Accommodation of a Central Arginine in a Transmembrane Peptide by Changing the Placement of Anchor Residues

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Supporting Information.

Figures.

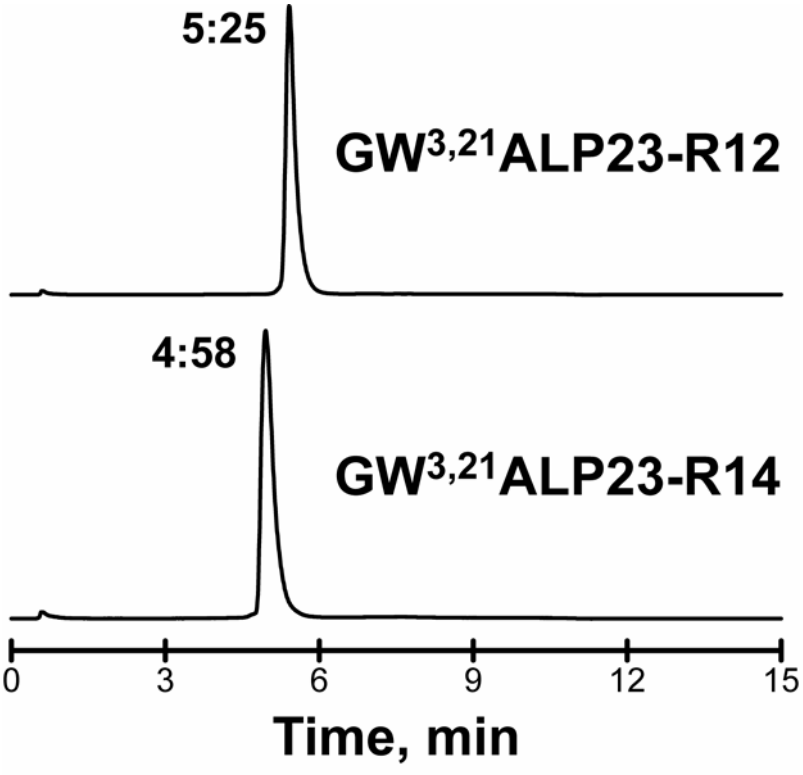

Figure S1. Analytical HPLC of $GW^{3,21}ALP23\text{-}R^{z}$.

