Electronic Supplementary Material (ESI) for RSC Advances.

Revised Version

Quantitative investigations of thermal and photoinduced J- and H-aggregation of hydrophobic spirooxazines in binary solvent through UV/VIS spectroscopy

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Supplementary Information Part

1)- Absorbance(λ_1) *vs* Absorbance(λ_2) diagrams

a)- Analysis of the H-aggregates of **1** vs concentration

They have been used to demonstrate the invariance of the H-aggregates spectra at various concentrations (from figure 2a of the main text):

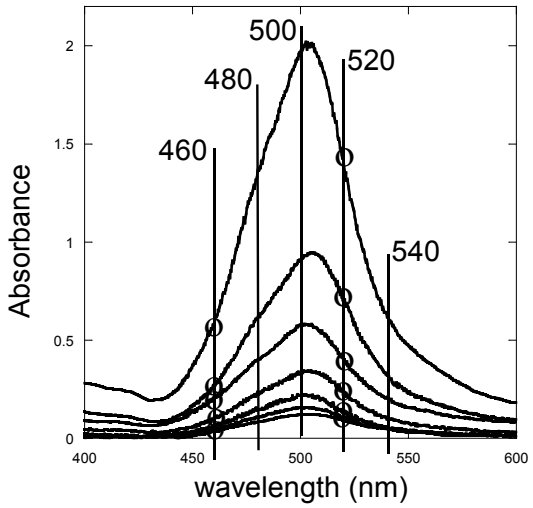

Figure 1S: Selection of the various wavelengths for the invariance check. For the sake of clarity only two wavelength (460and 520nm) are fully displayed. The circles illustrate the pick-up of the 7 absorbances values at 460 and 520nm.

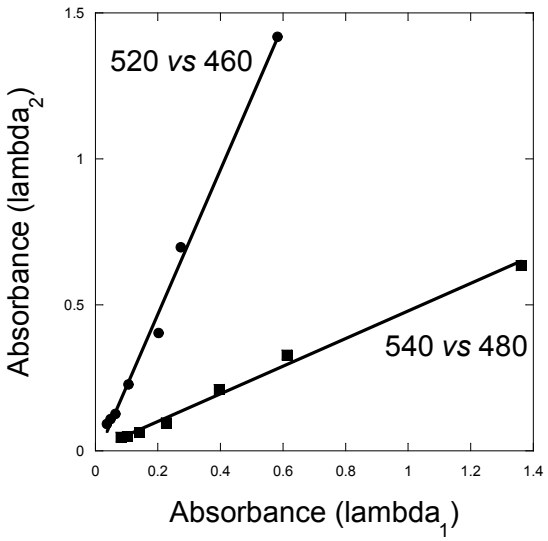

Figure 2S: Example of Abs vs Abs diagrams from figure 1S (only two line have been plotted).

For the linear analysis of the figure 1S Abs *vs* Abs diagrams, the selected 5 wavelengths have been plotted together (10 pairs). The linearity of the plots has been checked from the values linear regression coefficients.

Wavelengths (nm)	460	480	500	520	540
460	X	**.99833**	**.99835**	**.99696**	**.99644**
480		X	**.99993**	**.99865**	**.99644**
500			X	**.99895**	**.99690**
520				X	**.99842**
540					X

Table IS: Values of the linear regression coefficients of the various Abs *vs* Abs diagrams extracted from figure 1S. All the values are > 0.996 confirming the invariance of the shape of the 510nm band.

b)- Analysis of the H-aggregation spectral evolution of **1**

7 wavelengths have been selected on the figure 3 (main text) and 21 pairs have been checked for linearity.

wavelengths (nm)	476	511	536	581	591	626	661
476	X	**.99637**	**.99570**	**.98877**	**.99245**	**.99298**	**.99765**
511		X	**.98637**	**.99731**	**.99869**	**.99926**	**.99846**
536			X	**.97542**	**.98080**	**.98003**	**.99109**
581				X	**.99946**	**.99876**	**.99434**
591					X	**.99914**	**.99598**
626						X	**.99639**
661							X

Table IIS: Values of the linear regression coefficients of the various Abs vs Abs diagrams extracted from figure 3 (main text). All are higher than 0.980 confirming the linearity of all the diagrams, the presence of only two spectra and therefore the absence of any intermediate.

c)- Analysis of the H- and J-aggregation spectral evolution of **1** in presence of SDS

6 wavelengths have been selected on the figure 5 (main text) and 15 pairs have been checked for linearity.

