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SUPPLEMENTARY DATA

Gaining insight into the photophysical properties of a coumarin STP ester with potential for bioconjugation

M. González-Pérez,[a] S. Y. Ooi,[b] S. Martins,[a] João P. Prates Ramalho,[b] A. Pereira,[a,b] A. T. Caldeira [a,b]

[a] HERCULES Laboratory, Evora University, Largo Marquês de Marialva 8, 7000-809 Evora, Portugal

[b] Chemistry Department, School of Sciences and Technology, Evora University, Rua Romão Ramalho 59, 7000-671 Evora,, Portugal

***Corresponding author:**

Ana Teresa Caldeira, e-mail: atc@uevora.pt

Figure S1. Calculated UV-visible spectra for the *Z* and *E* isomers of C392STP (green and red, respectively) and for their mixture (*E/Z* 84/16) (black) and comparison with the experimental (blue) spectra in THF, methanol and water.

Table S1. Calculated electronic transition of the both isomers of C392STP in different solvents at PBE0/6-PBE0/311+G(2d,p) level of theory.

Table S2. Calculated energies for both isomers in different solvents at the B3LYP/6-31+G(d) theory level.

Table S3. Results of the statistical treatment of the Bakhshiev, Lippert-Mataga and Kawski-Chamma-Viallet correlations obtained considering the absobtion and emission frequencies in the solvents selected: slopes (m), intercepts (p) and correlation coefficients R^2 and adjR^2

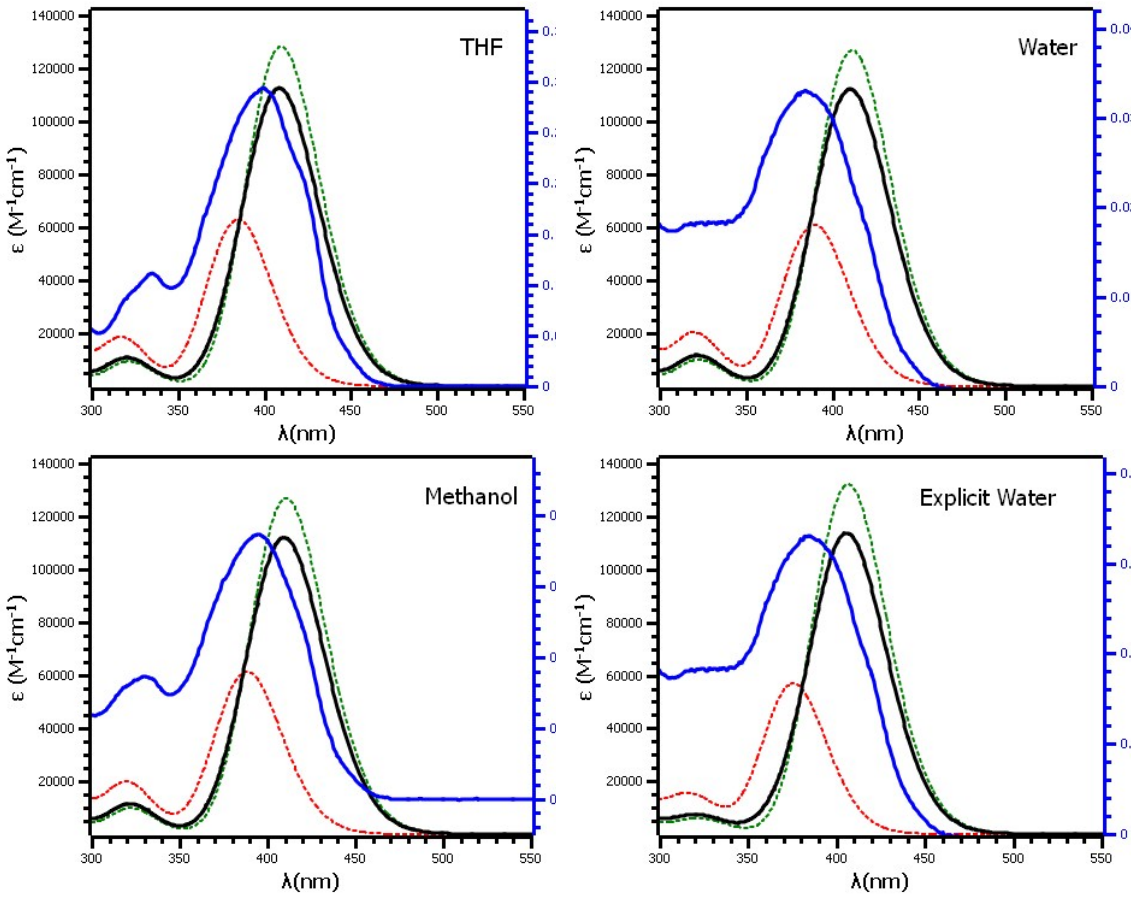

Figure S1. Calculated UV-visible spectra for the *Z* and *E* isomers of C392STP (green and red, respectively) and for their mixture (*E/Z* 84/16) (black) and comparison with the experimental (blue) spectra in THF, methanol and water.