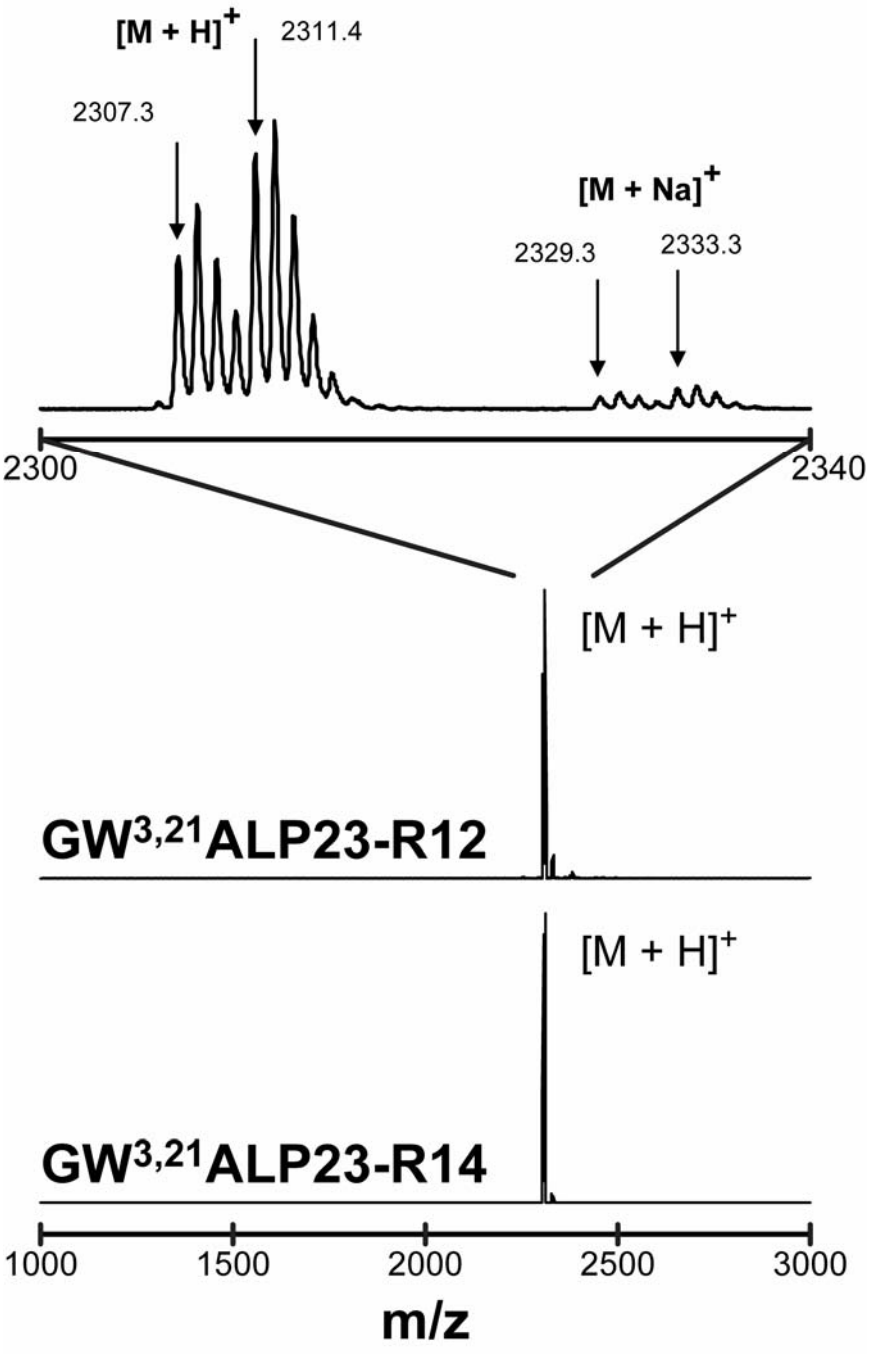

Figure S2. MALDI mass spectra of $GW^{3,21}ALP23\text{-}R^{z}$, containing two ^{2}H-labeled alanine residues.

