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Electronic Supplementary Information
4,4'-bis(2-benzoxazolyl)stilbene luminescent probe: assessment of aggregates formation through photophysics experiments and quantum-chemical calculations

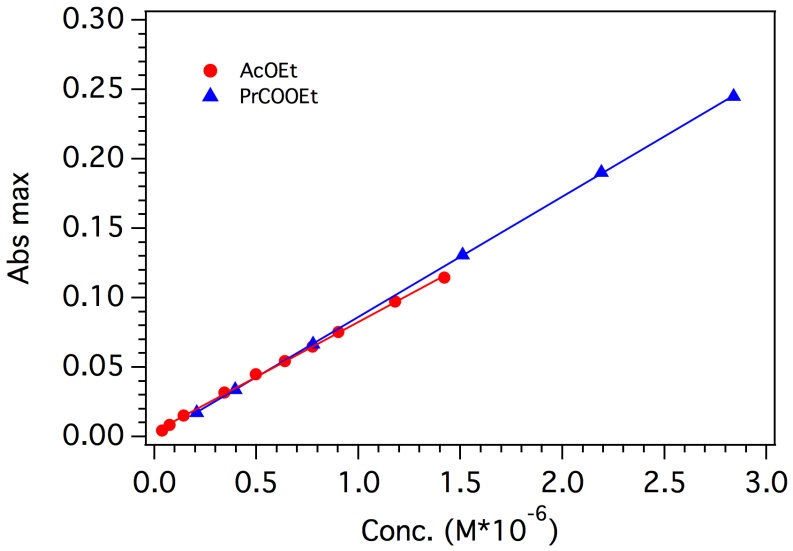

Figure S1 Absorbance maxima vs concentration for BBS solutions in AcOEt (red) and PrCOOEt (blue).

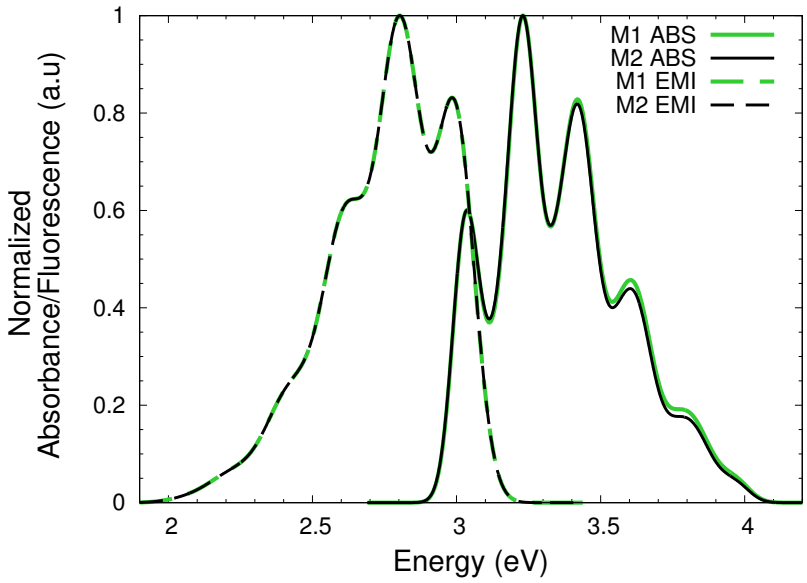

Figure S2 Calculated M06-2X/6-31+G* vibrationally resolved absorption and emission spectra of M1 and M2 in toluene, obtained by using the AH approach.

