

Supplementary Material (ESI) for Chemical Communications
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Synergistic assembly of hyperbranched polyethylenimine and fatty acids leading to unusual supramolecular nanocapsules

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Supplementary Materials

Chemical Communications

Methodology for dyes (CR and MO) extraction in phase transfer processes using the prepared molecular nanocapsules as well as UV-vis spectroscopy analysis:

Hyperbranched or linear PEI was mixed with Lauric acid (LA) or Palmitic acid (PA) in chloroform, and then 4ml of the micellar structure PEI-fatty acid chloroform solution was added to 4 ml of dye in water. The solution was shaken for 10 minutes and kept at room temperature in dark chamber overnight prior to measure. The concentrations of dyes in water were fixed ($[MO]=1.0 \times 10^{-4} M$, $[CR]=6.0 \times 10^{-5} M$), but the concentrations of PEI/Acid mixture were adjusted until only part of the dye in water was transferred into the chloroform phase. The water phase was measured by UV-vis spectrum, the remaining dye in water can be calculated, and the numbers of dye transferred into chloroform phase could be therefore obtained. (The mole extinction coefficients (ϵ) of Methyl Orange and Congo red in water were measured and found to be $2.16 \times 10^4 L/mol \text{ cm}$ (464 nm) and $2.50 \times 10^4 L/mol \text{ cm}$ (498 nm), respectively).

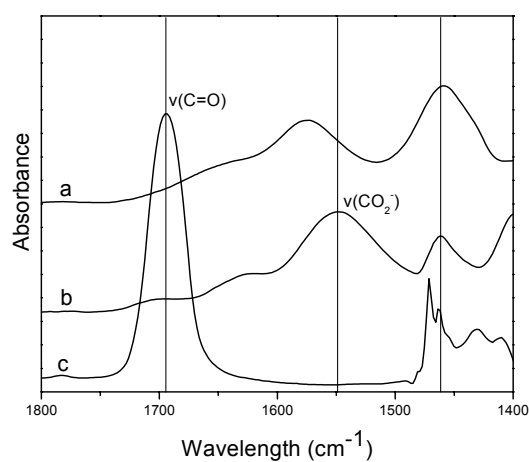


Fig .1 ATR-FTIR spectra of (a) neat PEI₂₃₂, (b) palmitic acid 60%+ PEI₂₃₂ (c) neat palmitic acid

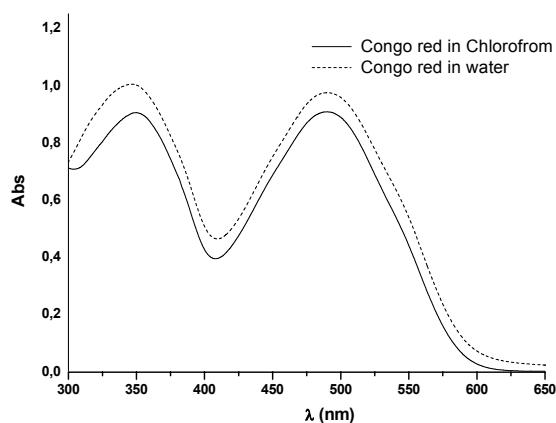


Fig. 2 The UV-vis spectra of Congo Red in water and Congo Red encapsulated by LA- PEI₂₃₂ molecular nanocapsule in chloroform .

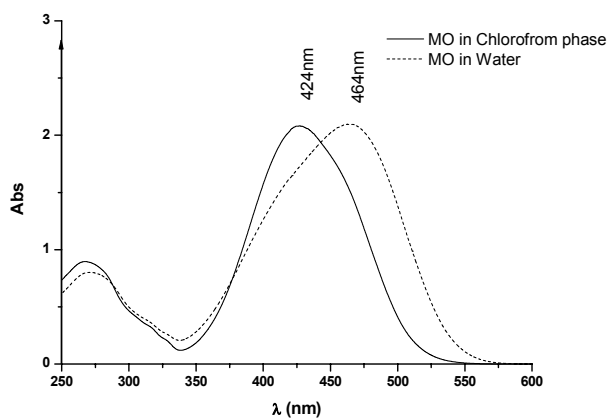


Fig. 3 The UV-vis spectra of Methyl Orange in water and Methyl Orange encapsulated by LA- PEI₂₃₂ molecular nanocapsule in chloroform.

Table 1 Data of the maximum number of hydrophilic dyes encapsulated by the micellar polymeric systems

Micellar structure ^a	M_n of PEI (x 10 ⁻⁴)	Number of Methyl orange ^b	Number of Congo red ^b
LA-PEI ₂₃₂	1	8.5	3.3
PA-PEI ₂₃₂	1	8.6	2.9
LA -PEI ₅₈₁	2.5	21.4	7.2
LA -LPEI ₃₄₈	1.5	1.2	0

^a Samples are mixture of Linear or Branched PEI with LA or PA . ^b Dye loading measured at LA or PA / amine groups in PEI = 0.6

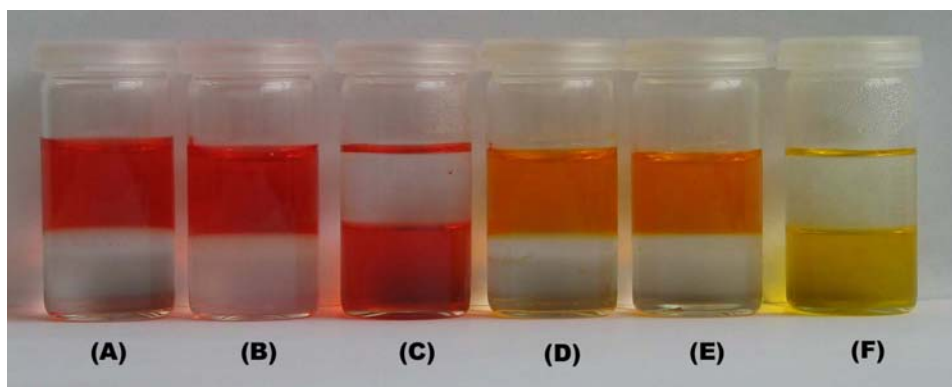


Fig. 4 Illustration of dye extraction processes (bottom layer: chloroform, upper layer: water). (A) Congo Red; only lauric acid (LA) in organic layer; (B) Congo Red; only PEI₂₃₂ in organic layer; (C) Congo Red; LA-PEI₂₃₂ nanocapsule in organic layer; (D) Methyl Orange; only LA in organic layer; (E) Methyl Orange; only PEI₂₃₂ in organic layer; (F) Methyl Orange; LA-PEI₂₃₂ nanocapsule in organic layer