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Photophysics of Crystal Violet Lactone in Reverse Micelles and Its Dual Behavior

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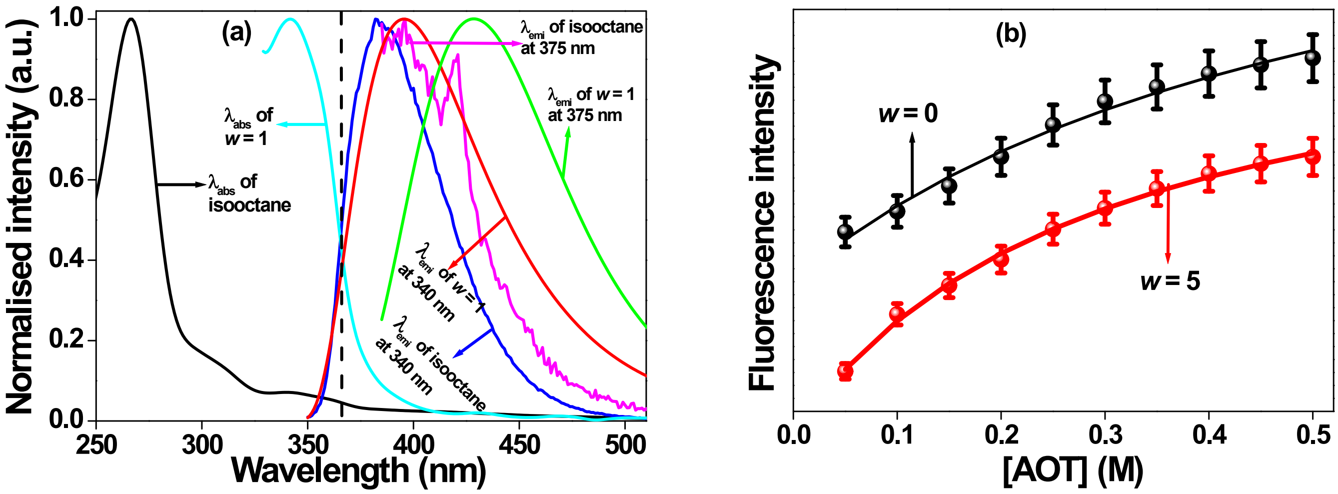

Fig. S1: (a) The change of absorption and emission spectra of CVL in isooctane and water RM (*w* = 1), (b) plot of fluorescence intensity of CVL in AOT/isooctane mixture (*w* = 0) and water RM (*w* = 5).