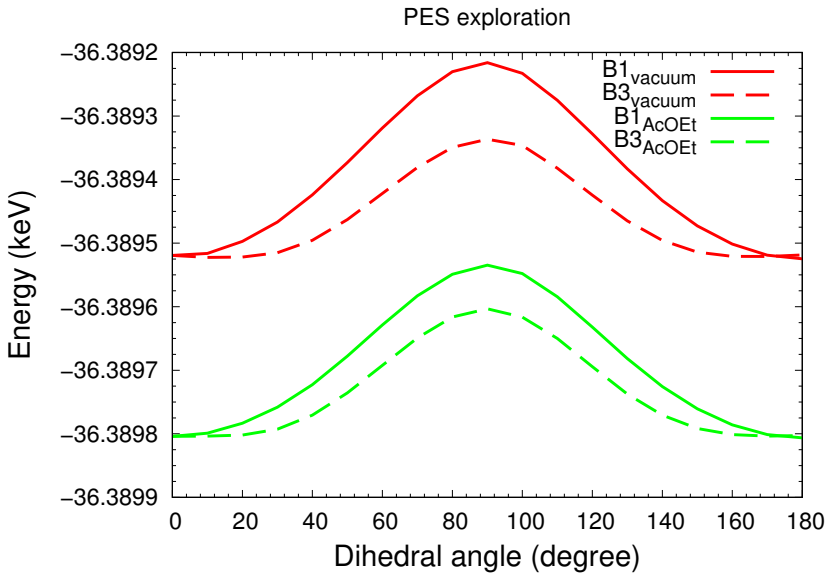

Figure S3 Scan around B1 and B3 bonds as reported in Figure 3 computed at M06-2X/6-31+G* level of theory in vacuum and in AcOEt.

Geometrical Parameter	Percentage Change $S_0 \rightarrow S_1$
B1	-1.97%
B2	-2.17%
B3	-4.08%
B4	4.47%
B5	-4.08%
B6	-2.17%
B7	-1.97%

Table S1 BBS M1 structure. Calculated M06-2X/6-31+G* bond length variation resulting from the excitation process. Data are obtained in toluene solution.

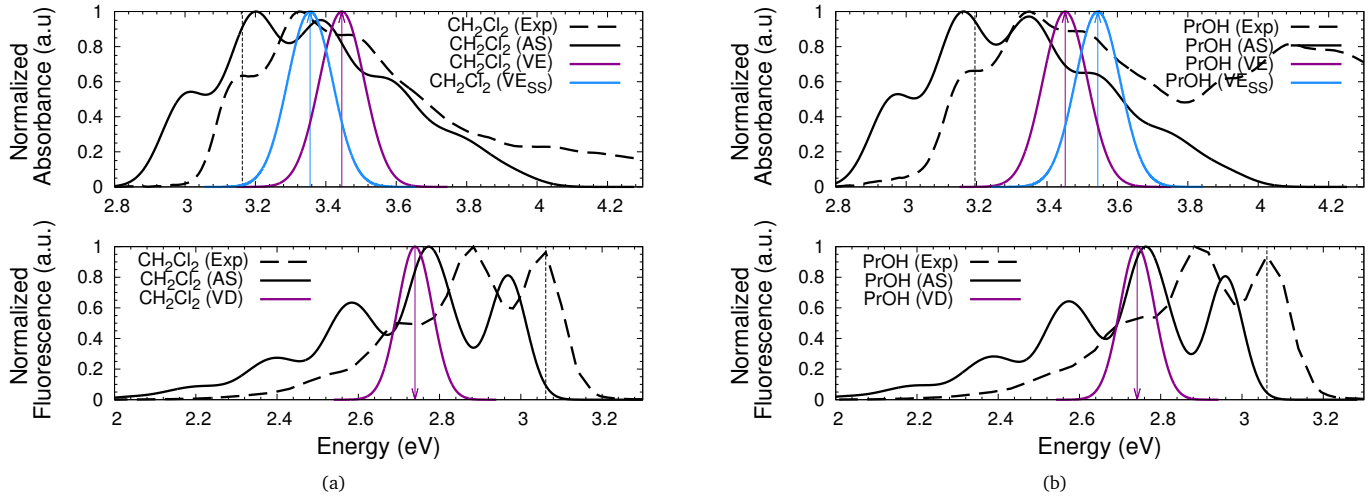

Figure S4 Calculated BBS absorption and emission spectra in various solvents obtained through vertical excitation (violet: solvent linear response, blue: state specific solvation) and the AS approach. All calculated spectra were obtained by summing oscillator strengths weighted Gaussian curves with a Full Width at Half Maximum (FWHM) of 0.15 and 0.1eV for the absorption and emission case respectively. Experimental spectra of diluted (10^{-5} M) solutions are also reported to comparison's sake.

