Proline Kink Angle Distributions for GWALP23 in Lipid Bilayers of Different Thickness

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Supporting Information.

Figure S1. MALDI mass spectra of a synthetic GWALP23-P12 peptide with two labeled alanines (Ala-d4) at different isotope abundance levels.

Figure S2. Reversed-phase HPLC chromatogram of a synthetic GWALP23-P12 peptide.

Figure S3. Representative ^{31}P NMR spectra of DOPC bilayers, with GWALP23-P12 incorporated.

Figure S4. ^{2}H NMR spectra for labeled Ala methyl groups C-terminal to the proline in GWALP23-P12, in oriented bilayers of DLPC, DMPC and DOPC. Sample orientation is $\beta = 0°$.

Figure S5. ^{2}H NMR spectra for labeled Ala methyl groups N-terminal to the proline in GWALP23-P12, in oriented bilayers of (left to right) DLPC, DMPC and DOPC. Sample orientation is $\beta = 0°$.

Figure S6. Segmental tilt distributions in DLPC and DOPC.

Figure S7. Distributions of proline-induced helix unwinding ("swivel") angles for GWALP23-P12 in (A) DLPC, (B) DMPC and (C) DOPC.

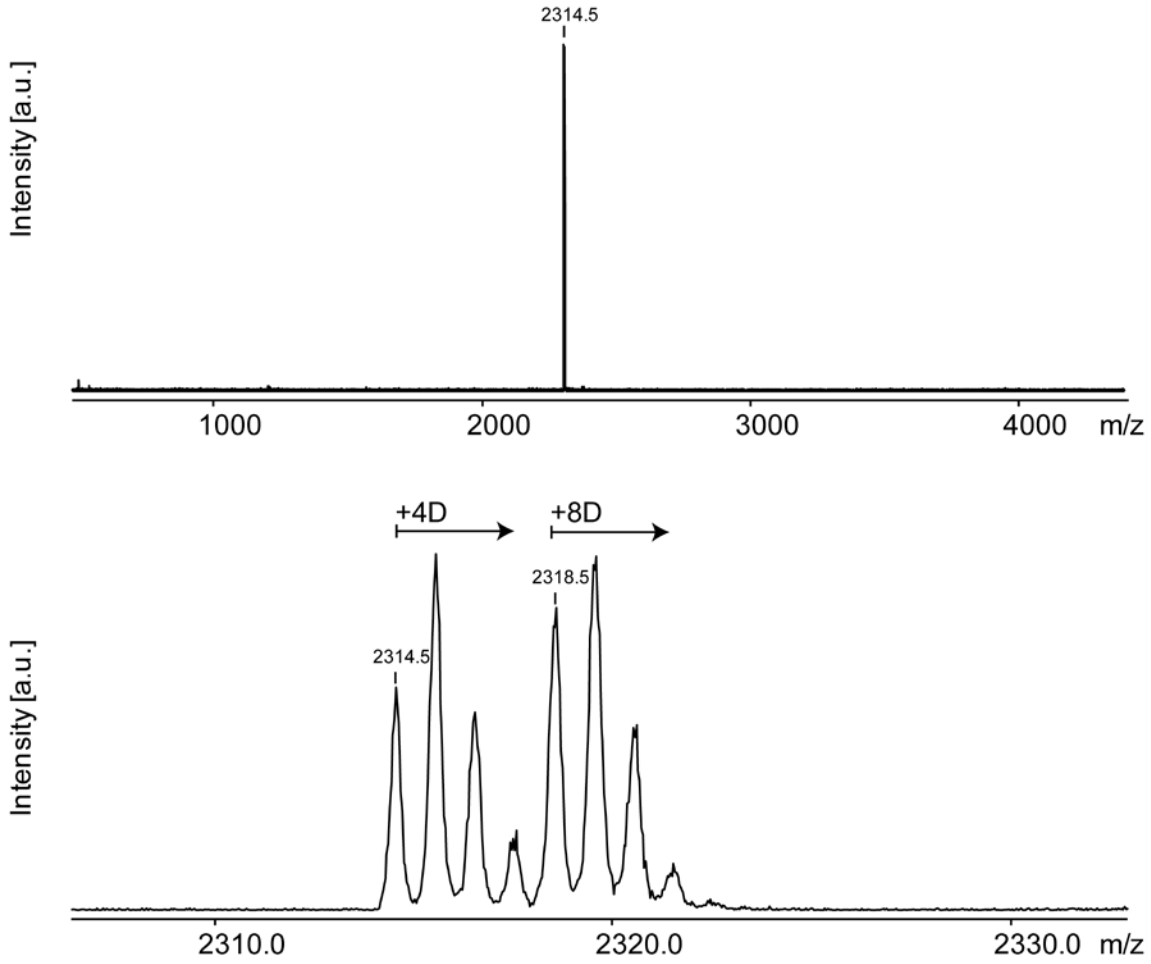

Figure S1. MALDI mass spectra of a synthetic GWALP23-P12 peptide with two labeled alanines (Ala-d4) at different isotope abundance levels.

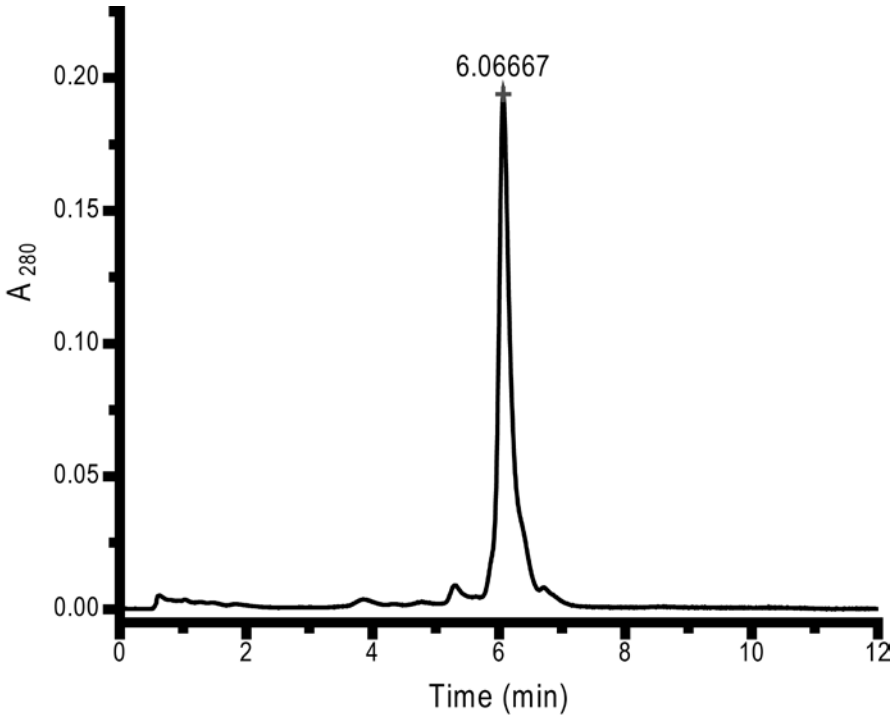

Figure S2. Reversed-phase HPLC chromatogram of a synthetic GWALP23-P12 peptide with ^{2}H-labeled alanines in two sequence positions.

