Supporting Information

Dynamic Structure of Disulfide-Removed Linear Analogs of Tachyplesin-I in the Lipid Bilayer from Solid-State NMR

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Table S1. Isotropic chemical shifts and secondary shifts (ppm) of ^{13}C- and ^{15}N-labeled sites in TPA4, TPF4 and TP-I.

		TPA4		TPF4		TP-I	
Residue	Site	δ_{iso}	$\Delta\delta_{iso}$	δ_{iso}	$\Delta\delta_{iso}$	δ_{iso}	$\Delta\delta_{iso}$
V6	Cα			58.1	-2.3	57.4/57.9	-3.0/-2.5
	Cβ			33.1	2.1		
	N			124.9			
A/F7	N			128.9			
G10	CO	169.7	-2.5	168.8	-3.4		
	Cα	44.4	0.5	43.6	-0.21	43.0	-0.8
	N	111.5		113.8			
I11	CO	173.6	-0.3	171.8	-2.1		
	Cα	56.8	-2.6	56.9	-2.4		
	Cβ	42.7	5.7	41.2	4.3		
	N	113.5		118.4			
A/F12	CO	173.4	-2.6	172.0	-1.9		
	Cα	50.0	-1.1	54.1	-2.2		
	Cβ	21.3	3.9	40.2	2.5		
	N	125.2					

Table S2: ^{1}H $T_{1\rho}$ values (ms) for various residues in TP-I, TPA4 and TPF4 bound to POPE/POPG membranes as a function of temperature. Not all samples were measured at all temperatures. Entry n.r. indicates that the resonance was not resolved. ^{1}H $T_{1\rho}$ was measured under an effective spin-lock field strength of 68.0 kHz.

Temp	TP-I		TPF4		TPA4		
(K)	V6	G10	V6	G10	G10	I11	A12
310		0.3					
308	4.3						
303		0.3					
298	4.7	0.4	6.6	4.6	8.4	7.6	9.1
283	4.0	1.1	5.5	3.6			
273	3.8		4.8	3.1	n. r.	5.9	5.8
263	4.1	2.4	4.6	3.1	n. r.	4.4	5.2
253			7.1	5.5	n. r.	4.5	5.7
243	4.8		8.2	7.2	n.r.	6.6	8.3

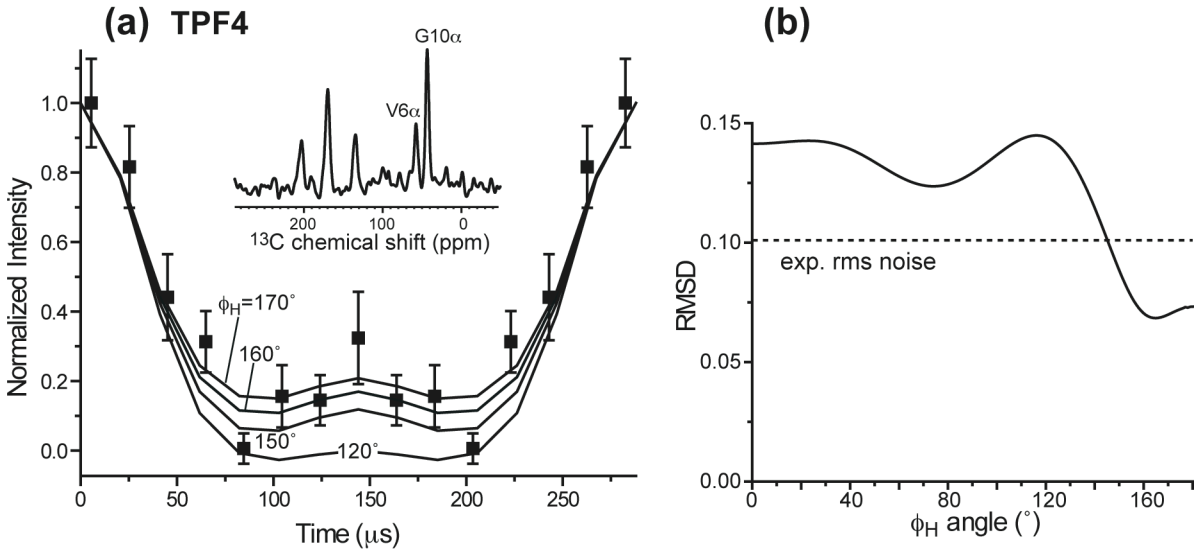

Figure S1. ϕ torsion angle of V6 in TPF4 from the HNCH experiment. (a) HNCH data, acquired under 3.472 kHz MAS at 233 K. (b) RMSD between the simulations and the experimental data. The best-fit ϕ_H angle is ±160°, which corresponds to a ϕ angle of –140° or –100°, both in the β-strand region of the Ramachandran diagram.

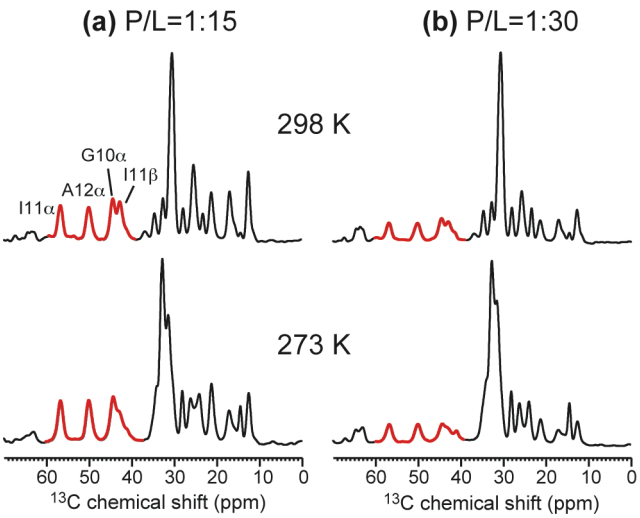

Figure S2. Comparison of ^{13}C CP-MAS spectra of TPA4 in POPE/POPG membranes at two peptide concentrations. (a) P/L=1:15. The spectra are the same as in Figure 5c, but scaled so that the lipid CH_2 peak is fully shown and its intensity is set to be the same in all spectra to serve as a reference to the peptide signal intensities. The TPA4 CP intensities (red) are unchanged between 298 K and 273 K, indicating the absence of motion at ambient temperature. (b) P/L=1:30. The peptide signal intensity is roughly half of those in (a), as expected for the half reduced concentration. The peptide CP intensities also remain unaffected by temperature. Thus, TPA4 is immobilized at 298 K even at the lower concentration. All spectra were measured under 5 kHz MAS.