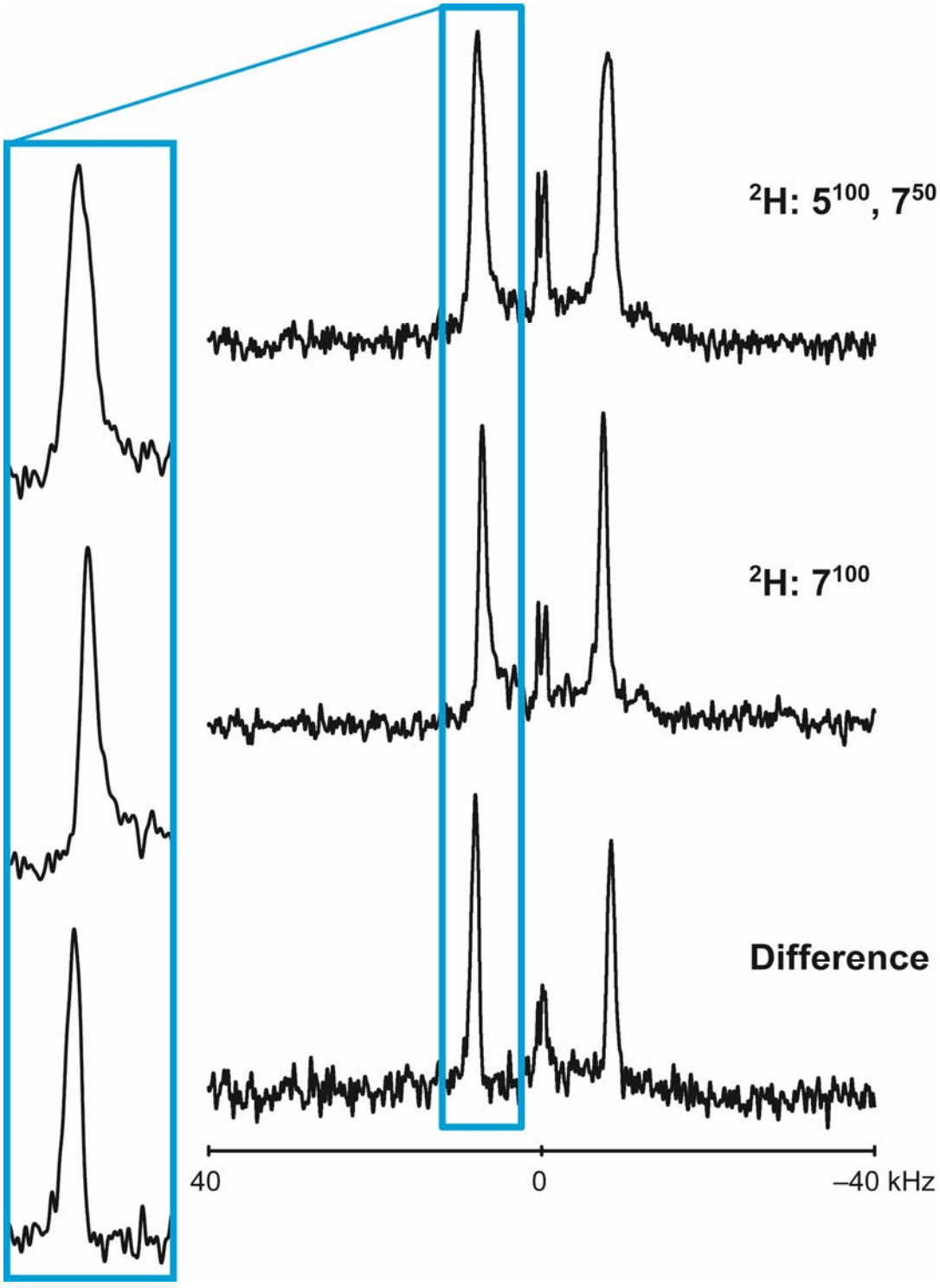

Figure S3. Difference spectra between double and single labeled peptides were used to assign the overlapping peaks. Sample is GW^{3,21}ALP23-R12 in DLPC; β=90°.