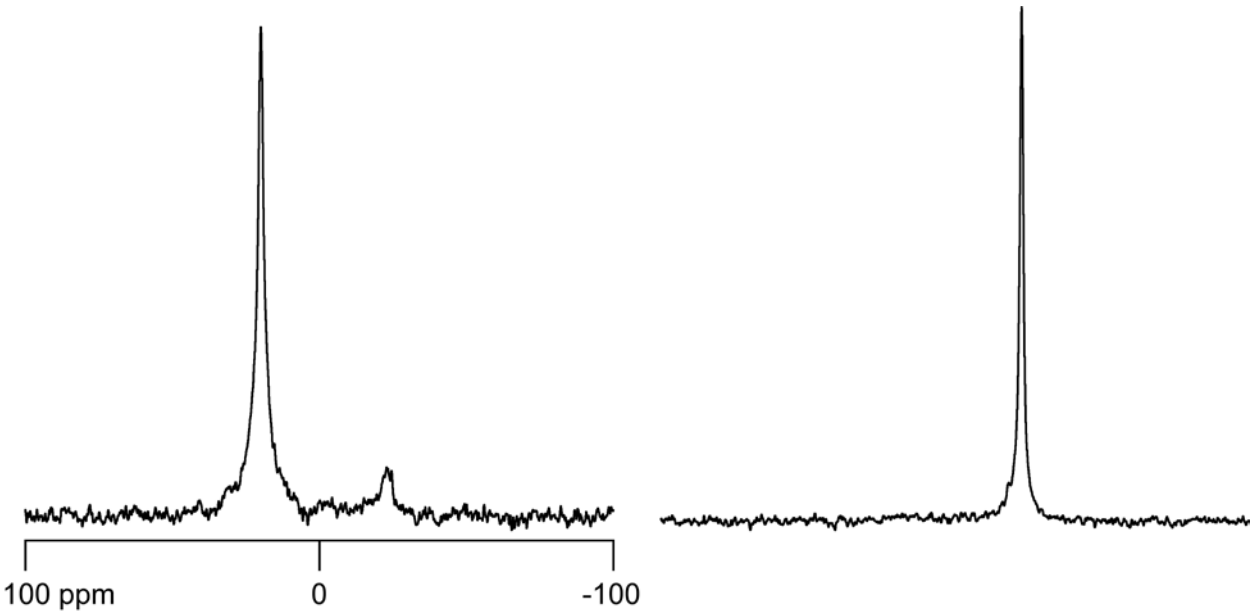

Figure S3. Representative ^{31}P NMR spectra of DOPC bilayers, with GWALP23-P12 incorporated, at β=0° (left) and β=90° (right) sample orientations.

