Supplementary Material (ESI) for Soft Matter

Supporting Information

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1 POPC and POPC/DMPS liposomes

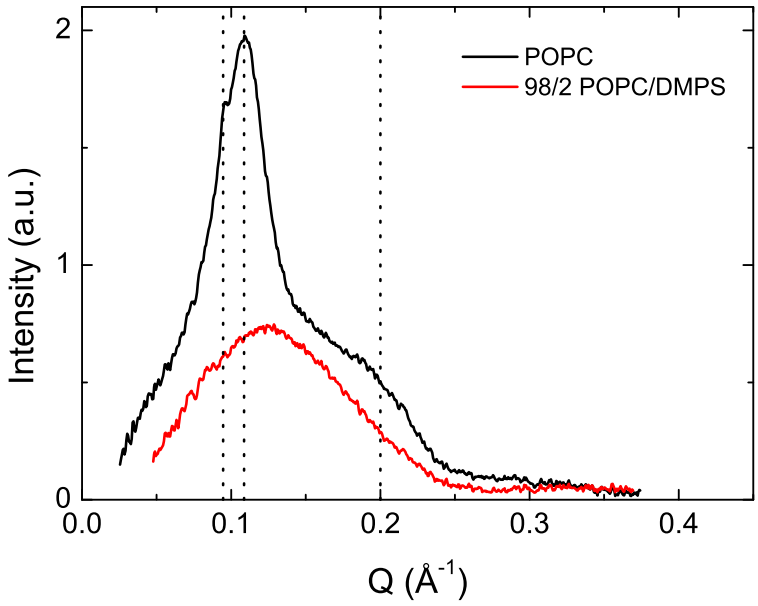

Figure 1: SAXS scattering intensity for POPC (black) and for POPC/DMPS (red) liposomes obtained as described in the text. Two main broad structural peaks around $Q = 0.1\text{Å}^{-1}$ (and a second order peak at $Q = 0.2\text{Å}^{-1}$) are present in POPC sample; they indicate that the samples are composed by multilamellar vesicles. These peaks disappear when liposomes were prepared in presence of a small fraction of ionic lipids (DMPS, 2% by weight) indicating, as expected, a strong correlation between lipid charge and particle morphology.

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2 Form factor for the SANS analysis

The internal structure of liposomes and nanoparticles is described by the form factor $F(Q, r, N)$ in Eq. 6 in the paper. Assuming an overall spherical particle shape, a single particle (the polidispersity is included at a later stage) is modelled in terms of a hollow-core, with radius r surrounded by a multilamellar shell with N repeating units. Each of them is composed by a lipid bilayer (with thickness $2(t_h + t_t)$) surrounded, on both sides, by an inter-bilayer region (with thickness t_{cw}) containing water and chitosan.

$$
\begin{aligned}
F(Q,r,N) = \\
& 4\pi \sum_{j=1}^{N} \left[\Delta\rho_{cw} \int_{r_j^A}^{r_j^B} x^2 \frac{\sin(Qx)}{Qx} dx + \Delta\rho_h \int_{r_j^B}^{r_j^C} x^2 \frac{\sin(Qx)}{Qx} dx + \right. \\
& \Delta\rho_t \int_{r_j^C}^{r_j^D} x^2 \frac{\sin(Qx)}{Qx} dx + \Delta\rho_h \int_{r_j^D}^{r_j^E} x^2 \frac{\sin(Qx)}{Qx} dx + \\
& \left. \Delta\rho_{cw} \int_{r_j^E}^{r_j^F} x^2 \frac{\sin(Qx)}{Qx} dx \right]
\end{aligned}
\tag{1}
$$

The integration limits are defined by:

- $r_j^A = r + 2(j-1)(t_h + t_t + t_{cw}) \equiv r + (j-1)d \rightarrow$ inner radius of the $j-$th repeating unit;
- $r_j^B = r_j^A + t_{cw} \rightarrow$ inner radius of the $j-$th lipid bilayer;
- $r_j^C = r_j^B + t_h \rightarrow$ outer radius of the $j-$th lipid bilayer headgroup;
- $r_j^D = r_j^C + 2t_t \rightarrow$ outer radius of the $j-$th lipid bilayer hydrophobic region;
- $r_j^E = r_j^D + t_h \rightarrow$ outer radius of the $j-$th lipid bilayer;
- $r_j^F = r_j^E + t_{cw} \equiv r_{j+1}^A \rightarrow$ outer radius of the $j-$th lipid bilayer;

In Eq. 1 three contrast terms are present: they are the differences between the scattering length density of the solvent ρ_s and that of each nanoparticle region:

- $\Delta\rho_{cw} = \rho_s - \rho_{cw}$ is the contrast for the interlayer region,
- $\Delta\rho_h = \rho_s - \rho_h$ is the contrast for the hydrophilic region of the lipid bilayer
- $\Delta\rho_t = \rho_s - \rho_t$ is the contrast for the hydrophobic region of the lipid bilayer

The contrast relative to the hollow core ($\Delta\rho_0 = \rho_s - \rho_0$) does not appear since the core region, is supposed to be filled by solvent only. It has then the same scattering length density of the solvent ρ_s and therefore null contrast. All the contrasts have been evaluated on the basis of the sample composition and have then been kept fixed during the fit procedure. A typical simultaneous fit of three SANS profiles related to the same sample in different lipids-solvents configurations is shown in Figure 2.

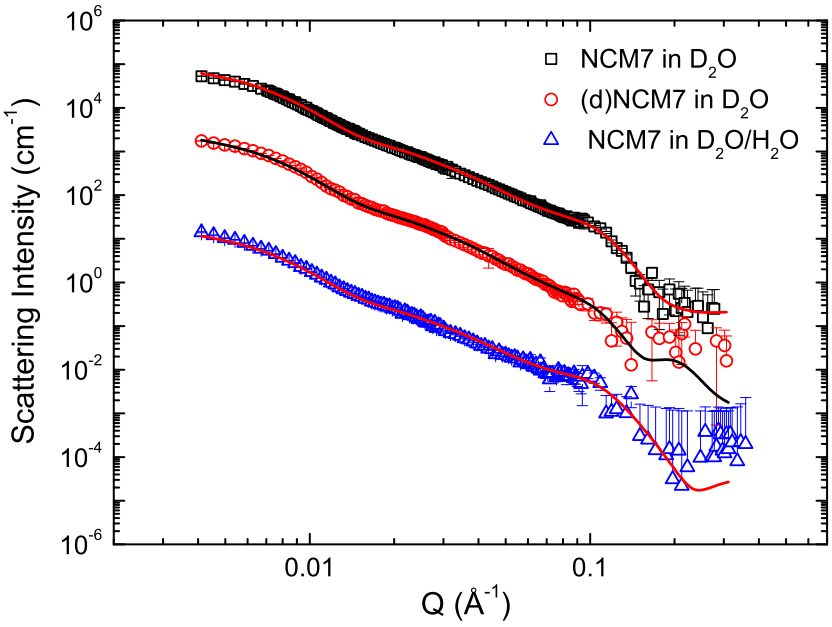

Figure 2: Scattering profiles of NCM7 particles using three different contrast configurations. The intensities have been rescaled to improve the visibility of the curves. The reduced χ^2 resulting from the fitting procedure is $\chi^2 = 0.7$