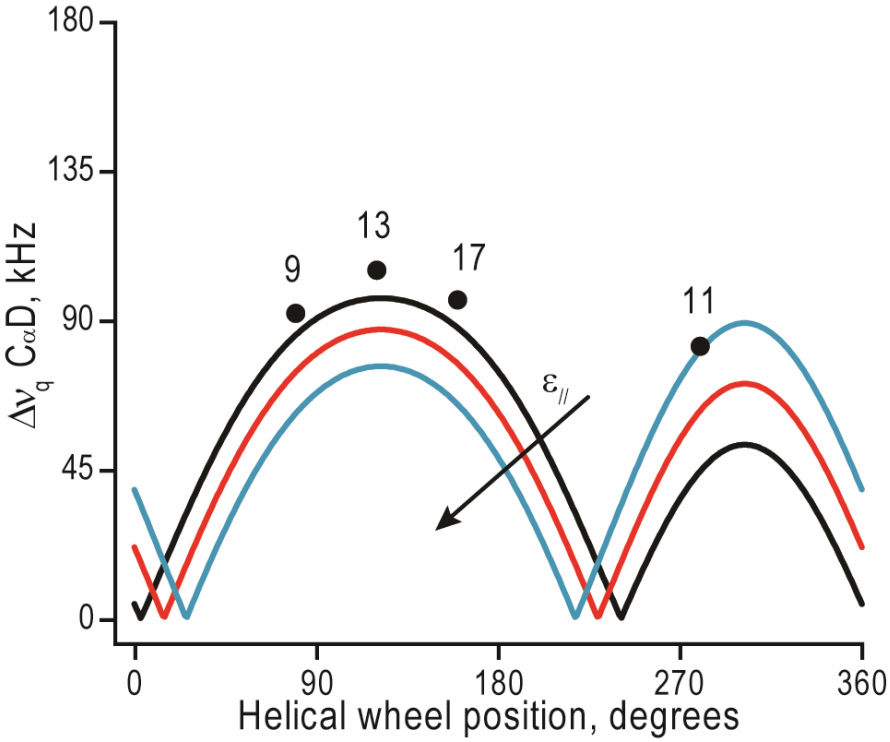

Figure S4. Helical wave plots for $C_\alpha D$ groups of $GW^{5,19}$ALP23-R14 in DOPC with different $\varepsilon_{//}$ values: 119º (black), 122º (red), 125º (blue).