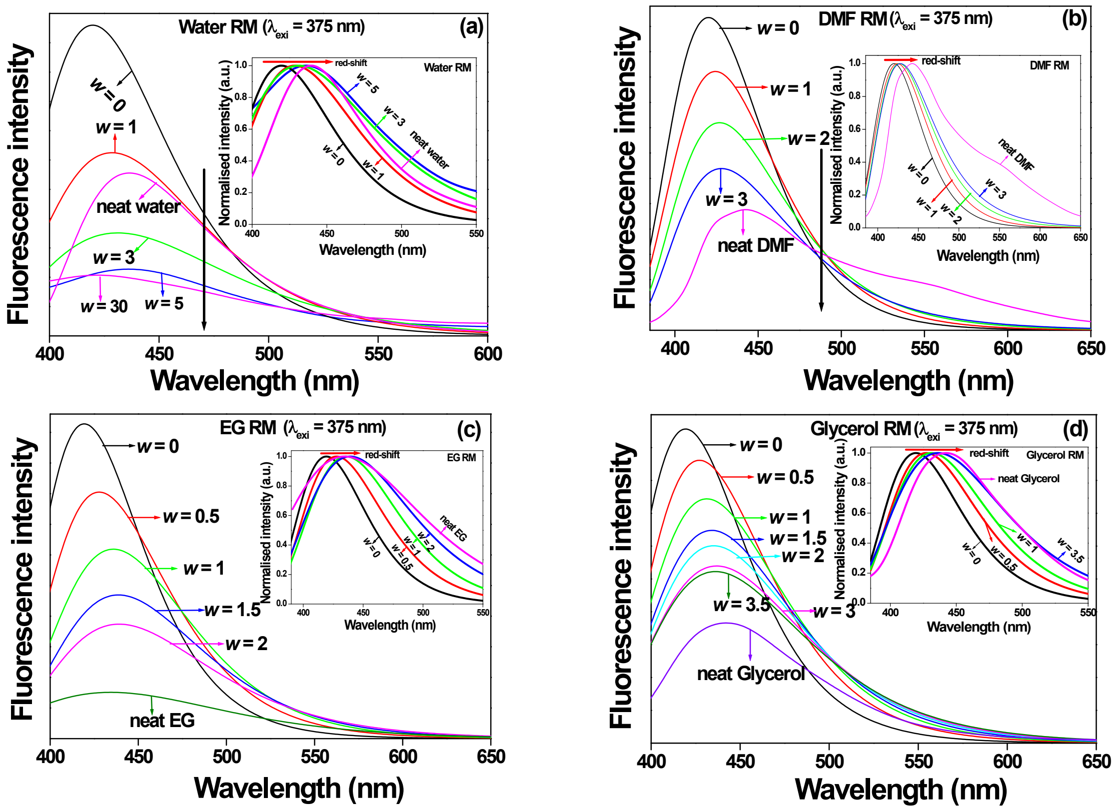

Fig. S2: The emission spectral profiles of CVL (λ_{exi} = 375 nm) in (a) water RM, (b) DMF RM, (c) EG RM and (d) glycerol RM with variation of respective '*w*' values and the corresponding neat solvents. Inset of the respective figure shows the change of the emission spectral shift.

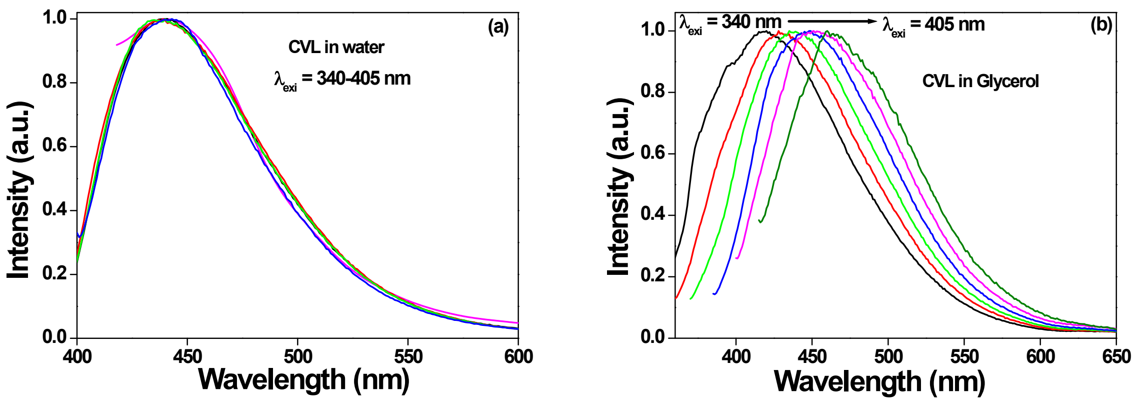

Fig. S3: The excitation wavelength dependent emission spectral shift of CVL in (a) water and (b) glycerol solvents.