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Table S1. Calculated electronic transition of the both isomers of C392STP in different solvents at PBE0/6-PBE0/311+G(2d,p) level of theory.

		λ/nm	Oscillator strength (f)	Key transitions
THF				
	S_1	409	1.773	H->L (99%)
E	S_2	324	0.046	H->L+1 (90%)
	S_3	320	0.085	H-2->L (86%)
	S_1	384	0.870	H->L (99%)
Z	S_2	324	0.093	H->L+1 (89%)
	S_3	314	0.175	H-2->L (84%)
Methanol				
	S_1	410	1.753	H->L (99%)
E	S_2	326	0.031	H->L+1 (89%)
	S_3	321	0.106	H-1->L (85%)
	S_1	388	0.847	H->L (99%)
Z	S_2	327	0.124	H->L+1 (92%)
	S_3	315	0.172	H-1->L (86%)
H_2O				
	S_1	411	1.753	H->L (99%)
E	S_2	326	0.030	H->L+1 (89%)
	S_3	321	0.109	H-1->L (42%)
	S_1	389	0.842	H->L (99%)
Z	S_2	327	0.132	H->L+1 (92%)
	S_3	315	0.175	H-1->L (87%)
H_2O explicit				
	S_1	406	1.826	H->L (99%)
E	S_2	329	0.045	H->L+1 (94%)
	S_3	316	0.046	H-1->L (85%)
	S_1	375	0.786	H->L (99%)
Z	S_2	324	0.123	H->L+1 (92%)
	S_3	309	0.130	H-1->L (86%)

Table S2. Calculated energies for both isomers in different solvents at the B3LYP/6-31+G(d) theory level.

Solvent	Energy (a.u)		ΔE (kcal mol^{-1})
	E isomer	*Z* isomer	
THF	-2474.5127	-2474.5002	7.41
Methanol	-2474.5264	-2474.5146	7.86
Water	-2474.5289	-2474.5172	7.33

Table S3. Results of the statistical treatment of the Bakhshiev, Lippert-Mataga and Kawski-Chamma-Viallet correlations obtained considering the absobtion and emission frequencies in the solvents selected: slopes (m), intercepts (p) and correlation coefficients R^2 and adjR^2.

Models						
Bakhshiev $\nu_{abs}-\nu_{em}=mf_B(\varepsilon_r,\eta)+p$;[a]						
	m	**p**	R^2	**adjR^2**	**n[b]**	**Solvents excluded**
Polar aprotic	1224 (266)	3838 (174)	0.8416	0.8020	**6**	**-**
Polar protic	3821 (1198)	1694 (986)	0.7178	0.6472	**6**	**7,8**
Polar	1263 (211)	3806 (157)	0.7822	0.7604	**12**	**7,8**
Lippert-Mataga $\nu_{abs}-\nu_{em}=mf_{LM}(\varepsilon_r,\eta)+p$ [c]						
	m	p	R^2	adjR^2	**n**	**Solvents excluded**
Polar aprotic	3488 (1153)	3834 (262)	0.6957	0.6196	**6**	**-**
Polar protic	11023 (3330)	1647 (964)	0.7326	0.6658	**6**	**7,8**
Polar	3624 (768)	3796 (200)	0.6897	0.6587	**12**	**7,8**
Kawski-Chamma-Viallet $\nu_{abs}+\nu_{em}=m_{KCV}\left[f_B(\varepsilon_r,\eta)+2g_{KCV}(\eta)\right]+p$ [d]						
	m	p	R^2	adjR^2	**n**	**Solvents excluded**
Polar aprotic	-1694 (217)	48375 (328)	0.9386	0.9232	**6**	**-**
Polar protic	-5766 (4616)	55081 (7534)	0.2806	0.1008	**6**	**7,8**

[a] $f_B(\varepsilon_r,\eta)=\left(2\eta^2-1/\eta^2+2\right)\left[(\varepsilon_r-1/\varepsilon_r+2)-\left(\eta^2-1/\eta^2+2\right)\right]$;

[b] number of solvents included in the correlation;

[c] $f_{LM}(\varepsilon_r,\eta)=(\varepsilon_r-1/2\varepsilon_r+1)-\left(\eta^2-1/2\eta^2+1\right)$;

[d] $g_{KCV}(\eta)=3/2\left[\left(\eta^4-1\right)/\left(\eta^2-1\right)^2\right]$