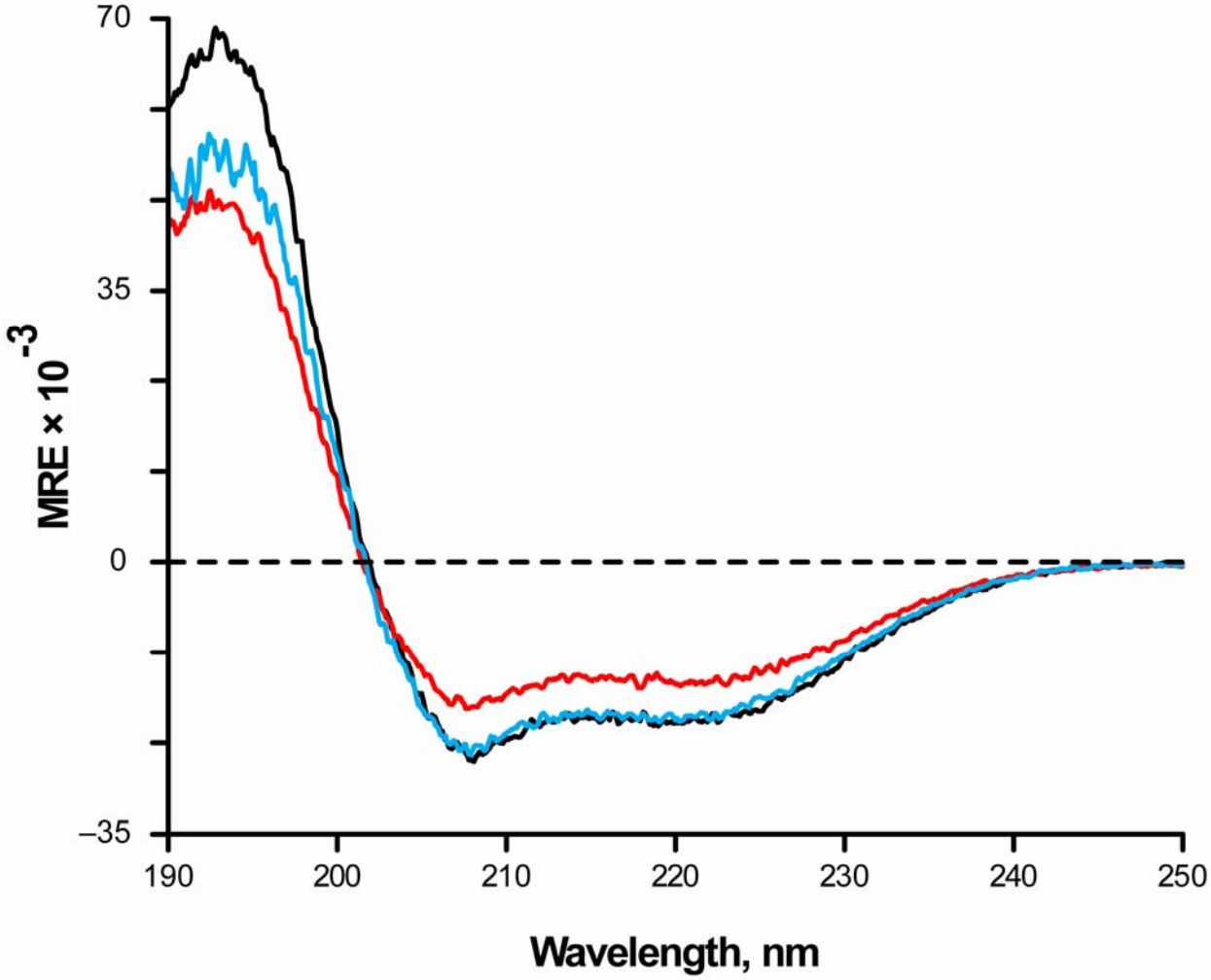

Figure S5. Circular dichroism spectra of $GW^{3,21}$ALP23 and -Arg^{Z} peptides in DLPC. Black: native sequence; Red: Z = 12; Blue: Z = 14.

