

Supporting information

Contrast-matched isotropic bicelles: a versatile tool to specifically probe the solution structure of peripheral membrane proteins using SANS.

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Table S1: Summary of the parameters used for the fitting procedure.

Name	Formula	MW (g/mol)	Volume (\AA^3)	SANS SLD (10^{-6}\AA^{-2})	SANS contrast in 100% D ₂ O (10^{-6}\AA^{-2})	SANS contrast in 42% D ₂ O (10^{-6}\AA^{-2})
h-DMPC	C ₃₆ H ₇₂ N O ₈ P	678	1090	0.28	-6.06	
Head	C ₁₀ O ₈ P N H ₁₄	308	336	2.24	-4.10	
Tail	C ₂₆ H ₅₈	370	754	-0.58	-6.92	
h-DHPC	C ₂₀ H ₄₀ N O ₈ P	454	660	0.67	-5.67	
Head	C ₁₀ O ₈ P N H ₁₄	308	336	2.24	-4.10	
Tail	C ₁₀ H ₂₆	146	324	-0.95	-7.29	
d-DMPC	C ₃₆ H ₅ N O ₈ P D ₆₇	745	1090	6.65		4.31
Head	C ₁₀ O ₈ P N H ₅ D ₉	317	336	5.05		2.71
Tail	C ₂₆ D ₅₈	428	754	7.39		5.05
d-DHPC	C ₂₀ H ₅ N O ₈ P D ₃₅	489	660	6.20		3.86
Head	C ₁₀ O ₈ P N H ₅ D ₉	317	336	5.05		2.71
Tail	C ₁₀ D ₂₆	172	324	7.38		5.04

The SLD of 42% (corresponding to the SANS matching point of most hydrogenated proteins) and 100% (corresponding to the SANS matching point of d-bicelles) D₂O are 2.34 and $6.34 \cdot 10^{-6} \text{\AA}^{-2}$ respectively.

Description of the “core-shell cylinder” form factor model:

$$P(Q, \alpha) = \frac{scale}{V_s} f^2(Q) + bkg \quad \text{Eq. S1}$$

where

$$f(Q) = \frac{2(\rho_c - \rho_s)V_c \sin \left[Q t_c \cos \frac{\alpha}{2} \right]}{\left[Q t_c \cos \frac{\alpha}{2} \right] \frac{J_1(Q r_c \sin \alpha)}{(Q r_c \sin \alpha)}} + \frac{2(\rho_s - \rho_{solv})V_s \sin \left[Q (t_c + 2t_s) \cos \frac{\alpha}{2} \right]}{\left[Q (t_c + 2t_s) \cos \frac{\alpha}{2} \right] \frac{J_1(Q (r_c + t_s) \sin \alpha)}{(Q (r_c + t_s) \sin \alpha)}} \quad \text{Eq. S2}$$

and

$$V_s = \pi(r_c + t_s)^2(t_c + 2t_s) \quad \text{Eq. S3}$$

where α is the angle between the axis of the cylinder and the Q -vector, V_s is the volume of the outer shell (*i.e.* the total volume, including the shell), V_c is the volume of the core, t_c is the thickness of the core, r_c is the radius of the core, t_s is the thickness of the shell, ρ_c , ρ_s , and ρ_{solv} are the scattering length densities of the core, the shell, and the solvent, respectively, and bkg is the background level. The outer radius of the shell is given by $r_c + t_s$ and the total length of the outer shell is given by $t_c + 2t_s$. J_1 is the first order Bessel function.

