Supplementary Information

Part 1: Light Scattering

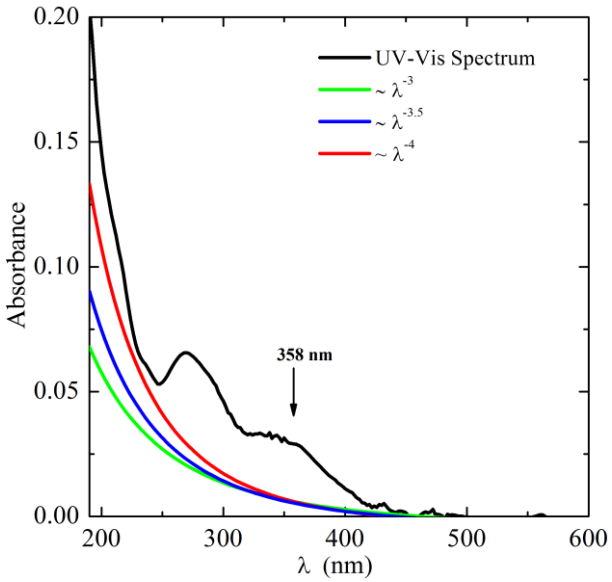

Figure S1: Absorbance spectrum of 0.9 µM of Prodan in water and three fits for the scattering using the function $a\lambda^{-x}$, with x = 3.7 (green), 4.0 (red) and 4.25 (blue)

Figure S1 illustrates the difficulty of subtracting a light scattering profile from the absorption spectrum of Prodan in water. Three different possible light scattering profiles are drawn, corresponding to functions $a\lambda^{-x}$, with x = 4.0 (red), 3.5 (blue) and 3.0 (green). It is impossible to evaluate which one is the correct one, as absorption bands are spread from 200 to 500 nm. Usually, different *x* values correspond to scattering particles of different dimensions.

It is important to notice that the intensity of the band at 358 nm is the less affected by light scattering, as mentioned in Results and Discussion. That is why it was the only one used for a quantitative analysis of the dependence of the optical spectrum on Prodan concentration (Figure 6).

Part 2: Electronic Transitions

*Table S1: Average values for electronic absorption transitions energies (in 10^3 cm^{-1}), wavelength (in nm), and its oscillator strengths for monomer and dimmer Prodan in water. Numbers in parentheses are standard deviations. *Transition n – π*. All other transitions are π – π*.*

Monomer				Dimmer			
Transition	Energy	λ	OS	Transition	Energy	λ	OS
1	28.48(3)	351	0.019(2)	1*	27.23(5)	367	0.001(1)
2	28.82(3)	347	0.480(8)	2*	27.31(5)	366	0.002(1)
3*	28.92(5)	346	0.022(7)	3	28.88(5)	346	0.051(3)
4	36.92(5)	271	0.593(6)	4	29.04(3)	344	0.042(2)
5	38.76(3)	258	0.609(11)	5	30.86(1)	324	0.266(20)
6	39.52(4)	253	0.346(11)	6	31.38(8)	319	0.598(17)
7	41.69(5)	240	0.245(9)	7	36.66(30)	273	0.615(75)
8	44.31(4)	225	0.008(3)	8	38.02(20)	263	0.475(50)
				9	39.20(20)	255	0.317(38)
				10	39.72(14)	252	0.440(34)
				11	40.90(20)	244	0.257(28)

For the monomer Prodan in water, the electronic absorption transition energies were calculated with ZINDO/CIS over 75 statistically uncorrelated configurations, composed by 1 explicit Prodan molecule embedded in the electrostatic field of the 290 water molecules represented as point charges. To take into account the effect of the Prodan aggregation, the electronic absorption transition energies were calculated in 75 statistically uncorrelated configurations, composed by 2 explicit Prodan molecules (dimmers selected from the liquid Prodan simulation) embedded in the electrostatic field of the self-consisted reaction field (SCRF) of the aqueous solution. The final values for the electronic absorption transition energies were calculated as an average over the 75 QM calculations.