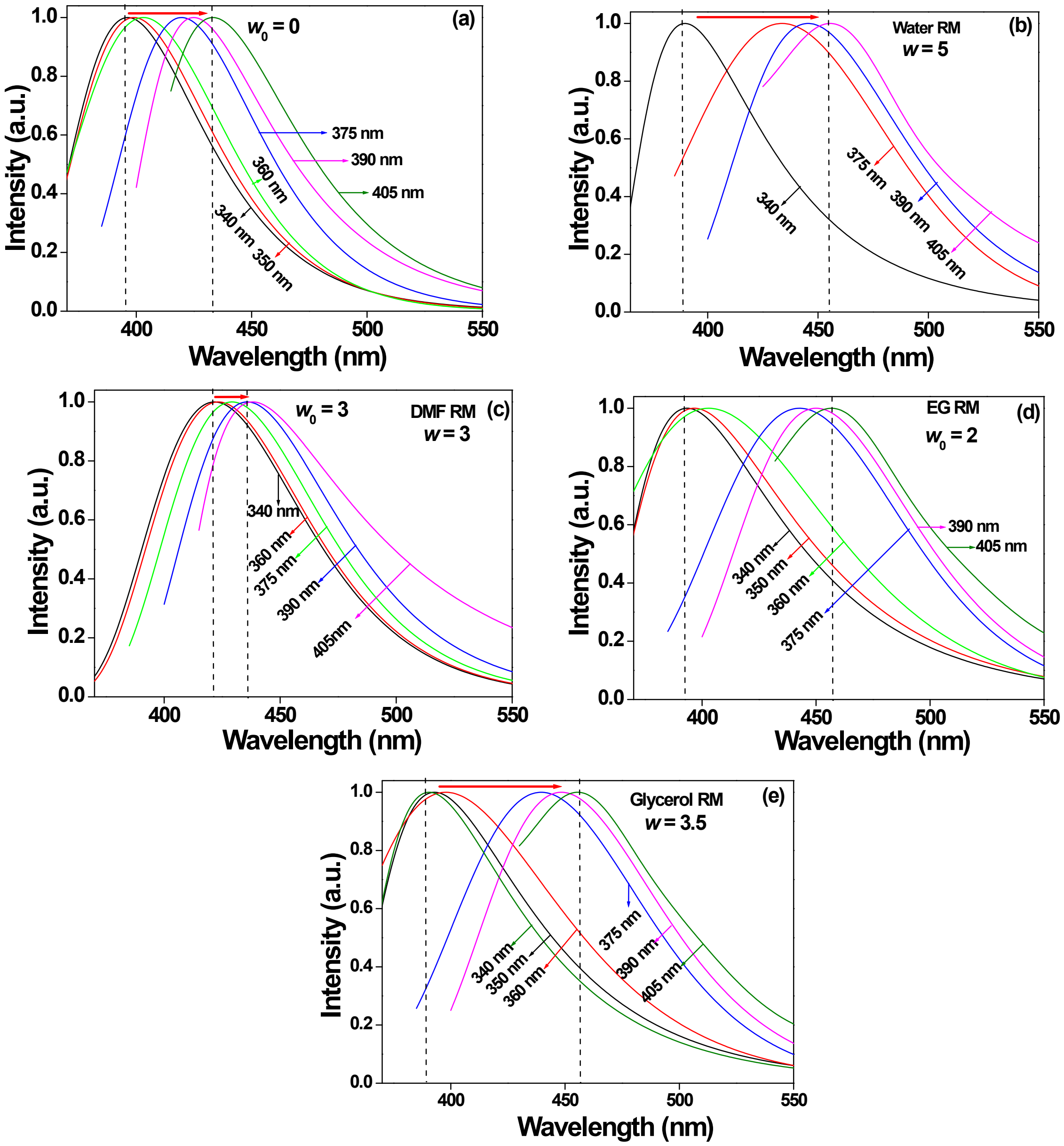

Fig. S4: The excitation wavelength dependent emission spectral shift of CVL in (a) isooctane/AOT system, (b) water RM, (c) DMF RM, (d) EG RM and (e) glycerol RM (λ_{exi} = 340 to 405 nm).

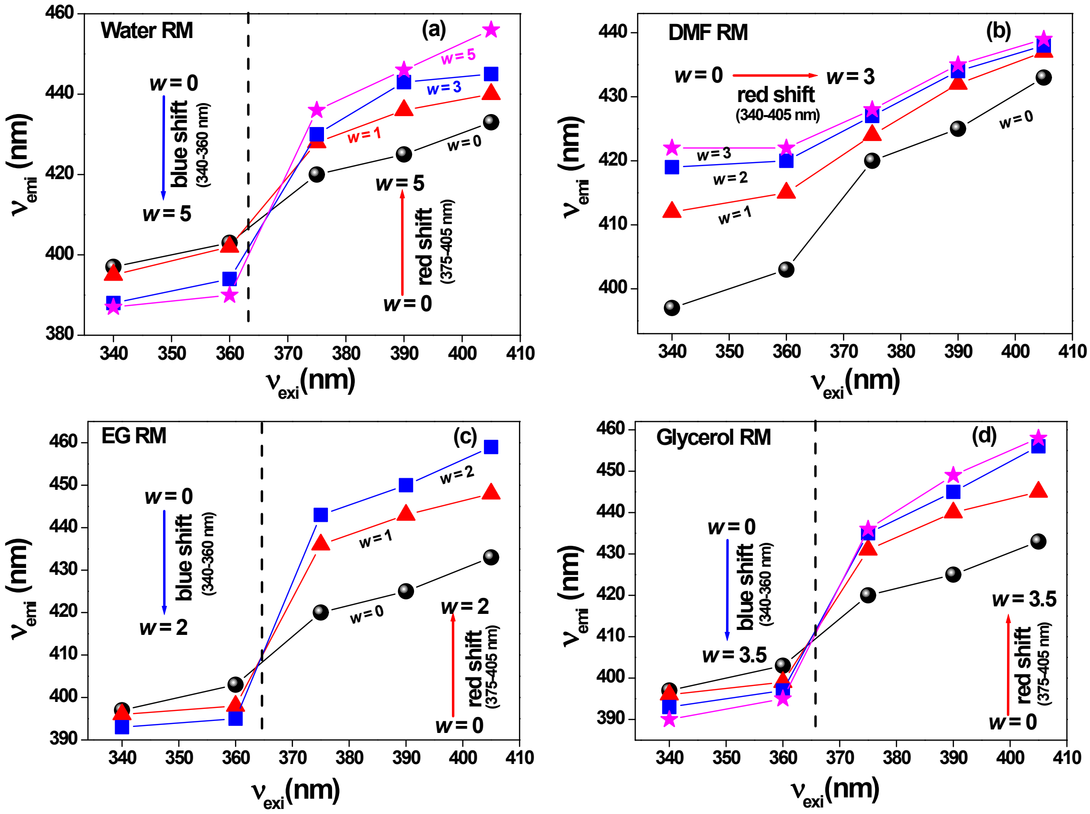

Fig. S5: The change of emission spectral shift of CVL with the change in excitation wavelengths in (a) water RM, (b) DMF RM, (c) EG RM and (d) glycerol RM.