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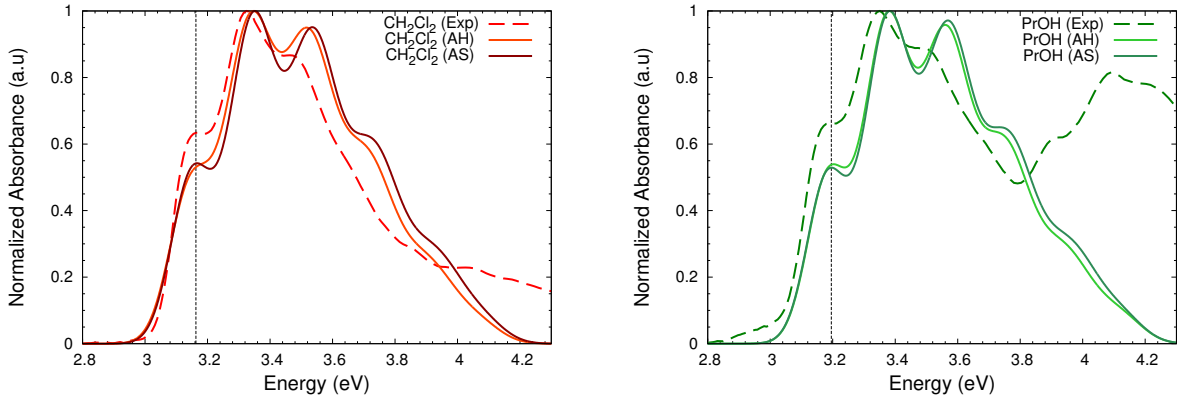
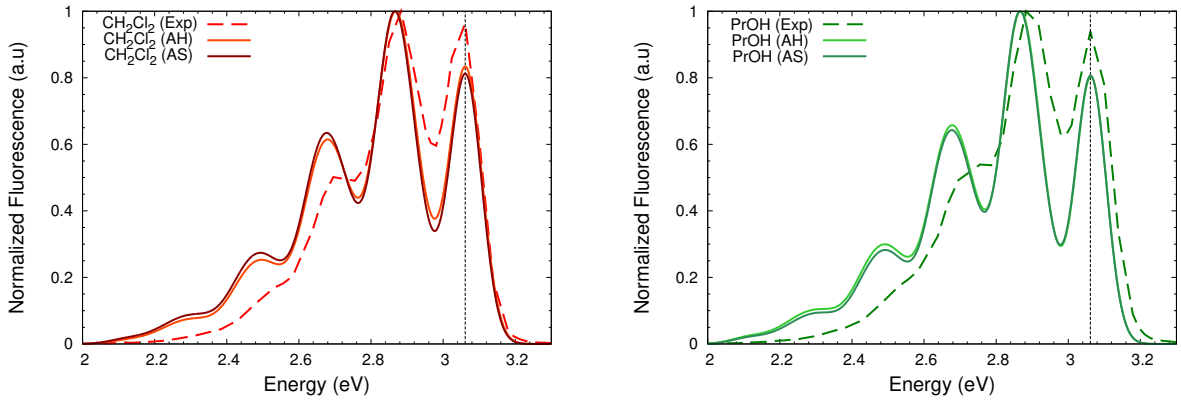


