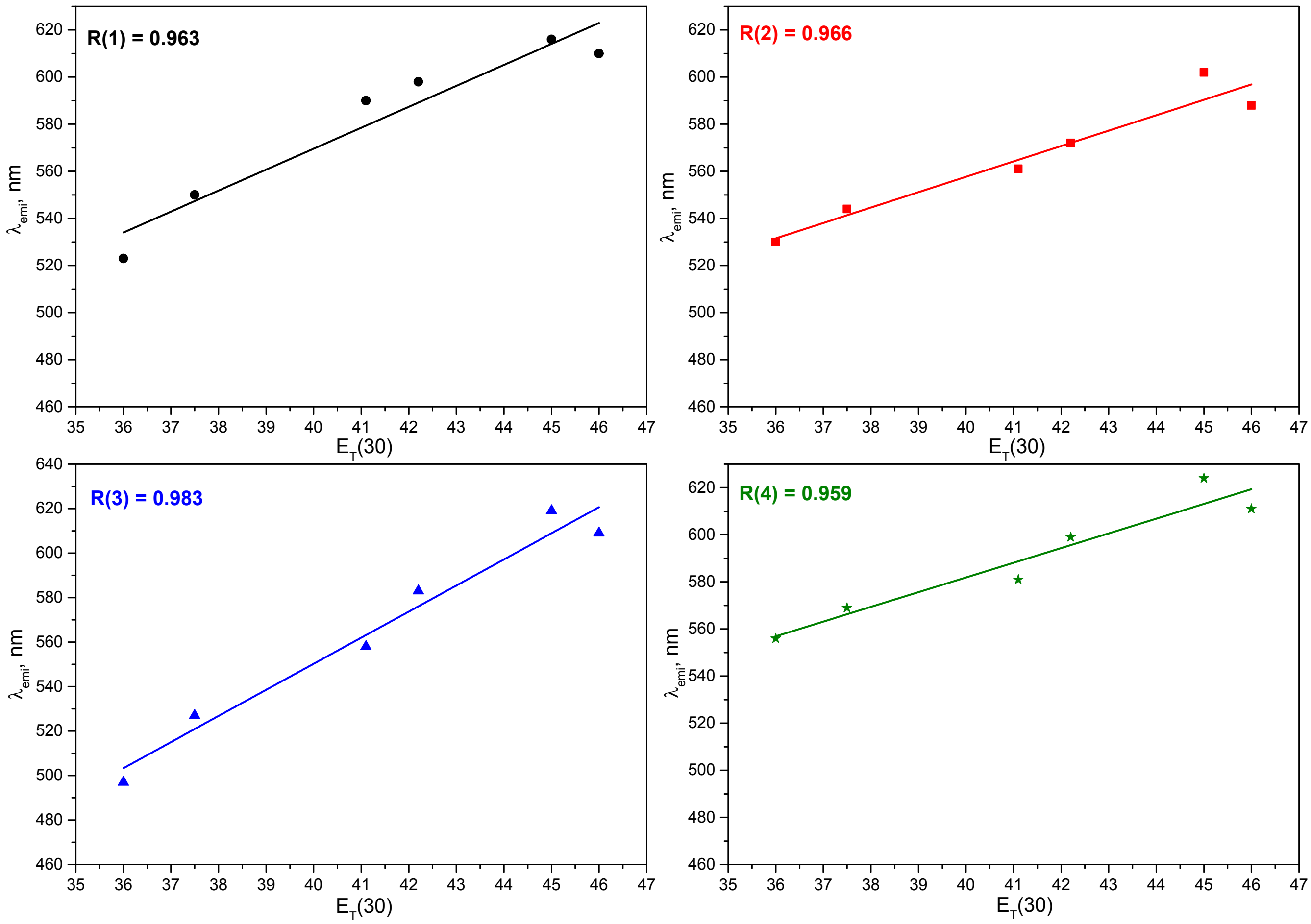

Figure S1. Linear correlation between $E_T(30)$ values [taken from Ch. Reichardt, E. Harbusch-Gornert, *Liebigs Ann. Chem.*, **1983**, 721 – 743] and the experimental positions of λ_{emi} for compounds **1-4** in every solvent used.