Electronic supplementary information (ESI)

Self-assembled systems of water soluble metal 8-hydroxyquinolates with surfactants and conjugated polyelectrolytes

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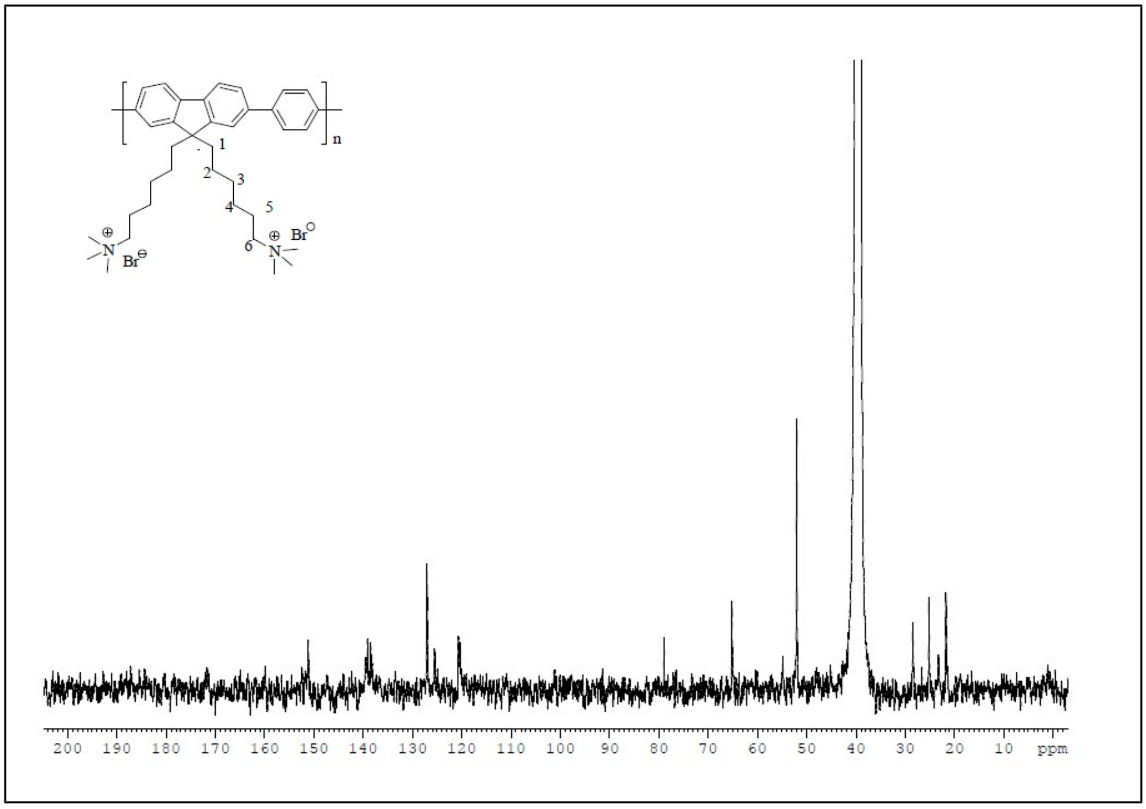

Fig. S1. ^{13}C NMR spectrum of the batch of the conjugated polyelectrolyte HTMA-PFP used in this study.