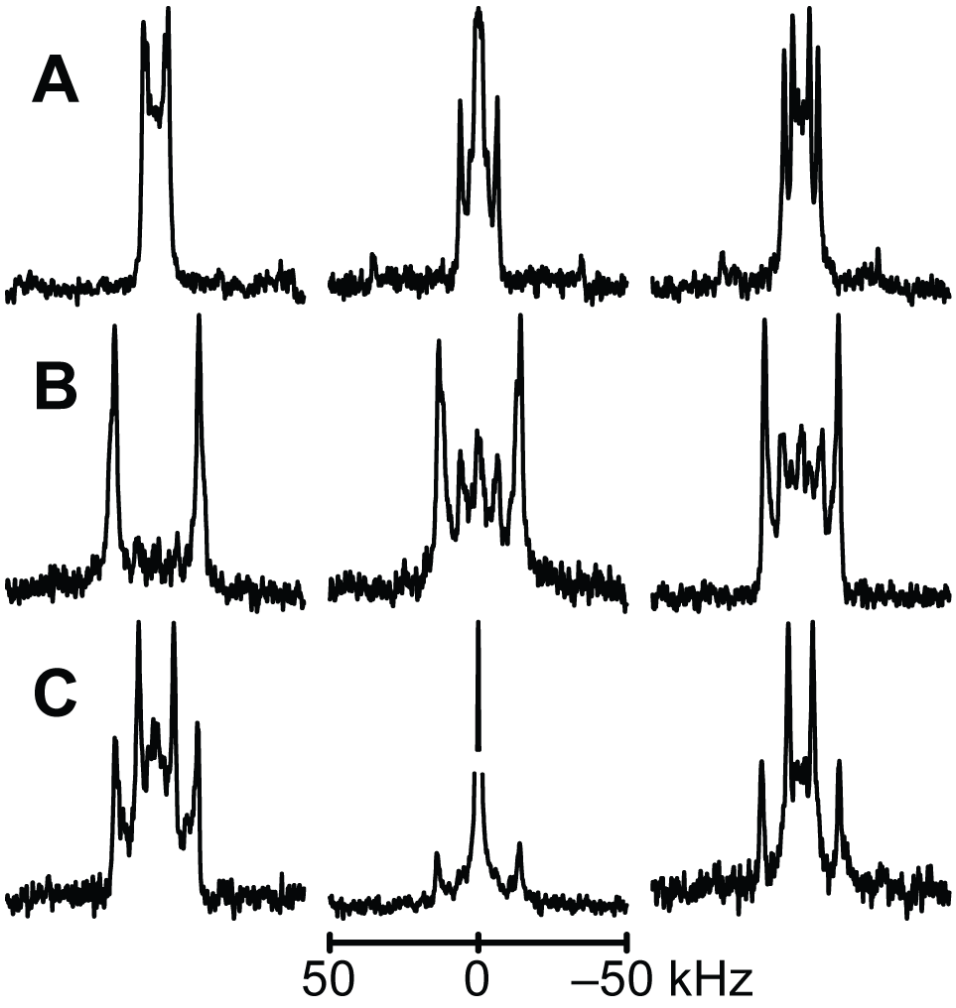

Figure S4. ^{2}H NMR spectra for labeled Ala methyl groups C-terminal to the proline in GWALP23-P12, in oriented bilayers of DLPC, DMPC and DOPC. Sample orientation is β = 0°. Deuterium isotope levels in the labeled alanines are: A. 100% Ala^{17}, 50% Ala^{21}. B. 100% Ala^{15}, 50% Ala^{13}. C. 100% Ala^{16}, 50% Ala^{15}.

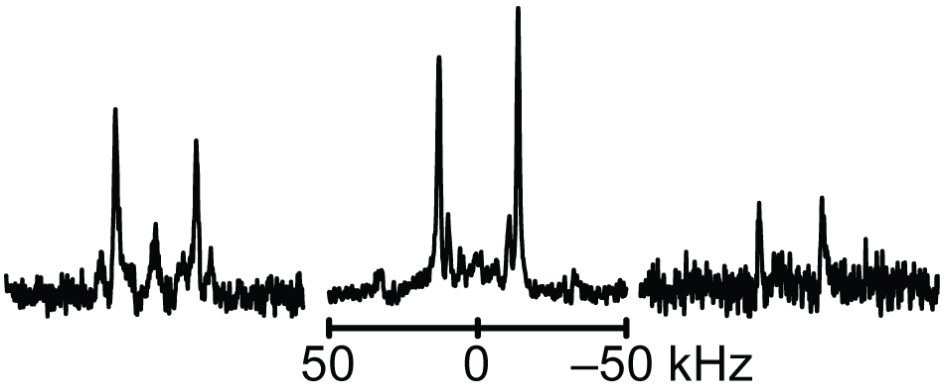

Figure S5. ^{2}H NMR spectra for labeled Ala methyl groups N-terminal to the proline in GWALP23-P12, in oriented bilayers of (left to right) DLPC, DMPC and DOPC. Sample orientation is $\beta = 0°$. The deuterium isotope abundance is 100% in Ala^{7} and 50% in Ala^{9}.