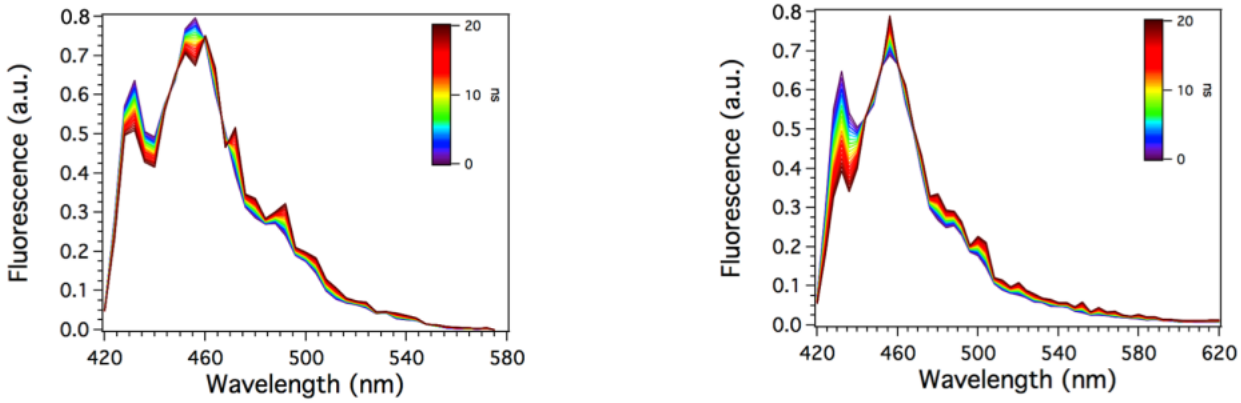
(a) (b)

Figure S5 Calculated vibrationally resolved absorption spectra of M1 in different solvents using the AH and AS approach are compared with the experimental spectra of diluted (10^{-5} M) solutions. All calculated spectra were obtained by summing normalized molar absorption coefficient weighted Gaussian curves with a Full Width at Half Maximum (FWHM) of 0.15 eV for each calculated energy value.



(a) (b)

Figure S6 Calculated vibrationally resolved emission spectra of M1 in different solvents using the AH and AS methods are compared with the experimental spectra of diluted (10^{-5} M) solutions. All calculated spectra were obtained by summing normalized energy emitted by one mole per second weighted Gaussian curves with a Full Width at Half Maximum (FWHM) of 0.1 eV for each calculated energy value.



(a) (b)

Figure S7 Time-resolved emission spectra of BBS 10^{-5} M in (a) AcOEt and (b) PrCOOEt.

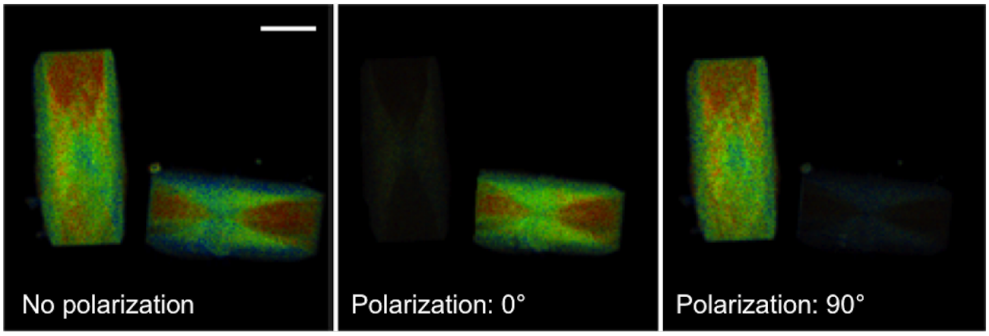


Figure S8 Pseudo-colour confocal images of BBS crystals fluorescence upon polarized light irradiation at 405 nm. Scale bar: 50 μm.