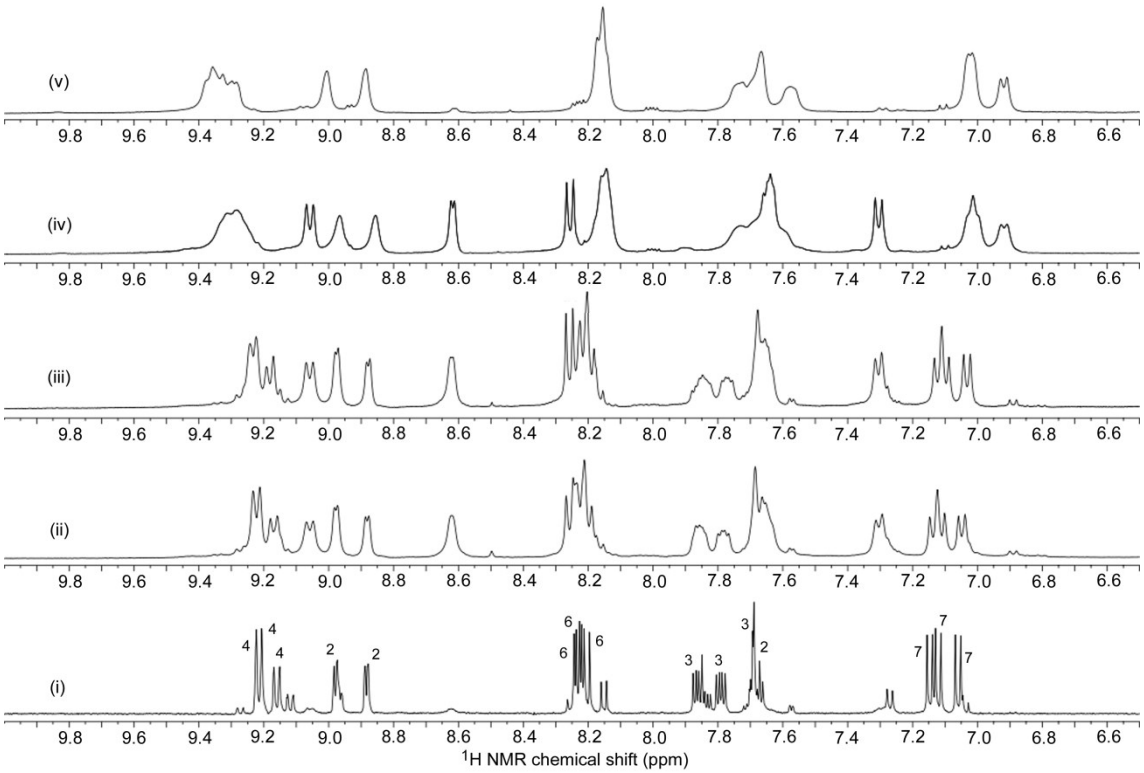

Fig. S2. Expansion 6.5-10 ppm of the ^{1}H NMR spectra (500 MHz) of D_2O solutions of (i) Al^{3+}/8-HQS 2.5:7.5 mmol dm^{-3}, pH 5.7 (ii) Al^{3+}/8-HQS/CTAB 2.5:7.5:0.50 mmol dm^{-3}, (iii) Al^{3+}/8-HQS/CTAB 2.5:7.5:1.0 mmol dm^{-3}, (iv) Al^{3+}/8-HQS/CTAB 2.5:7.5:5 mmol dm^{-3} and (v) Al^{3+}/8-HQS/CTAB 2.5:7.5:10 mmol dm^{-3}, temp. 298 K.