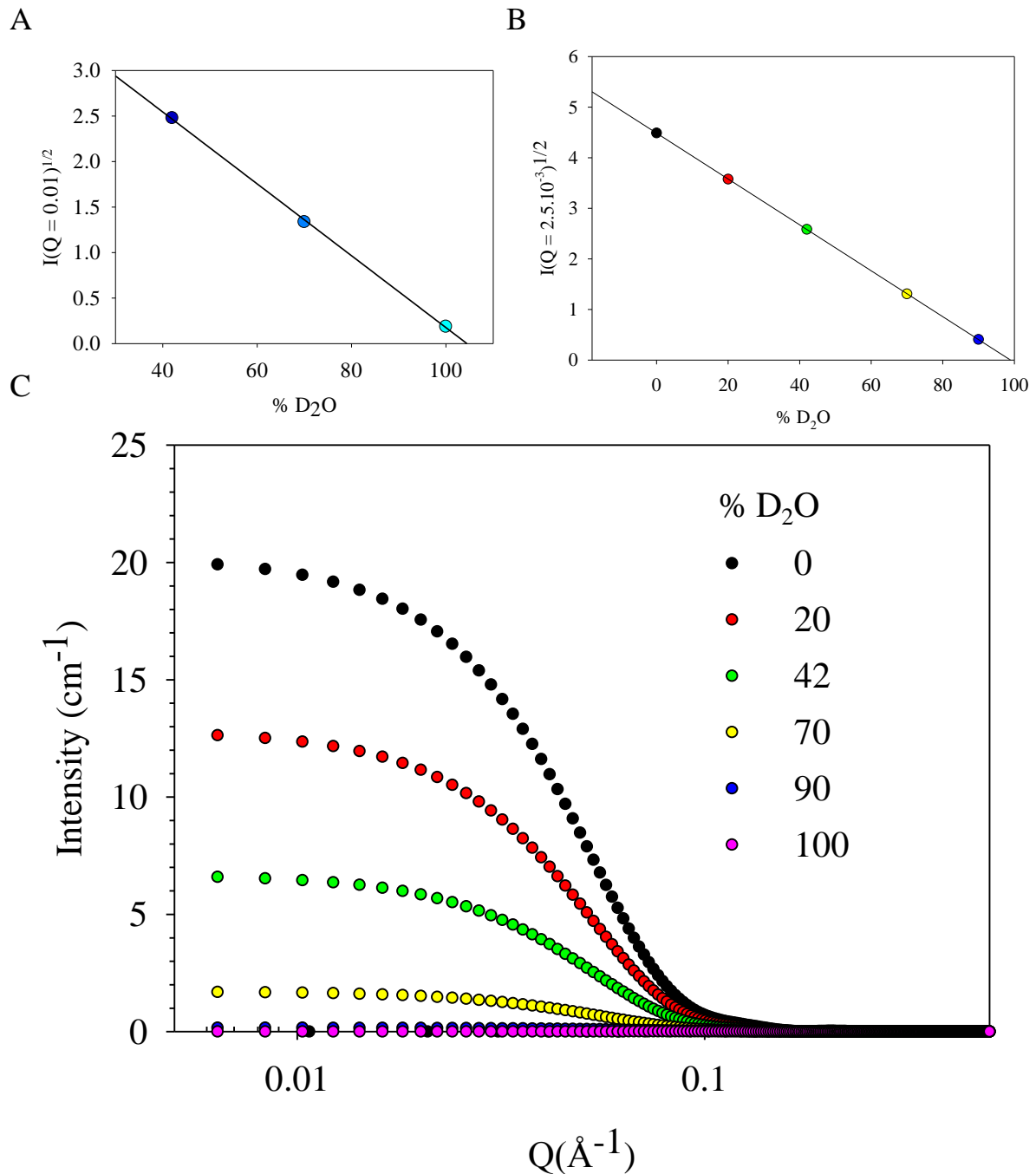


Figure S1: (A) Square root of $I(Q = 0.01 \text{ \AA}^{-1})$ versus the percentage of D₂O plot obtained with the experimental data of d-bicelles in 42, 70, and 100% D₂O (see Figure 3). Experimental match-point is 104% D₂O. (B) Square root of $I(Q = 2.5 \cdot 10^{-3} \text{ \AA}^{-1})$ versus the percentage of D₂O plot obtained with theoretical data generated with the "core-shell cylinder" model. Theoretical match-point is 99% D₂O. (C) Simulated SANS intensities of the "core-shell cylinder" model in 0 (black), 20 (red), 42 (green), 70 (yellow), 90 (dark blue), and 100 (magenta) % D₂O.