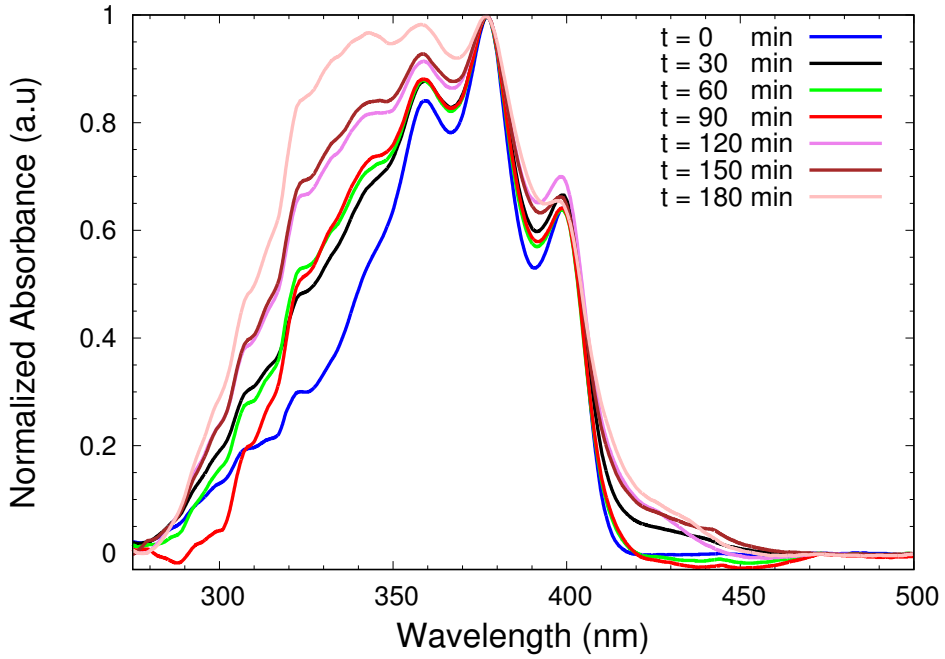


Figure S9 UV-Vis absorption spectra of a COC film containing the 0.5 wt.% of BBS during an annealing experiments aimed at favouring the formation of dye aggregates. The spectra are normalized to the absorption intensity attributed to the isolated BBS molecules at 377 nm.

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Table S2 M06-2X/6-31+G* in AcOEt vertical excitation energies (in eV) and oscillator strengths (f) of M1, M2 and of different dimeric structures (ST:Stacked, SL:Slide, HB:Herringbone) extracted from the crystal structure[20] and not optimized.

	States			
	S1	**S2**	**S3**	**Orientation**
E	*3.5919*	*4.4314*	*4.7968*	*M1*
f	*2.6596*	*0.0000*	*0.0348*	
E	*3.5912*	*4.4383*	*4.8014*	*M2*
f	*2.6398*	*0.0017*	*0.0383*	
E	*3.4768*	*3.5984*	*4.1755*	*ST1*
f	*0.0000*	*5.2302*	*0.0332*	
E	*3.4687*	*3.5988*	*4.1639*	*ST2*
f	*0.0017*	*5.2021*	*0.0320*	
E	*3.4700*	*3.5992*	*4.1752*	*ST3*
f	*0.0002*	*5.1907*	*0.0199*	
E	*3.5757*	*3.6091*	*4.4172*	*SL1*
f	*0.0053*	*5.2718*	*0.0003*	
E	*3.5758*	*3.6076*	*4.4198*	*SL2*
f	*0.0067*	*5.2487*	*0.0014*	
E	*3.5743*	*3.6078*	*4.4196*	*SL3*
f	*0.0024*	*5.2328*	*0.0002*	
E	*3.5850*	*3.6028*	*4.4222*	*HB1*
f	*2.0329*	*3.3032*	*0.0004*	
E	*3.5848*	*3.6023*	*4.4236*	*HB2*
f	*2.0345*	*3.2812*	*0.0004*	
E	*3.5844*	*3.6019*	*4.4289*	*HB3*
f	*2.0417*	*3.2533*	*0.0018*	