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Supporting Information

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Determination of the CMC in presence of TEA

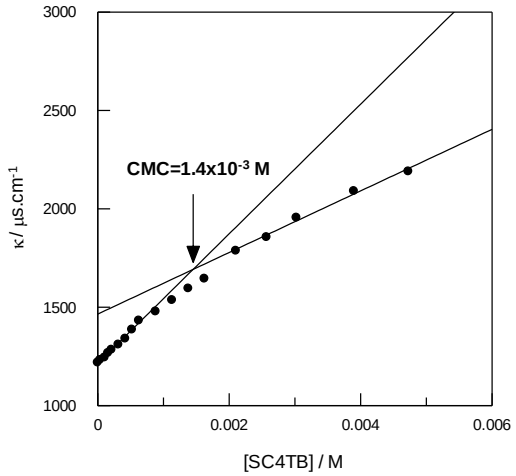


Figure S1. Plot of the electrical conductivity of SC4TB in presence TEA ($3x10^{-3}$ M).

PBS buffer and Na^+ influence on DMSI fluorescence spectra.

Figure S-2. Fluorescence spectra of DMSI (10 μM) in the absence and the presence of different PBS buffer concentrations at pH=6.90. [Buffer]=0; 0.1mM; 0.5mM; 1.0mM; 5.0mM; 10mM; 50mM and 10mM.

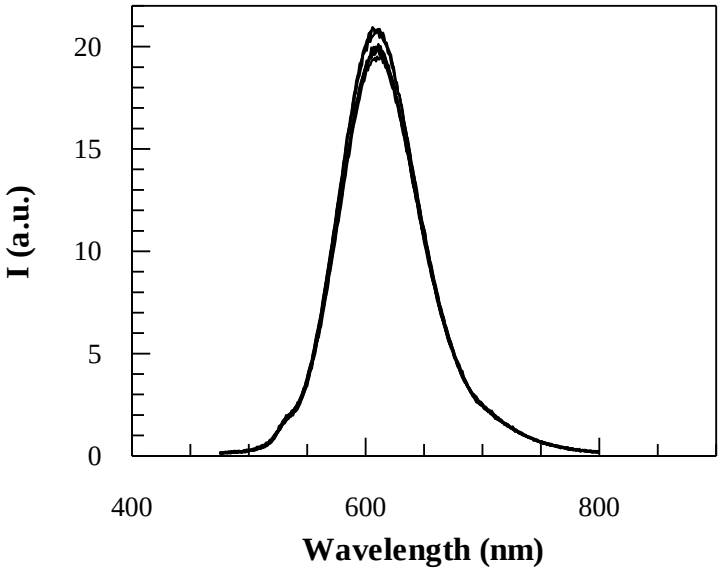
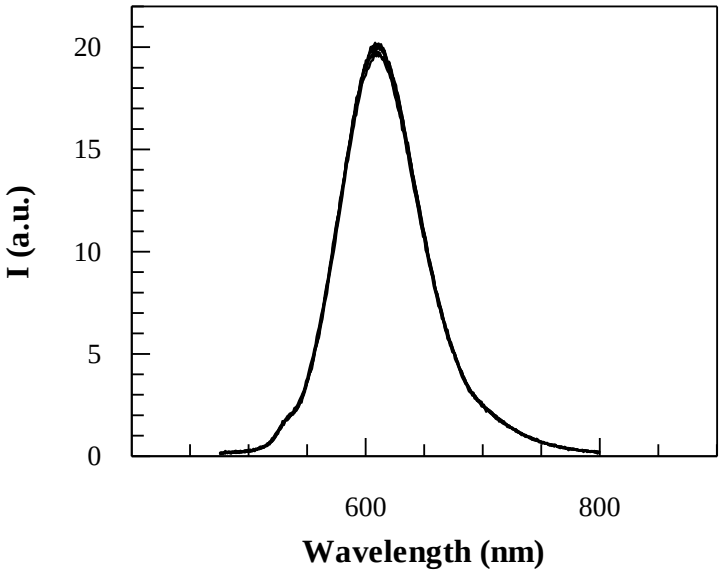


Figure S-3. Fluorescence spectra of DMSI (10 μM) in the presence of 10mM PBS buffer (pH=6.90) at different NaCl concentrations. [NaCl]=1mM; 15mM; 30mM; 60mM; 90mM; 100mM.



Influence of DMSI on the critical micelle concentation of SC4TB.

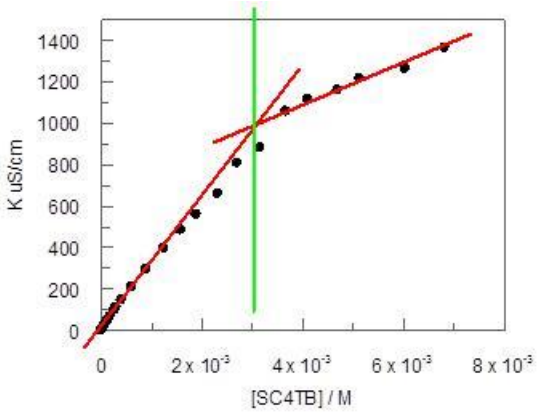


Figure S-4. Conductimetric determination of CMC for SC4TB in the absence of additives at 25ºC. cmc=3mM.