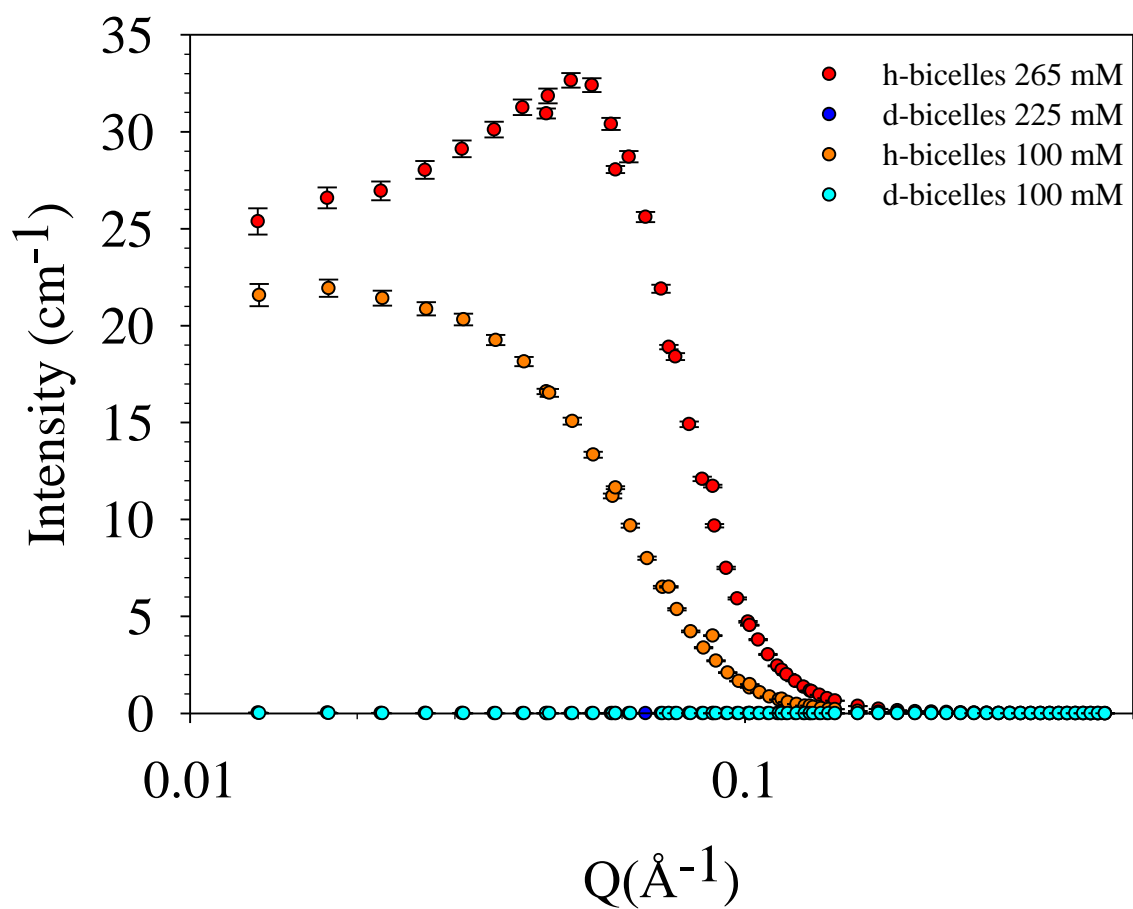


Figure S2: SANS intensities measured for $q = 1$ h-bicelles at 20°C for a total DMPC/DHPC concentration of 265 ($q_{\text{eff}} = 1.05$) (red) and 100 ($q_{\text{eff}} = 1.1$) (orange) mM and for $q = 1$ contrast-matched d-bicelles at 225 ($q_{\text{eff}} = 1.05$) (dark blue) and 100 ($q_{\text{eff}} = 1.1$) (cyan) mM in 100% D_2O d-TNE buffer. At 265 mM, the structure peak is observed for h-bicelles. The contrast-matched d-bicelles are superimposed and close to zero intensity.