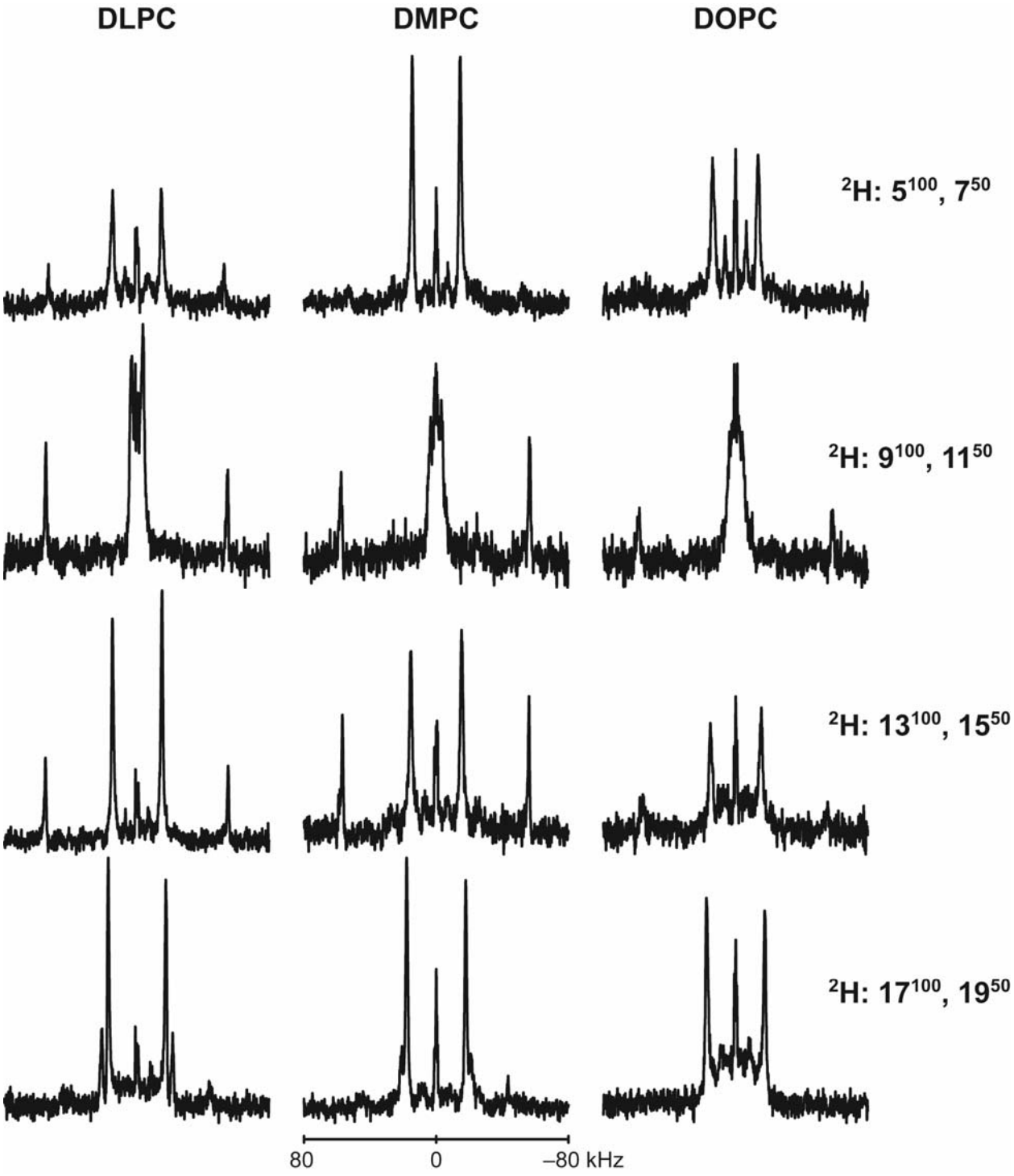

Figure S6. Deuterium NMR spectra of GW^{3,21}ALP23-R12 in DLPC, DMPC, DOPC. Sample orientation is β =0°.