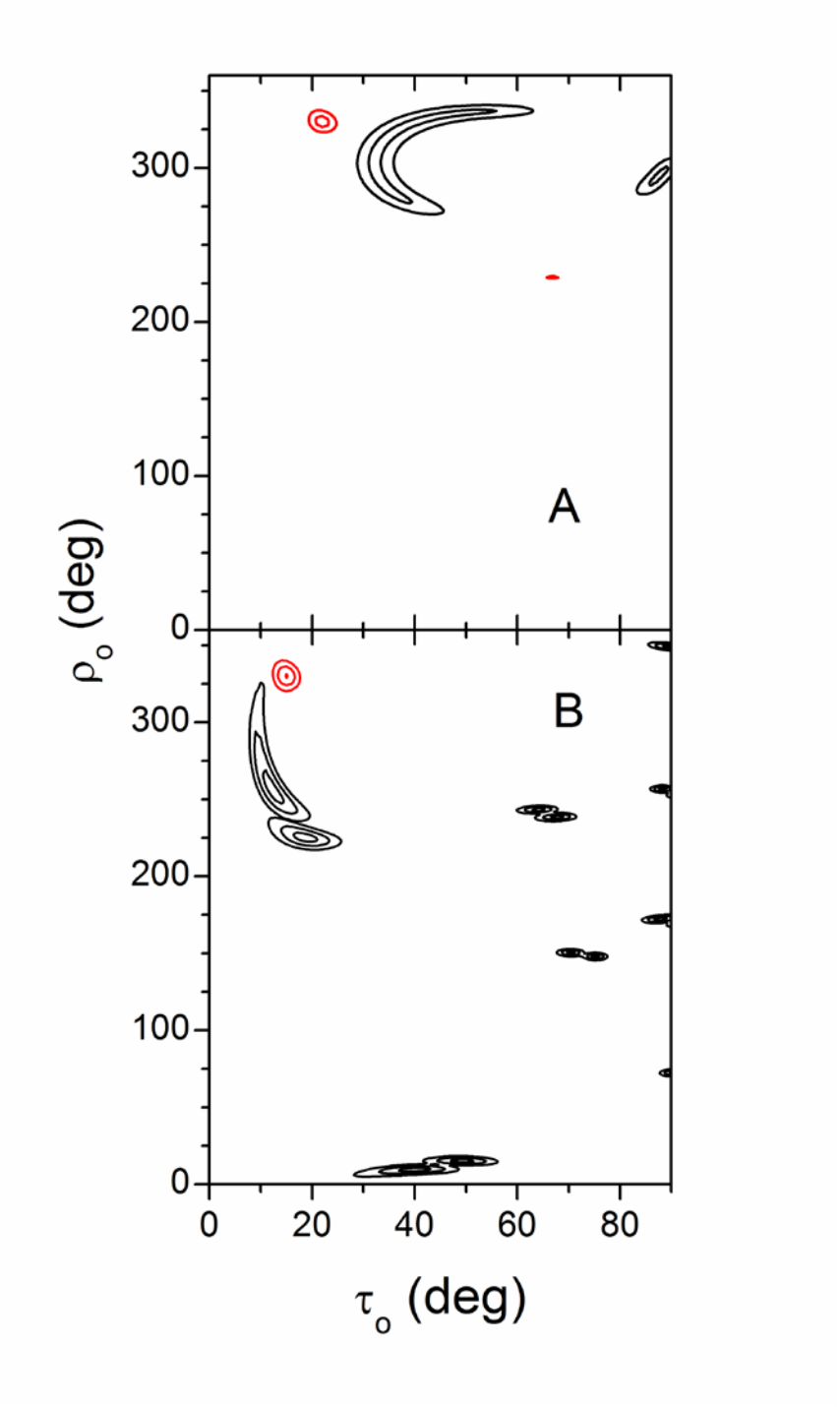

Figure S6. Segmental tilt in DLPC and DOPC. RMSD plots for the tilt of the N-terminal (black) and C-terminal (red) helical segments of GWALP23 P12 in oriented bilayers of (A) DLPC, and (B) DOPC. RMSD is plotted at contour levels of 1, 2 and 3 kHz, as a function of τ and ρ values for the optimum S_{zz} in semi-static calculations.