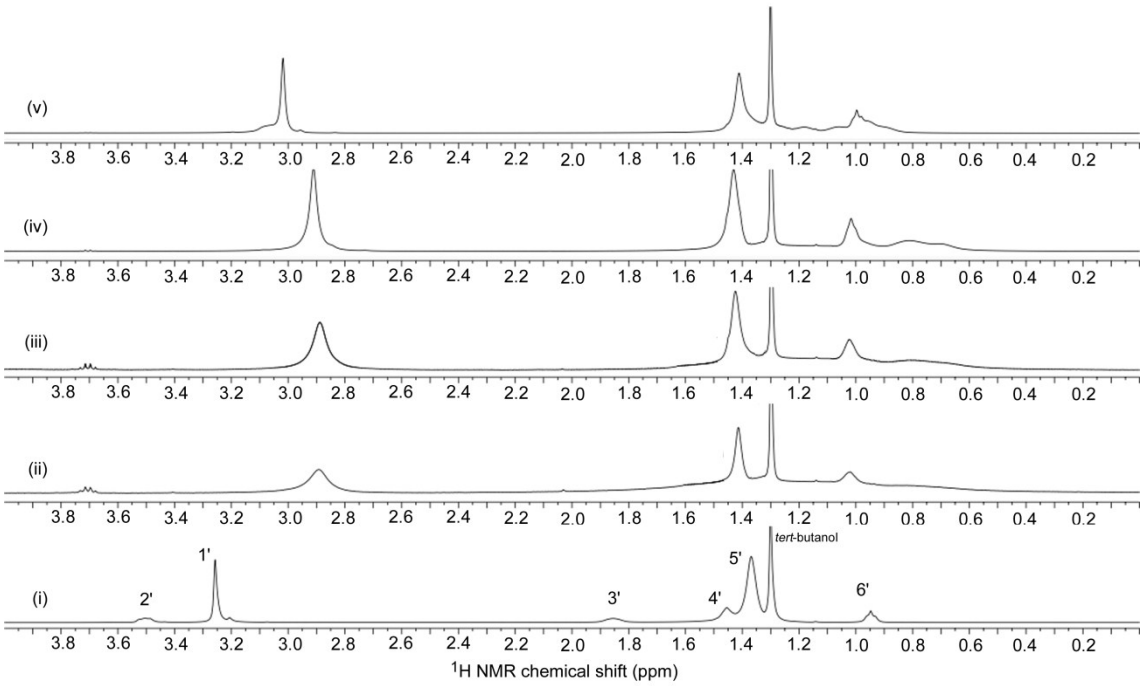

Fig. S3. Expansion 0-4 ppm of the ^{1}H NMR spectra (500 MHz) of D_2O solutions of (i) CTAB 5 mmol dm^{-3}, (ii) Al^{3+}/8-HQS/CTAB 2.5:7.5:0.5 mmol dm^{-3}, (iii) Al^{3+}/8-HQS/CTAB 2.5:7.5:1 mmol dm^{-3}, (iv) Al^{3+}/8-HQS/CTAB 2.5:7.5:5 mmol dm^{-3} and (v) Al^{3+}/8-HQS/CTAB 2.5:7.5:10 mmol dm^{-3}, temp. 298 K.

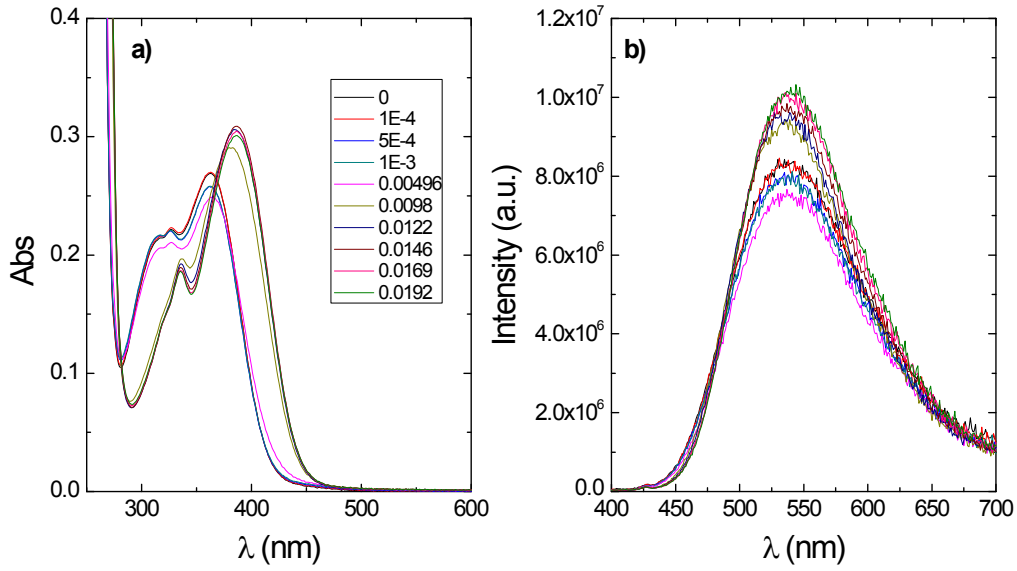

Fig. S4. Effect of DTAB on the (a) absorption and (b) PL (λ_{exc}=367 nm) spectra of Zn(II):8-HQS (1:2), at pH 6.