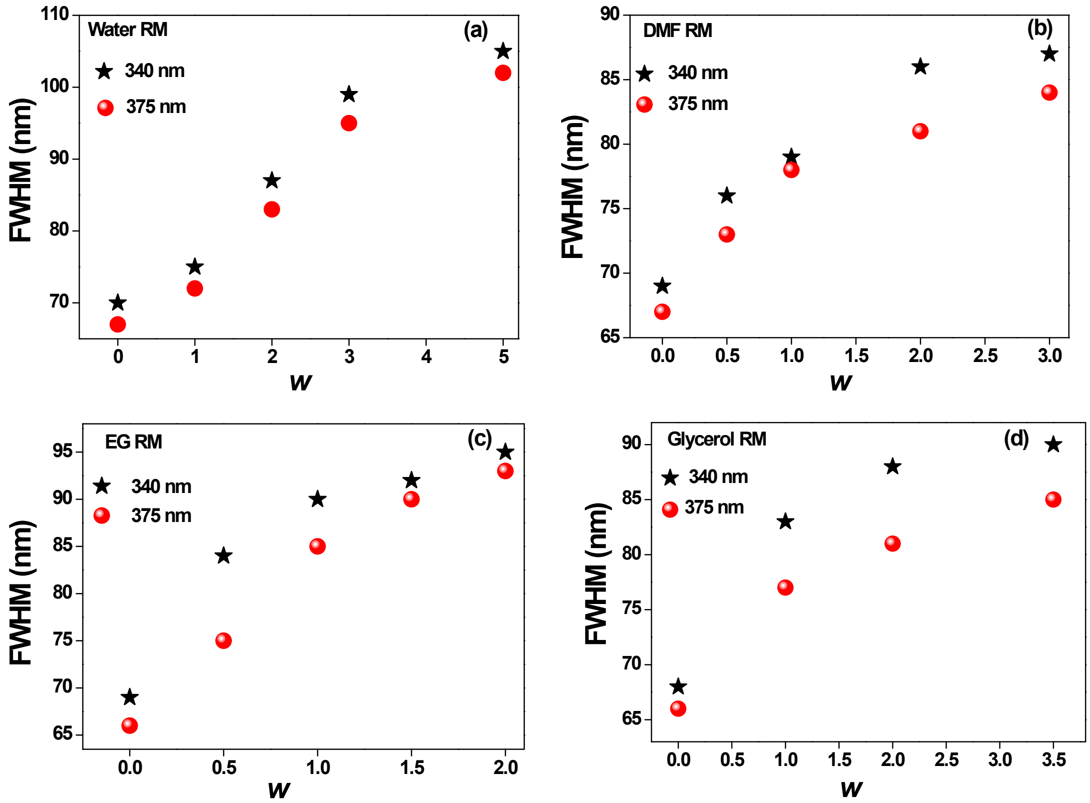

Fig. S6: Plot of FWHM of the fluorescence emission spectra of CVL against variation of '*w*' values in (a) water RM, (b) DMF RM, (c) EG RM and (d) glycerol RM at different excitation wavelengths.

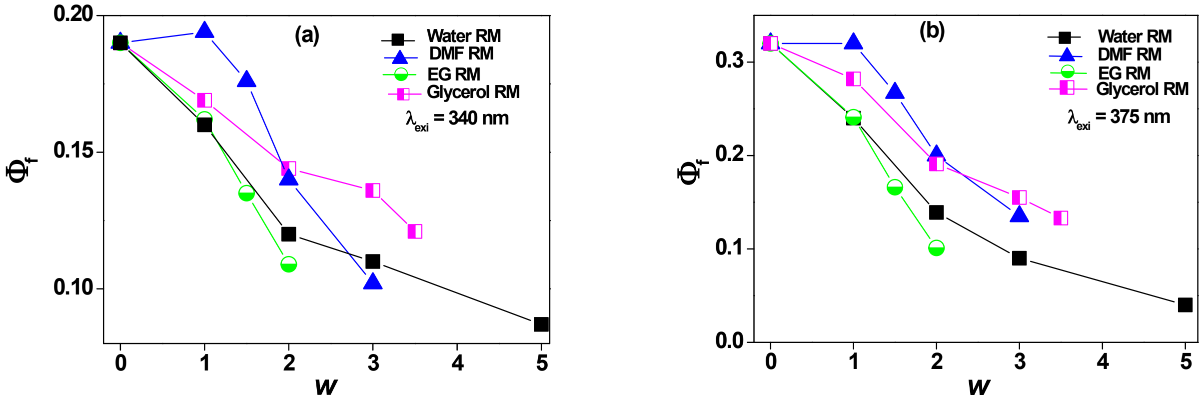

Fig. S7: The change of fluorescence quantum yield (ϕ_f) values of CVL against variation of '*w*' values in presence of different reverse micelles at different excitation wavelengths at (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

