Roles of Arginine and Lysine Residues in the Translocation of a Cell-Penetrating Peptide from ^{13}C, ^{31}P and ^{19}F Solid-State NMR

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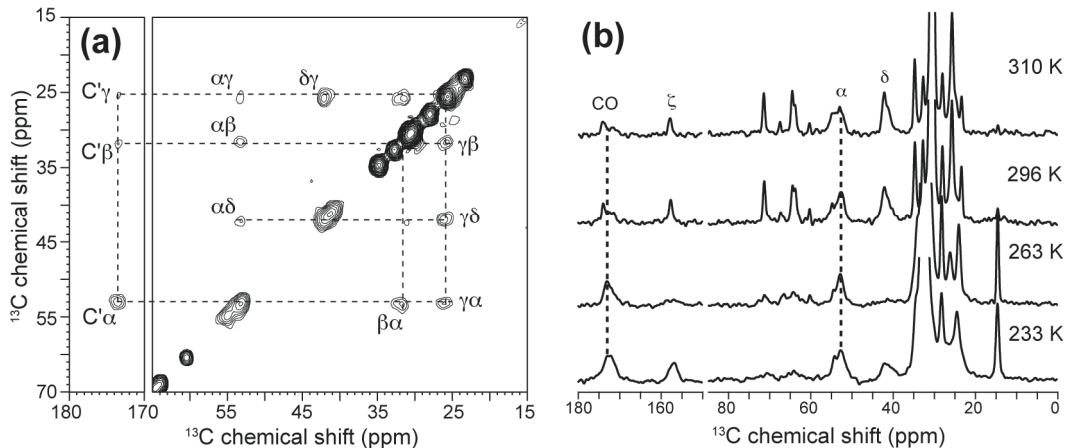
Figure S1. ^{13}C spectra of Arg$_{10}$-labeled penetratin in POPC/POPG (8:7) membranes. (a) 2D ^{13}C-^{13}C DARR spectra measured at 303 K. (b) Temperature-dependent 1D ^{13}C CP-MAS spectra.
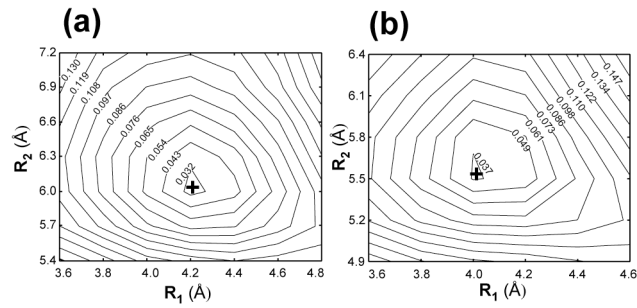
Figure S2. Root-mean-square deviations between the calculated and experimental ^{13}C-^{31}P REDOR intensities. (a) Arg$_{10}$ Cζ. (b) Lys$_{13}$ Cε. The REDOR curve fitting used a combination of a short distance (R_1) and a long distance (R_2) at a 1:1 ratio. Best-fits are 6.0 Å and 4.2 Å for Arg$_{10}$ Cζ (minimum RMSD = 0.029), and 5.5 Å and 4.0 Å for Lys$_{13}$ Cε (minimum RMSD = 0.036).

Table S1. ^{13}C chemical shifts of penetratin Arg_{10} in DMPC/DMPG (8:7) at 303 K and 243 K, and in POPC/POPG (8:7) at 303 K.

Site	DMPC/DMPG		POPC/POPG
	303 K	234 K	303 K
CO	173.4	173.0	173.5
Cα	53.2	52.7	53.3
Cβ	31.5	31.3	31.9
Cγ	25.8	25.0	25.9
Cδ	42.2	41.5	42.1
Cζ	157.8	157.0	157.8