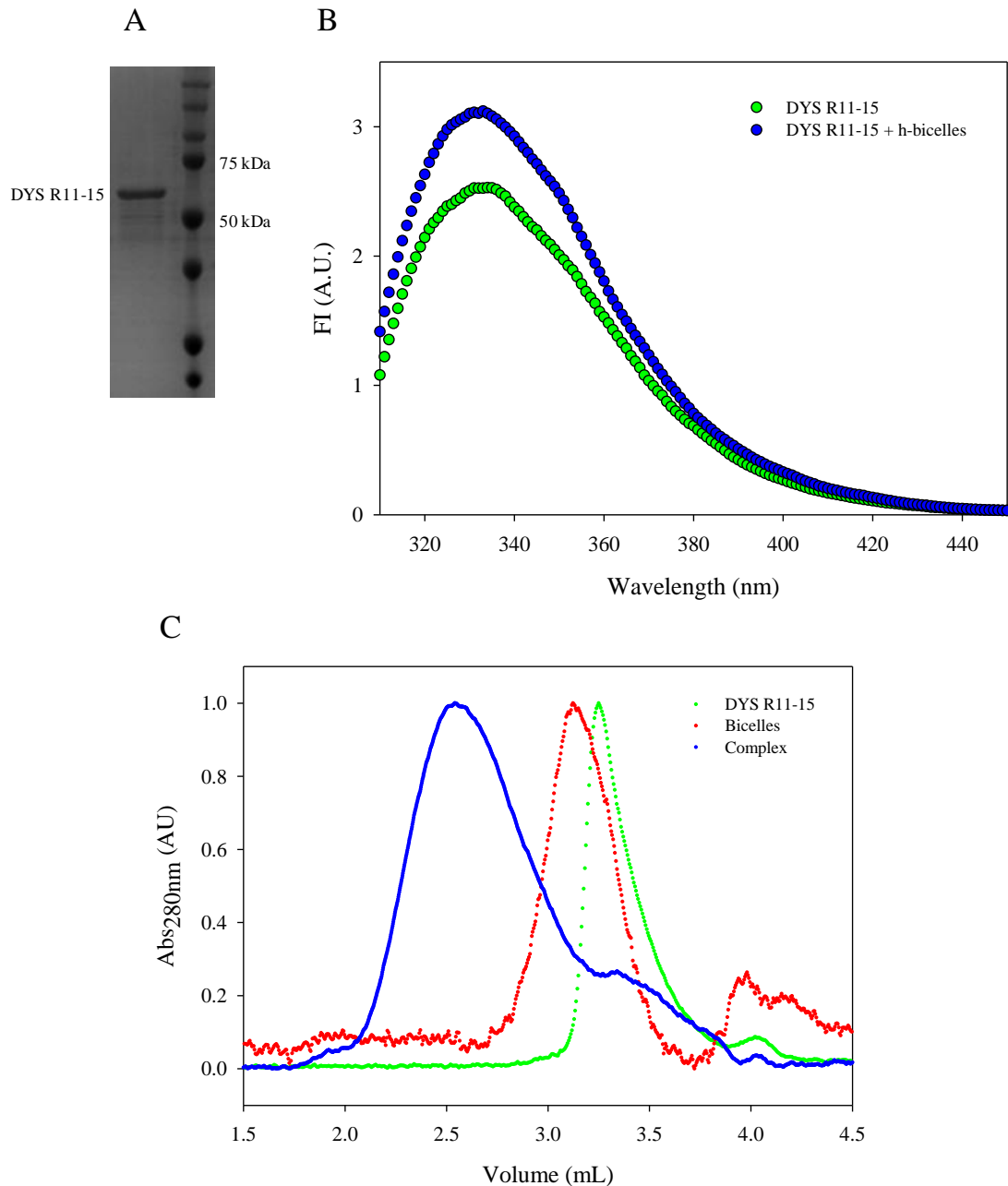


Figure S3: (A): SDS-PAGE analysis of DYS-R11-15, assessing the purity and the expected molecular weight of the protein. (B): Tryptophan intrinsic fluorescence variation of DYS-R11-15 alone (green) or in the presence of h-bicelles (blue). Fluorescence intensity variation is attributed to a modification in the tryptophan environment due to lipid binding. (C) Chromatographic (HPLC) co-elution (Abs_{280nm} detector) of DYS-R11-15 bound to h-bicelles (blue) versus the elutions of h-bicelles (red) or DYS R11-15 (green) alone. Top of the peaks was normalized to the unity for clarity.