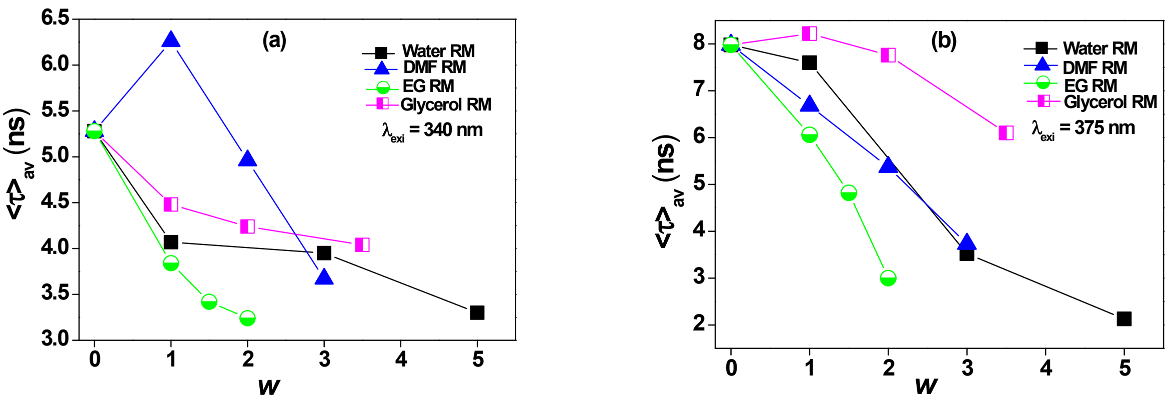

Fig. S8: The change of average fluorescence lifetime (<τ_f>) values of CVL against variation of '*w*' values in presence of different reverse micelles at different excitation wavelengths at (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

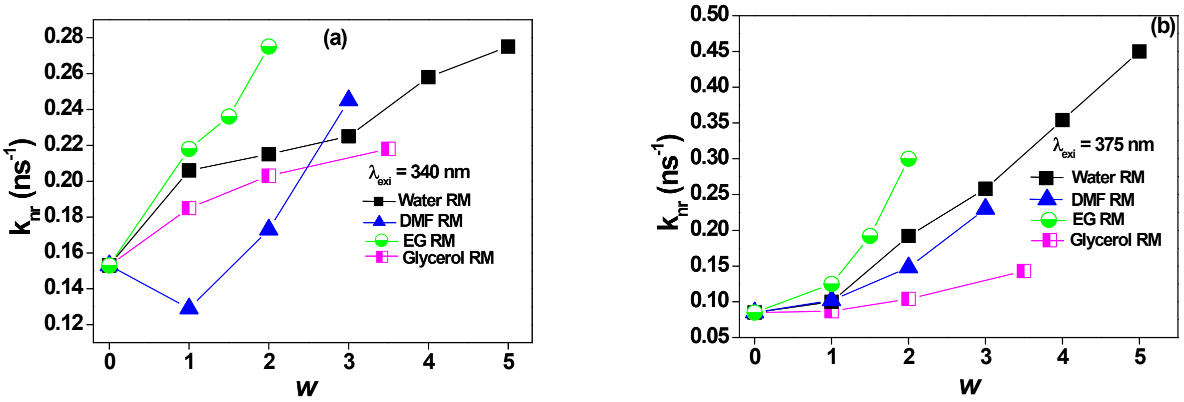

Fig. S9: The change of non-radiative decay rate constant (k_{nr}) values of CVL against variation of '*w*' values in presence of different reverse micelles at different excitation wavelengths at (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