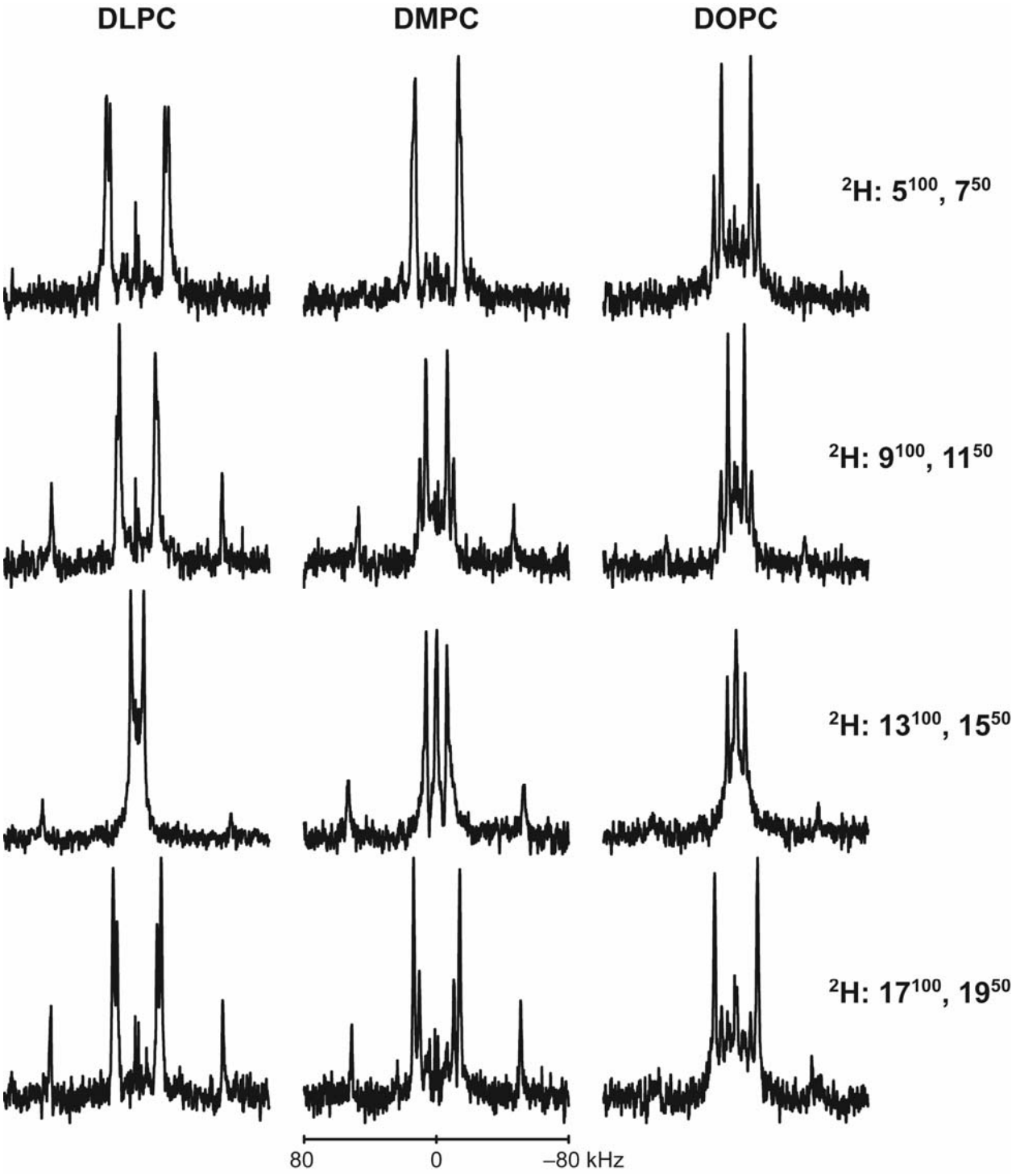

Figure S7. Deuterium NMR spectra of GW^{3,21}ALP23-R14 in DLPC, DMPC, DOPC. Sample orientation is β =0°.

