Supplemental Information

Investigating partitioning of free versus macrocycle bound guest into a model POPC lipid bilayer

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Table S1: NR median fit results and 68% confidence limits for measurements with avobenzone.

	100 μM incubation		Rinse	
	POPC-d_{31}	POPC	POPC-d_{31}	POPC
Substrate				
Thickness silicon oxide (Å)	10.2±0.6	8.5±0.5	9.4±1.0	8.9±1.0
Substrate roughness, σ (Å)	2.4 ± 0.3		3 ± 1	
Bilayer				
Thickness sub-membrane space (Å)	0.4±0.4	0.5±0.4	0.4±0.4	0.8±0.3
Substrate-proximal hydrocarbon thickness (as-prepared) (Å)	15.7±0.6	16.7±0.5	15.9±0.9	17.9±0.5
Substrate-distal hydrocarbon thickness (as-prepared) (Å)	14.5±0.5	13.3±0.5	13.7±0.9	12.6±0.5
Thickness change per leaflet after adding avobenzone	+0.5±0.2	+0.6±0.2	+0.7±0.3	+0.4±0.2
Bilayer completeness, as-prepared	1.00±0.01	1.00±0.01	1.00±0.01	1.00±0.01
Bilayer completeness, with avobenzone	0.99±0.01	1.00±0.01	1.00±0.01	1.00±0.01
Avobenzone				
Peak of avobenzone CVO from bilayer center (Å)	10 ± 3		7± 3	
Surface volume density (Å³/Å²)	3.0 ± 0.5 ~1 avobenzone per 2.7 lipids in outer leaflet		3.8 ± 0.4 ~1 avobenzone per 2.1 lipids in outer leaflet	

Table S2: NR median fit results and 68% confidence limits for measurements with avobenzone : Calix[8] – PO_3H_2.

|	100 µM incubation		Rinse	
	POPC-d_{31}	POPC	POPC-d_{31}	POPC
Substrate				
Thickness silicon oxide (Å)	11±1	7±1	11±1	7±1
Substrate roughness, σ (Å)	4.6 ± 0.5		4.8 ± 0.5	
Bilayer				
Thickness sub-membrane space (Å)	1±2	1.0±0.6	2±2	1±1
Substrate-proximal hydrocarbon thickness (as-prepared) (Å)	13±1	16±1	13±1	16±1
Substrate-distal hydrocarbon thickness (as-prepared) (Å)	14±1	13±1	14±1	13±1
Thickness change per leaflet after adding avobenzone : Calix[8]	+0.1±0.2	-0.3±0.1	+0.4±0.3	-0.4±0.1
Bilayer completeness, as-prepared	1.00±0.01	1.00±0.01	1.00±0.01	1.00±0.01
Bilayer completeness, with avobenzone : Calix[8]	0.99±0.01	0.99±0.01	0.99±0.01	0.99±0.01
Avobenzone : Calix[8]				
Peak of avobenzone CVO from bilayer center (Å)	11± 3		10± 3	
Surface volume density of avobenzone (Å³/Å²)	2.3 ± 0.6 ~1 avobenzone per 3.0 lipids in outer leaflet		2.5 ± 0.4 ~1 avobenzone per 2.8 lipids in outer leaflet	
Surface volume density of Calix[8] (Å³/Å²)	0.7±0.5 (not significant)		0.6±0.5 (not significant)	
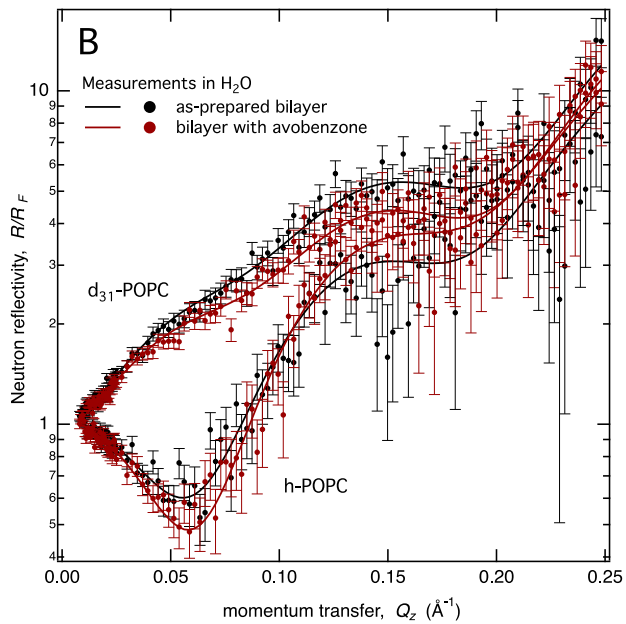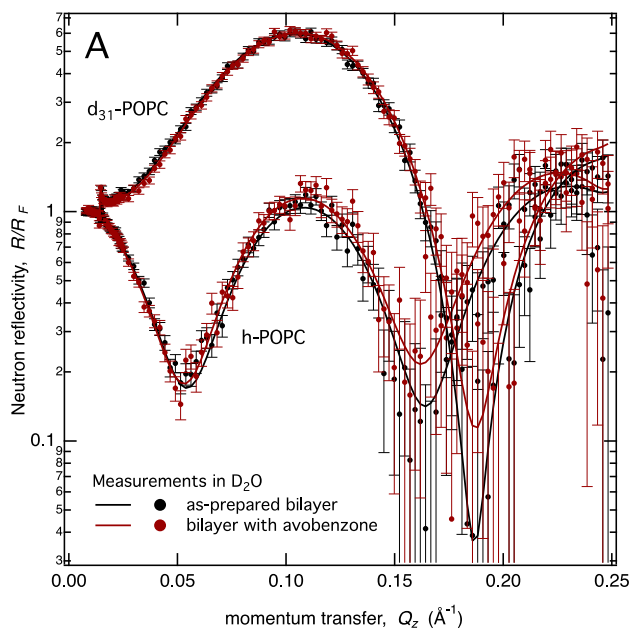
Figure S1: Fresnel-normalized neutron reflectivity curves for two independent measurements of a h-POPC and a d_{31}-POPC bilayer, as-prepared and while incubating 100 μM avobenzone. Each condition was characterized using two isotopically distinct bulk solvents, (A) H_2O and (B) D_2O. Significant changes in the reflectivity were observed for most combinations of bilayer and bulk solvent upon addition of avobenzone. The entire set of 8 reflectivity curves was analysed simultaneously using one structural model. Combining two measurement with bilayers that differ in their lipid chain deuteration was essential in resolving avobenzone in the lipid bilayer core. Qualitatively similar reflectivities were recorded after rinsing and for the complex of avobenzone and Calix[8] − PO_3H_2 during incubation and after rinsing.