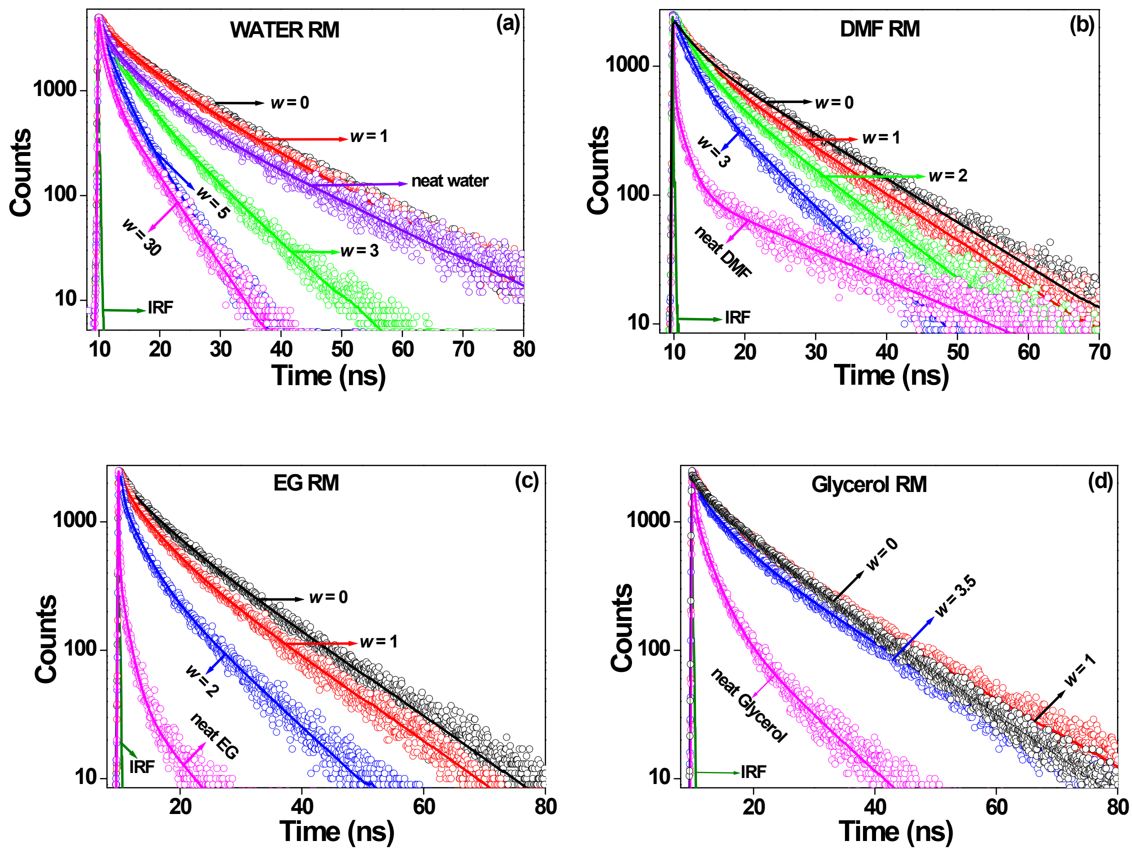

Fig. S10: The fluorescence emission decay profiles of CVL (λ_{exi} = 375 nm) in (a) water RM, (b) DMF RM, (c) EG RM and (d) glycerol RM with variation of respective '*w*' values.

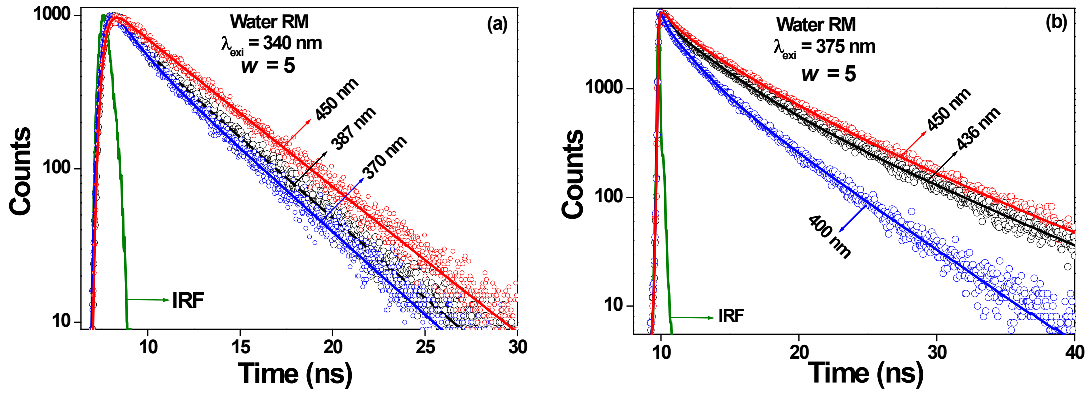

Fig. S11: The emission wavelength dependent fluorescence emission decays of CVL in water RM at two different excitation wavelengths (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