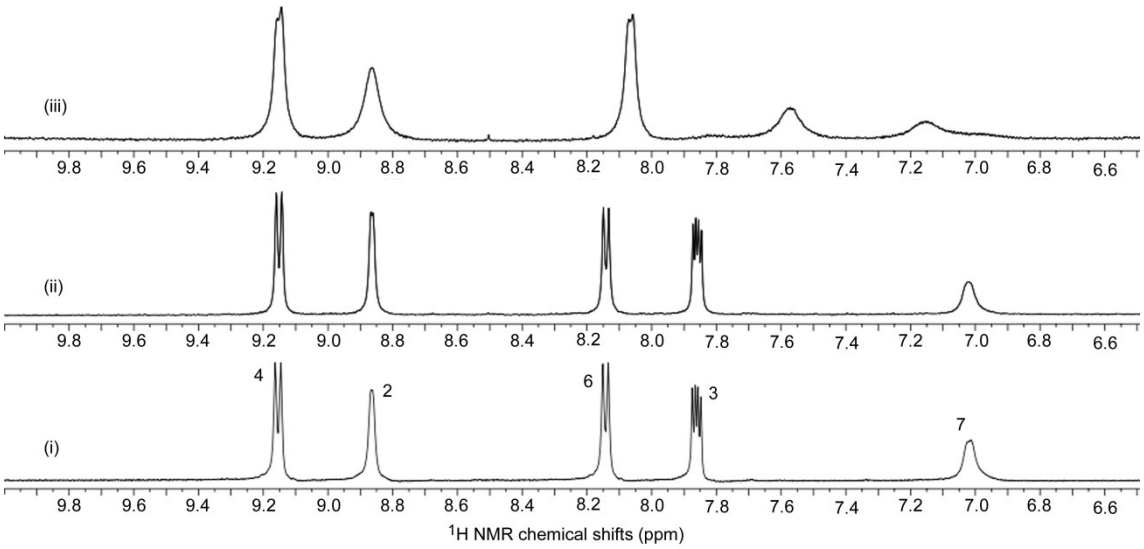

Fig. S5. Expansion of the 6.5-10 ppm region of the ^{1}H NMR spectra of D_2O solutions of (i) Zn^{2+}/8-HQS 5:10 mmol dm^{-3}, pH 6.1 (ii) Zn^{2+}/8-HQS/DTAB 5:10:5.0 mmol dm^{-3}, (iii) Zn^{2+}/8-HQS/DTAB Zn^{2+}/8-HQS/DTAB 5:10:20 mmol dm^{-3}, temp. 298 K.

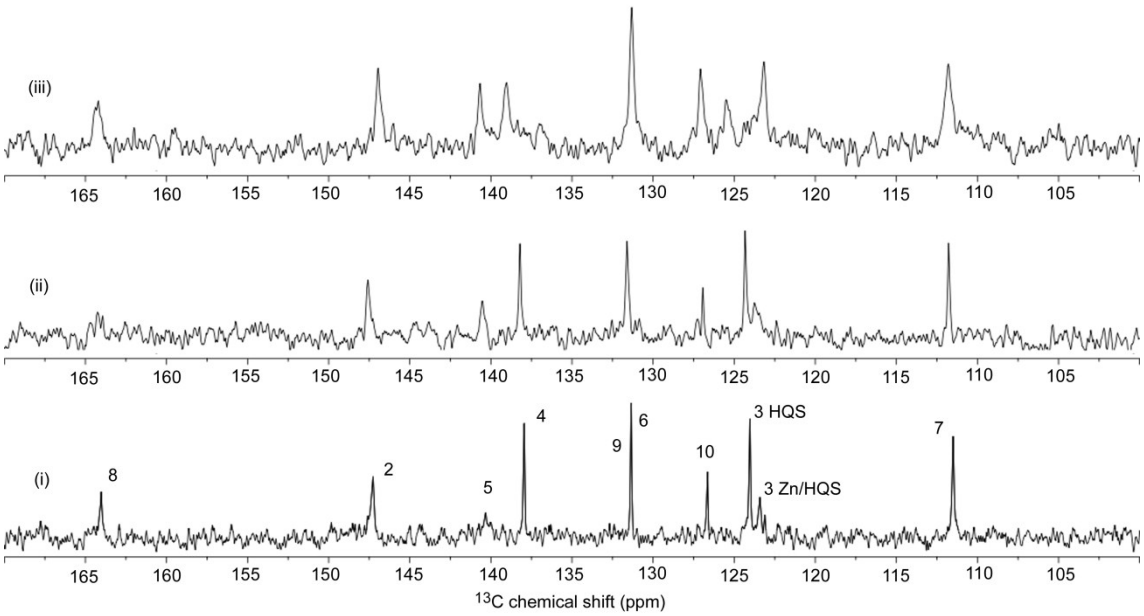

Fig. S6. Expansion 100-170 ppm of the ^{13}C NMR spectra of D_2O solutions of (i) Zn^{2+}/8-HQS 5:10 mmol dm^{-3}, pH 6.1 (ii) Zn^{2+}/8-HQS/DTAB 5:10:5.0 mmol dm^{-3}, (iii) Zn^{2+}/8-HQS/DTAB.