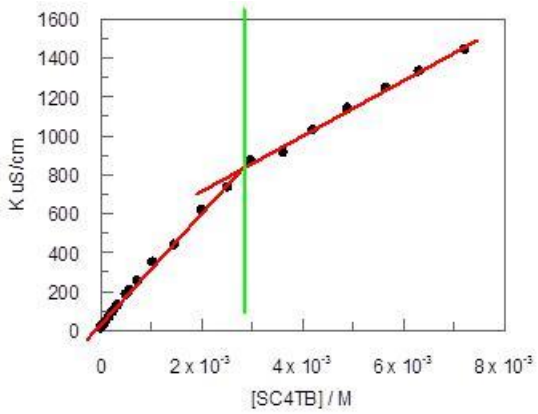


Figure S-5. Conductimetric determination of CMC for SC4TB in the presence of 0.1mM of DMSI at 25ºC. cmc=3mM.

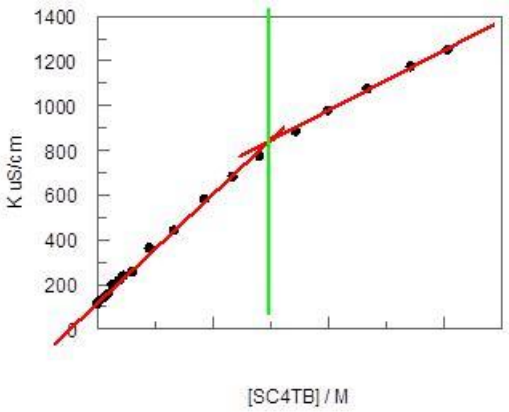


Figure S-6. Conductimetric determination of CMC for SC4TB in the presence of 1.0mM of DMSI at 25ºC. cmc=3mM

Derivation of distribution model

Based in Scheme 3 of the manuscript the following set of equations can be proposed:

$$[\mathrm{H}]_0 = [\mathrm{H}]_\mathrm{w} + [\mathrm{H}]_\mathrm{M} + [\mathrm{HG}]_\mathrm{w} + [\mathrm{HG}]_\mathrm{M} \quad (1)$$

$$[\mathrm{G}]_0 = [\mathrm{G}]_\mathrm{w} + [\mathrm{G}]_\mathrm{M} + [\mathrm{HG}]_\mathrm{w} + [\mathrm{HG}]_\mathrm{M} \quad (2)$$

Above the CMC and if CMC >> $[\mathrm{G}]_0$

$$[\mathrm{H}]_\mathrm{M} = [\mathrm{H}]_0 - \mathrm{CMC} \quad (3)$$

$$K^\mathrm{w}_{\mathrm{H:G}} = \frac{[\mathrm{HG}]_\mathrm{w}}{[\mathrm{H}]_\mathrm{w}[\mathrm{G}]_\mathrm{w}} \qquad K^\mathrm{M}_{\mathrm{H:G}} = \frac{[\mathrm{HG}]_\mathrm{M}}{[\mathrm{H}]_\mathrm{M}[\mathrm{G}]_\mathrm{W}} \qquad K^\mathrm{M}_\mathrm{S} = \frac{[\mathrm{G}]_\mathrm{M}}{[\mathrm{H}]_\mathrm{M}[\mathrm{G}]_\mathrm{w}} \quad (4)$$

By combining the above expressions a quadratic equation is obtained that allows determination of the concentration of monomeric free host:

$$\mathrm{a}[\mathrm{H}]_\mathrm{w}{}^2 + \mathrm{b}[\mathrm{H}]_\mathrm{w} + \mathrm{c} = 0 \quad (5)$$

with:

$$\mathrm{a} = K^\mathrm{w}_{\mathrm{H:G}}$$

$$\mathrm{b} = 1 + \left(K^\mathrm{M}_\mathrm{S} + K^\mathrm{M}_{\mathrm{H:G}} + K^\mathrm{w}_{\mathrm{H:G}}\right)[\mathrm{H}]_\mathrm{M} + K^\mathrm{w}_{\mathrm{H:G}}([\mathrm{G}]_0 - [\mathrm{H}]_0)$$

$$\mathrm{c} = \left(K^\mathrm{M}_\mathrm{S} + K^\mathrm{M}_{\mathrm{H:G}}\right)[\mathrm{H}]_\mathrm{M}{}^2 + \left\{([\mathrm{G}]_0 - [\mathrm{H}]_0)\,K^\mathrm{M}_{\mathrm{H:G}} - K^\mathrm{M}_\mathrm{S}[\mathrm{H}]_0 + 1\right\}[\mathrm{H}]_\mathrm{M} - [\mathrm{H}]_0$$

The concentration of free guest is given by:

$$[G]_w = \frac{[G]_0}{(1 + K_{MG}[H]_M + K_M^{1:1}[H]_M + K_W^{1:1}[H]_w)} \quad (6)$$

and the concentration of the complexes is given by the respective equations for the equilibrium constants (equation 4).