	362	443	512	582	617	668
362	X	**.99703**	**.98472**	.42372	.15559	**.98070**
443		X	**.99039**	.43090	.12835	**.98647**
512			X	.51285	.00702	**.99941**
582				X	.75155	.53979
617					X	.02242
668						X

Table IIIS: Values of the linear regression coefficients of the various Abs *vs* Abs diagrams extracted from figure 6 (main text). Those higher than 0.980 are displayed in bold. For these wavelengths, linearity is insured. Note however the lack of correlation for 582 and 617nm.

d)- Abs vs Abs diagram analysis of the photo-induced aggregation of **2**

	376	480	519	609	668	675
376	X	**.97994**	**.97337**	.61729	**.82557**	**.87184**
480		X	**.99740**	.69969	**.88417**	**.92361**
519			X	.74489	**.91143**	**.94513**
609				X	**.94730**	**.91531**
668					X	**.99553**
675						X

Table IVS: Values of the linear regression coefficients of the various Abs *vs* Abs diagrams extracted from figure 8 (main text). Those higher than 0.825 are displayed in bold showing the linearity. Note the lack of correlation for 609nm with 376, 480 and 519nm.

2)-Kinetic analysis of the H-aggregation of **1**

Because the kinetic of the aggregation is monitored by an UV/visible spectrophotometer, the absorbance is a linear function of the concentration of the aggregates. The normalized evolution is given by: $Y = (Abs(t) - Abs_\infty) / (Abs_0 - Abs_\infty)$. This is a decreasing function going from Y = 1 at t = 0 to Y = 0 at $t \rightarrow \infty$.

Table VS provides a brief summary of some of the most common expressions used in the literature for fitting aggregation kinetic data displayed on figure 4A (main text).

entry	integrated equation	parameters	F (10^{-5})	figure
1 A-E	$Y= \exp[-(kt)^n]$	k; n	27.9	3S
2 F-W	$Y=((k_1/k_2)+A_0)/(1+(k_1/k_2A_0)\exp(k_1+k_2A_0)t)$	k_1; k_2A_0	9.35	4S
3 SKa	$Y=\exp\{-[\alpha/t][\exp(\beta t^2)-1]\}$	α; β	24.4	5S
4 SKd	$Y=\exp\{[\alpha t][\exp(-\beta t^2)-1]\}$	α; β	1.82	4A

Table VS : List of integrated 2-parameters equations used to check the figure 4a kinetic record. A-E: Avrami-Erofe'ev; F-W: Finke-Watzky; SKa: Skrdla "acceleratory"; SKd: Skrdla "deceleratory". The normalized evolution is given by: $Y = (Abs(t) - Abs_\infty) / (Abs_0 - Abs_\infty)$. F: residual least squares.

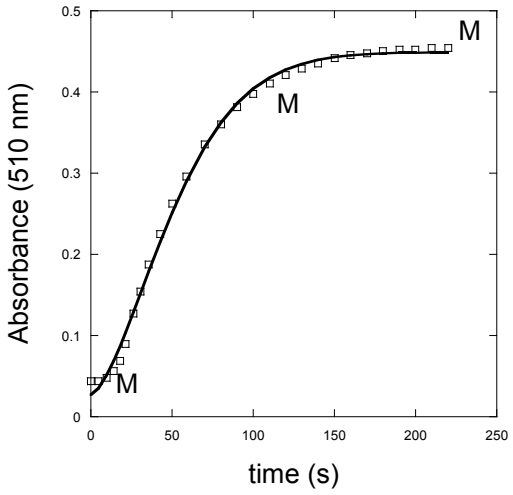

Figure 3S: Attempt to fit the aggregation kinetics with the Avrami-Erofe'ev equation using A_0 = 2.72e-2; A_{inf} = 4.49e-1; k = 1.67e-02; n =1.57. Note in "M" the misfit zones.

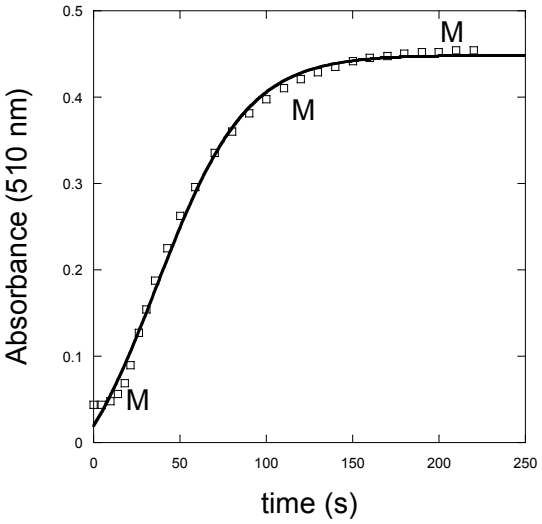

Figure 4S: Attempt to fit the aggregation kinetics with the Finke-Watzky equation using Abs_0 = 1.94e-02; Abs_{inf} = 4.49e-01; $k_2[A_0]$= 3.08e-2; k_1 = 7.56e-3. Note in "M" the misfit zones.