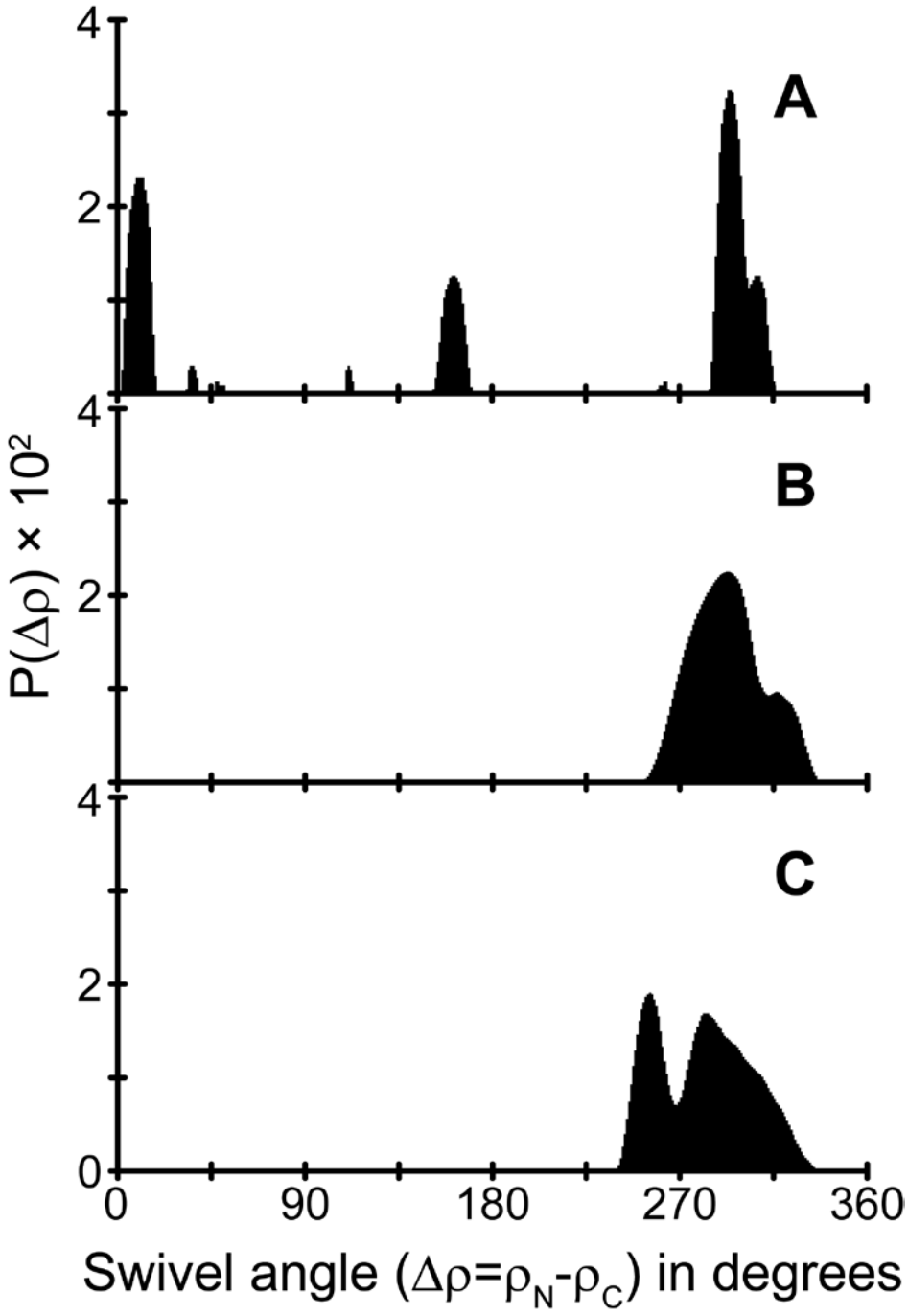

Figure S7. Distributions of proline-induced helix unwinding ("swivel") angles, calculated from rmsd (τ ,ρ) analysis of the N- and C-terminal segments of GWALP23-P12 in (A) DLPC, (B) DMPC and (C) DOPC.