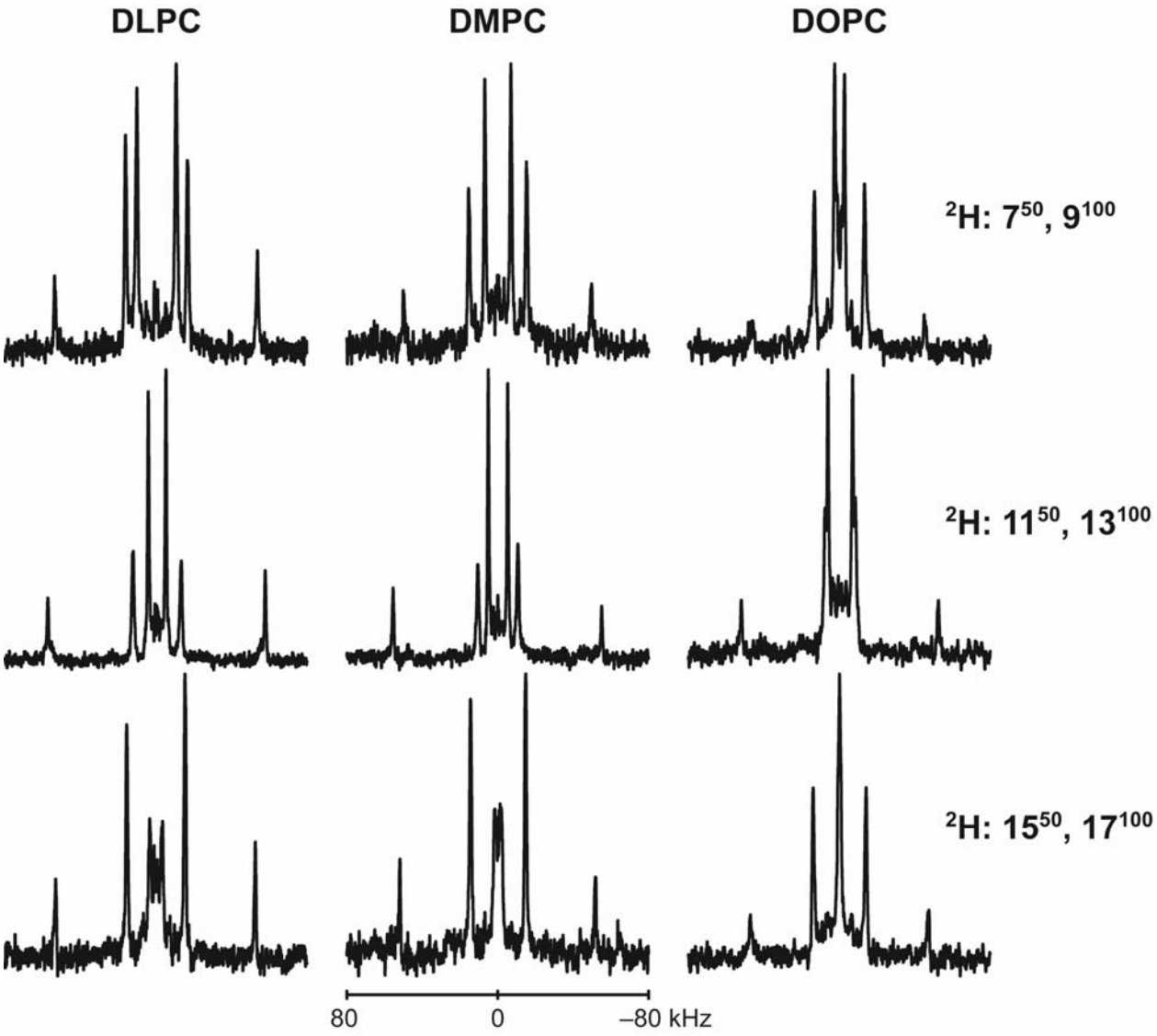

Figure S8. Deuterium NMR spectra of GW^{5,19}ALP23-R14 in DLPC, DMPC, DOPC. Sample orientation is β =0°.

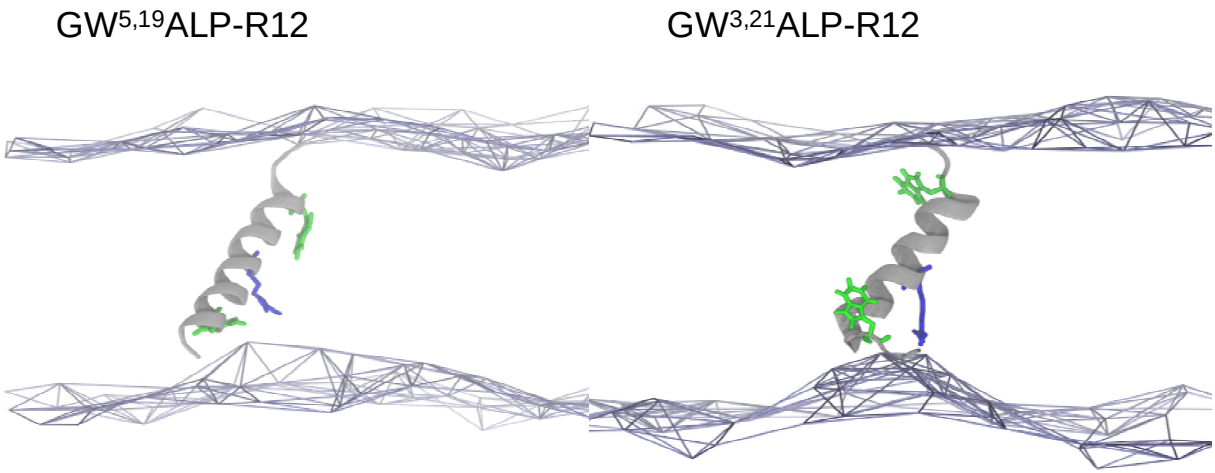

Figure S9. Final snapshots from 50 ns atomistic MD simulations in DPPC of N-terminally snorkeling forms of R12 modified peptides $GW^{5,19}$ALP23-R12 and $GW^{3,21}$ALP23-R12, with peptide backbone in grey cartoon, Trp residues green, and Arg residues blue. Bilayer phosphate head groups are rendered as a grey network.