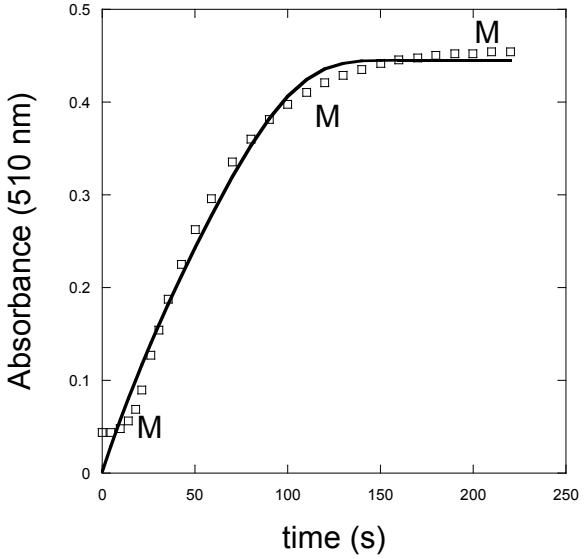

Figure 5S: Attempt to fit the aggregation kinetics with the Skrdla "acceleratory" equation using Abs_0 = 1.38e-03; Abs_{inf} = 4.45e-01; alpha = 1.30e+02; beta = 1.05e-04. Note in "M" the misfit zones.

3)-Kinetic analysis of the aggregation of **1** in presence of SDS (from figure 9A).

The Skrdla "decelerative" equation has been used to fit the kinetic record.

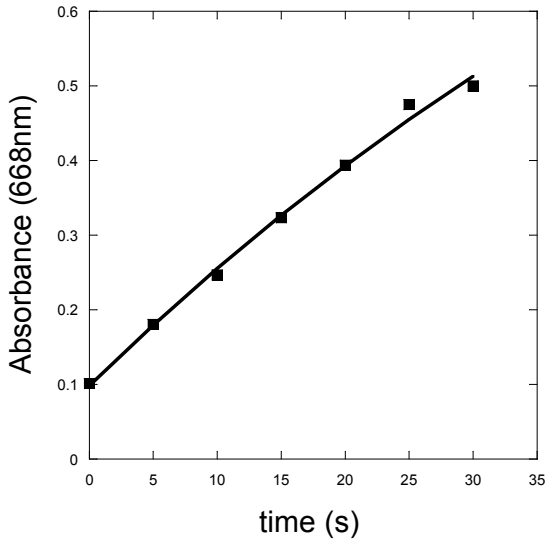

Figure 6S: Fit of the aggregation kinetics of **1** in presence of SDS with the Skrdla "decelerative" equation using Abs_0 = 9.83e-02; Abs_{inf} = 1.34; α = 1.36e-2; β= 0.2.

4)-Kinetic analysis of the photo-induced aggregation of **2** in presence of SDS (from figure 9B).

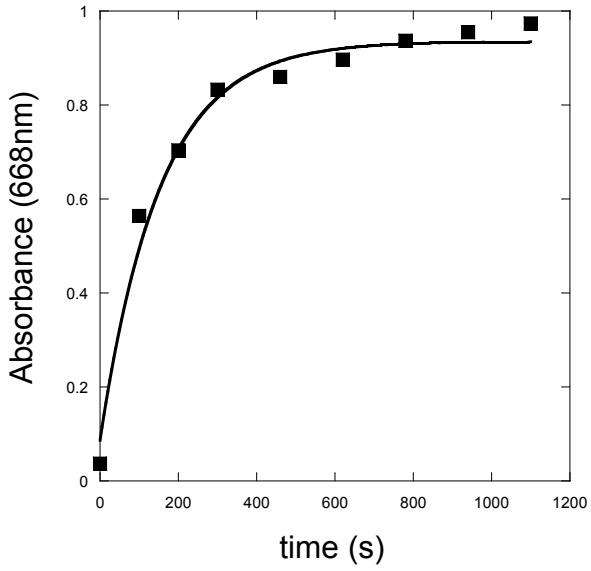

Figure 7S: Fit of the photo-induced aggregation kinetics of **2** in presence of SDS with the Skrdla "decelerative" equation using Abs_0 =6.64e-2; Abs_{inf} =0.93; α =0.007; β=0.2.