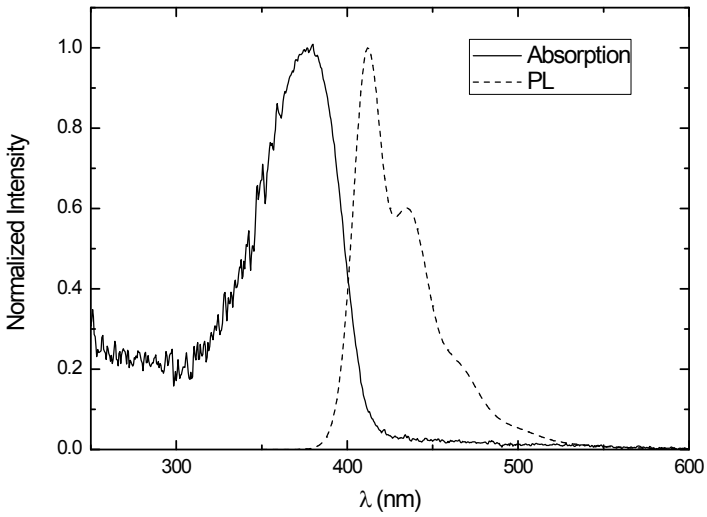

Fig. S7. Absorption and PL (λ_{exc}= 380 nm) spectra of HTMA-PFP in $C_{12}E_5$ (1×10^{-4} M) micellar solution.

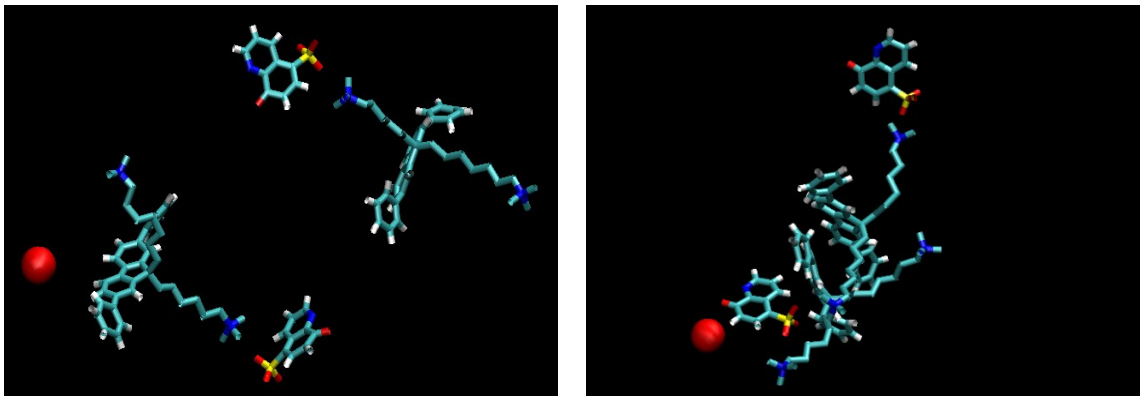

Fig. S8. (a) and (b)A(3) left and A(4) right showing the competing interaction between HTMA-PFP(monomer) and 8-HQS which reduces the frequency of 8-HQS interactions with Zn(II).