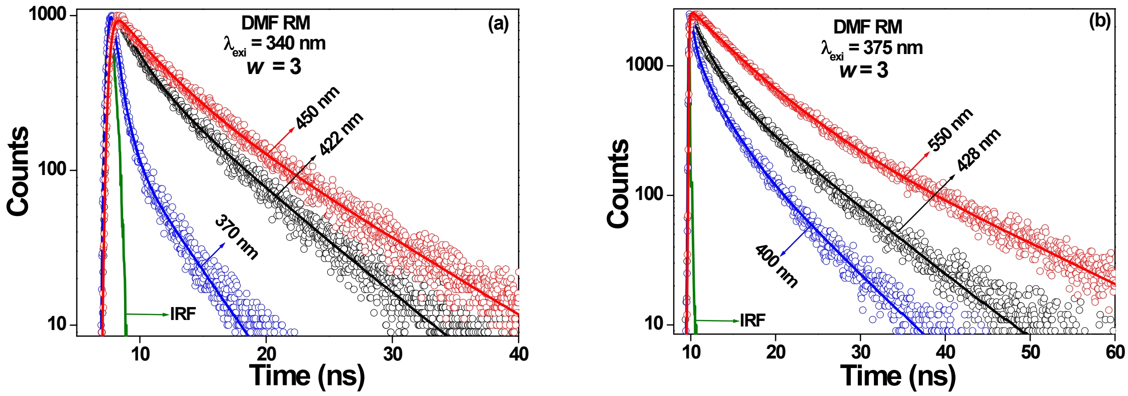

Fig. S12: The emission wavelength dependent fluorescence emission decays of CVL in DMF RM at two different excitation wavelengths (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

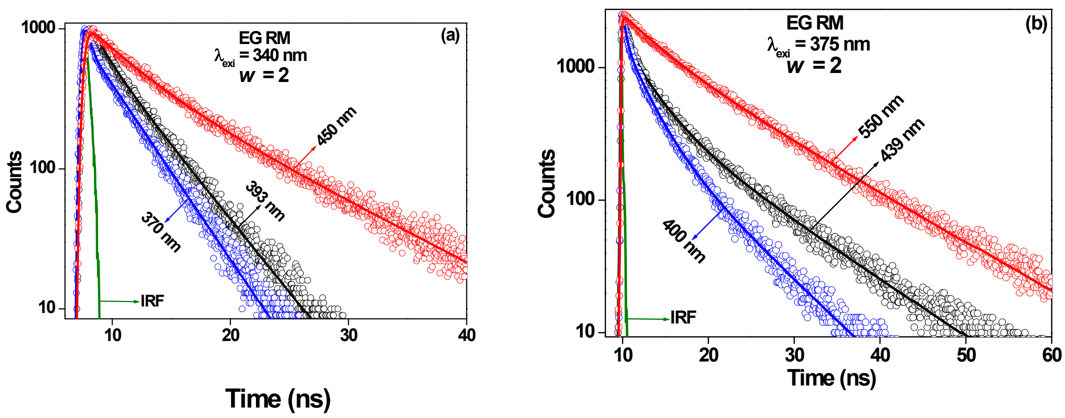

Fig. S13: The emission wavelength dependent fluorescence emission decays of CVL in EG RM at two different excitation wavelengths (a) λ_{exi} = 340 nm and (b) λ_{exi} = 375 nm.

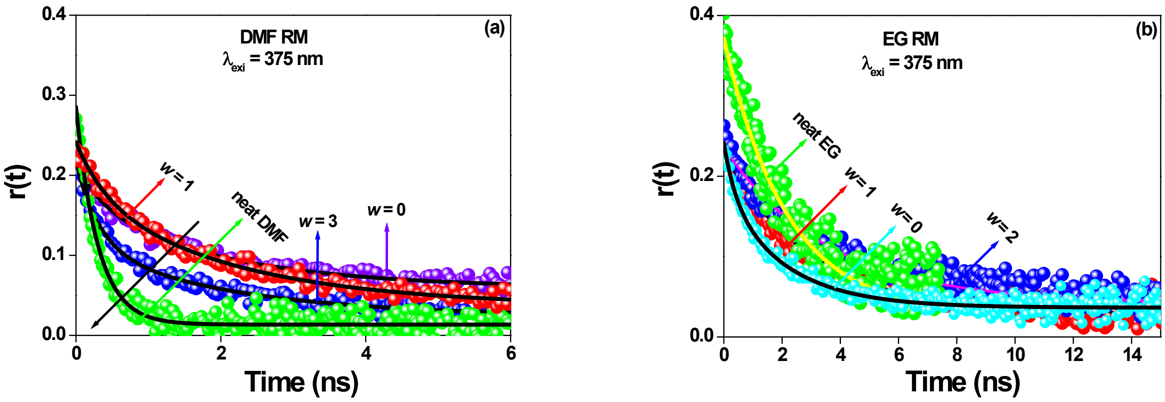

Fig.S14: The time-resolved fluorescence anisotropy decays of CVL in (a) DMF RM and (b) EG RM at λ_{exi} = 375 nm.

