

Supporting Information

Reversible Sheet – Turn Conformational Change of a Cell-Penetrating Peptide in Lipid Bilayers Studied by Solid-State NMR

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Table S1. Intensity fractions of sheet and turn peaks of (I3, N9)-labeled penetratin in DMPC/DMPG (8:7) membranes at P/L = 1:15 and 1:30.

T (K)	P/L = 1:15				P/L = 1:30			
	I3 α		N9 α		I3 α		N9 α	
	Sheet	Turn	Sheet	Turn	Sheet	Turn	Sheet	Turn
243	0.75	0.25	0.63	0.37	0.60	0.40	0.50	0.50
263	0.75	0.25	0.64	0.36	0.77	0.23	0.51	0.49
283	0.79	0.21	0.66	0.34	0.65	0.35	0.44	0.56
288	0.73	0.27	0.36	0.64	-	-	-	-
293	0.67	0.33	0.27	0.73	0.31	0.69	0.20	0.80
298	0.50	0.50	0.28	0.72	0.12	0.88	0.03	0.97
303	0.50	0.50	0.27	0.73	0.19	0.81	0.17	0.83
305	0.41	0.59	0.15	0.85	-	-	-	-
310	0.24	0.76	0.12	0.88	0.05	0.95	0.06	0.94

Table S2: ^{13}C chemical shifts (ppm) of penetratin in DMPC/DMPG bilayers at 310 K and 243 K.

residue	site	310 K	243 K
I3	CO	173.8	172.3
	C α	60.2	57.4
	C β	36.3	39.8
	C γ	26.2	26.4
	C δ	15.7	15.2
	C ϵ	11.4	12.7
I5	CO	-	172.2
	C α	59.2	57.5
	C β	36.8	40.1
	C γ	25.6	26.5
	C δ	15.7	15.9
	C ϵ	11.3	12.7
Q8	CO	-	172.8
	C α	54.6	53.4
	C β	31.4	33.8
	C γ	27.9	31.6
	C δ	-	177.7
N9	CO	173.9	-
	C α	52.2	49.4
	C β	36.6	38.8
	C γ	175.6	-
K13	CO	174.2	171.7
	C α	54.4	53.1
	C β	31.5	35.3
	C γ	22.7	22.8
	C δ	27.2	27.2
	C ϵ	39.8	39.7