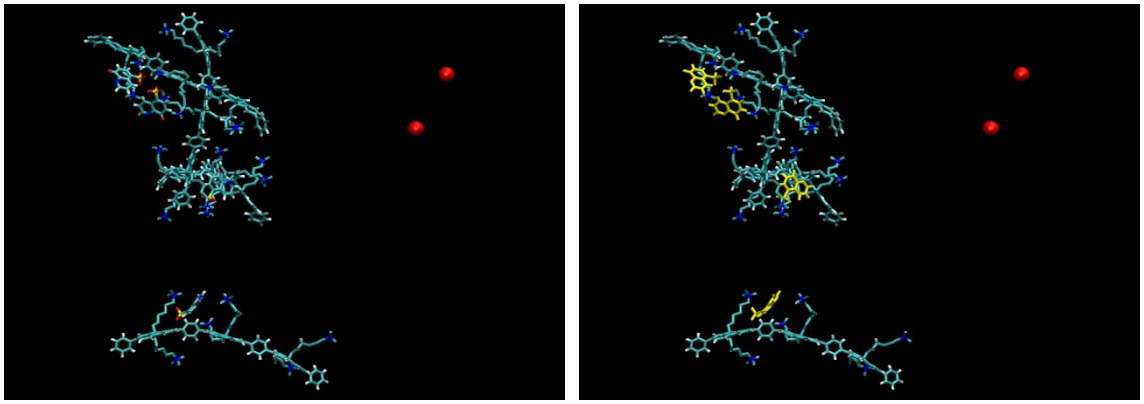

Fig. S9. Left and right images show the dissociation of $[Zn(8\text{-}QS)_2]^{2-}$ in the presence of HTMA-PFP(trimer;) the right schematic shows the same representation with 8-QS ligand shown in yellow to demonstrate encapsulation by HTMA-PFP(trimer).

Table S1. Selected bond lengths (Å) and angles (degrees) calculated at the B3LYP/6-31G(d,p) level with PCM (water)[a] for the meridional $[Al(8\text{-}HQS)_3]^{3-}$ complex in the presence or absence N,N,N-trimethyl-N-propylammonium counterions.

Bond lengths	**$[Al(8\text{-}HQS)_3]^{3-}$ + counterions**	**$[Al(8\text{-}HQS)_3]^{3-}$**	**Angles**	**$[Al(8\text{-}HQS)_3]^{3-}$ + counterions**	**$[Al(8\text{-}HQS)_3]^{3-}$**
$Al\text{-}O_I$	1.878	1.885	$O_I\text{-}Al\text{-}N_I$	80.84	80.75
$Al\text{-}O_{II}$	1.870	1.870	$O_{II}\text{-}Al\text{-}N_{II}$	83.04	83.74
$Al\text{-}O_{III}$	1.884	1.887	$O_{III}\text{-}Al\text{-}N_{III}$	82.56	83.55
$Al\text{-}N_I$	2.109	2.111	$O_I\text{-}Al\text{-}O_{II}$	93.46	92.70
$Al\text{-}N_{II}$	2.078	2.073	$N_I\text{-}Al\text{-}O_{III}$	89.09	89.95
$Al\text{-}N_{III}$	2.063	2.046	$N_{II}\text{-}Al\text{-}N_{III}$	171.70	173.67

[a] Polarizable Continuum Model.[55,56]

Table S2. Mulliken charges for selected atoms calculated at the B3LYP/6-31G(d,p) level with PCM (water)[a] for the meridional $[Al(8\text{-}HQS)_3]^{3-}$ complex in the presence or absence of N,N,N-trimethyl-N-propylammonium counterions.

Atom	Mulliken Charge $[Al(8\text{-}HQS)_3]^{3-}$ + counterions	Mulliken Charge $[Al(8\text{-}HQS)_3]^{3-}$
Al	0.962	0.957
O_I	-0.677	-0.678
O_{II}	-0.674	-0.676
O_{III}	-0.681	-0.685
N_I	-0.578	-0.577
N_{II}	-0.562	-0.560
N_{III}	-0.560	-0.557
S_I	1.18	1.11
S_{II}	1.15	1.12
S_{III}	1.17	1.11

[a] Polarizable Continuum Model. [55,56]

Table S3. Dihedral angles (degrees) in the N,N,N-trimethyl-N-propylammonium counterions in the B3LYP/6-31G(d,p) optimized geometries.

Dihedral angle	$[Al(8\text{-}HQS)_3]^{3-}$ + counterions /PCM	$[Al(8\text{-}HQS)_3]^{3-}$ + counterions /vacuo
N-C4-C5-C6	179.982	178.981
	177.179	179.784
	179.878	179.889
C1-N-C4-C5	177.954	174.961
	178.709	176.393
	177.700	175.632
C2-N-C3-C1	118.555	118.555
	118.635	118.635
	118.481	118.481