Determination of partition coefficient of CVL in AOT/isooctane mixture (*w* = 0) and water RMs (*w* = 5):

From the plot of fluorescence intensity against different concentration of the used surfactant (AOT), we have calculated the partition coefficient values of the dye molecule in different microenvironments by using the following equation[1]:

$$I = \frac{I_0(\phi_f + \phi_b K_p[AOT])}{(1 + K_p[AOT]} \quad (1)$$

The parameters 'I_0' and 'I' 'represents the fluorescence intensity in absence of the surfactant and in presence of the respective concentration of the added surfactant. 'φ_f' and 'φ_b' denotes the fluorescence quantum yields of CVL molecule in neat isooctane and in bound to the micellar interface. 'K_p' is the partition coefficient value of CVL. [AOT] is the concentration of AOT surfactant in the medium. Using the equation, we have found in all the cases the 'K_P' value >1 which indicates the dye molecule resides at the micellar interface and not to the isooctane solvent. The partition coefficient (Kp) is defined as:

$$K_p = \frac{[CVL]_{interface}}{[CVL]_{isooct}} \quad (2)$$

Where, $[CVL]_{interface}$ and $[CVL]_{isooct}$ represents the concentration of CVL at interfacial region of the RMs and the isooctane respectively.

Table S1: Partition coefficient values (K_P) of CVL at different '*w*' values:

System	'*w*' value	Partition coefficient (K_P) in M^{-1}
Water/AOT/isooctane	0	1.8
	5	3.4

Reference:

1. J. Phys. Chem. B 2011, 115, 5971–5979

Table S2: The photophysical parameters of CVL in different reverse micelles (RM) and in neat solvents (λ_{exi} = 375 nm).

System	w	λ_{max}^{emi} (nm)	ϕ_f #	τ_1 (ns)	a_1	τ_2 (ns)	a_2	τ_3 (ns)	a_3	$<\tau>$# (ns)	χ^2
CVL in AOT/isooctane mixture	0	420	0.32	0.51	0.24	5.34	0.29	13.42	0.47	7.98	1.24
CVL in water	-	440	0.07	0.97	0.40	5.32	0.40	15.45	0.20	5.60	1.06
CVL in water/AOT/ isooctane RM	1	428	0.24	1.05	0.25	6.04	0.41	14.26	0.34	7.60	1.15
	3	430	0.09	0.49	0.30	3.35	0.43	8.07	0.27	3.77	1.11
	5	436	0.04	0.36	0.32	1.91	0.45	4.74	0.23	2.06	1.16
	30	420	0.03	0.20	0.40	1.83	0.36	4.78	0.24	1.90	1.02
CVL in DMF	-	438	0.001	0.08	0.91	1.54	0.07	18.36	0.02	0.55	1.14
CVL in DMF/AOT/ isooctane RM	1	424	0.32	0.90	0.25	4.87	0.39	12.71	0.36	6.70	1.11
	2	427	0.20	0.82	0.29	4.46	0.42	11.17	0.29	5.35	0.98
	3	428	0.14	0.70	0.38	3.87	0.44	9.80	0.18	3.73	1.01
CVL in EG	-	445	0.004	0.03	0.96	1.30	0.03	7.12	0.01	0.14	1.07
CVL in EG/AOT/ isooctane RM	1	436	0.24	0.85	0.32	4.83	0.38	13.17	0.30	6.06	1.08
	2	439	0.10	0.51	0.48	3.05	0.35	9.87	0.17	3.00	1.09
CVL in glycerol	-	440	0.083	0.32	0.62	2.51	0.31	9.65	0.07	1.65	1.13
CVL in glycerol/AOT/ isooctane RM	1	431	0.28	1.07	0.27	6.11	0.37	15.76	0.36	8.22	1.10
	2	435	0.19	0.86	0.29	5.67	0.37	15.93	0.34	7.76	1.08
	3.5	436	0.13	0.52	0.34	4.30	0.35	14.28	0.31	6.10	0.98

#Experimental Error of ±5% $<\tau> = a_1\tau_1 + a_2\tau_2 + a_3\tau_3$

Table S3: The excitation wavelength dependent fluorescence emission spectral shift of CVL at different '*w*' values in different RMs.

System	*w*	Variation of excitation wavelength (nm)	Emission spectral shift (nm)
AOT/isooctane mixture	0	340 nm to 405 nm	37
Water RM	1		46
	3		52
	5		69
DMF RM	1		24
	2		19
	3		17
EG RM	1		48
	2		64
Glycerol RM	1		50
	2		63
	3.5		66