Supporting information

Structural Elucidation of Cell-Penetrating Penetratin Peptide in Model Membranes at Atomic Level: Probing Hydrophobic Interactions in the Blood-Brain-Barrier

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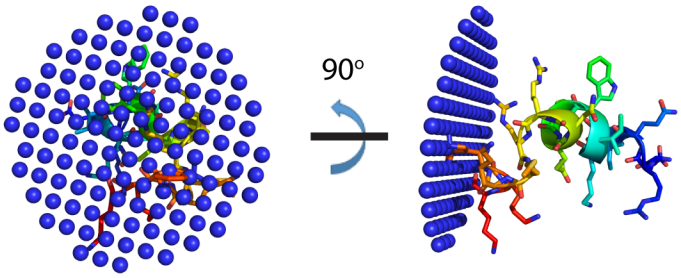

Figure S1: Prediction of DK17 peptide position in the membrane system as predicted using OPM server. The blue spheres in the figure correspond to dummy atoms that represents phosphate head group.

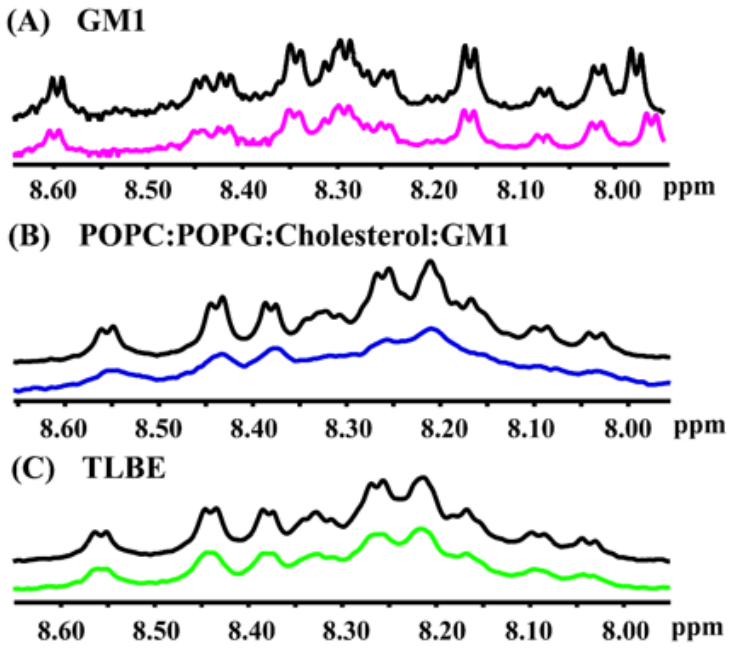

Figure S2: Interaction of DK17 with various LUVs using ^{1}H NMR. LUV-induced line broadening of DK17 (in 10 mM Na_2HPO_4 buffer of pH 4.5) was noted for the amide proton resonances upon titration with each lipid at 288 K. In all cases the free peptide resonances were represented as black and broadened NMR signals were denoted as different respective colors (A-C).

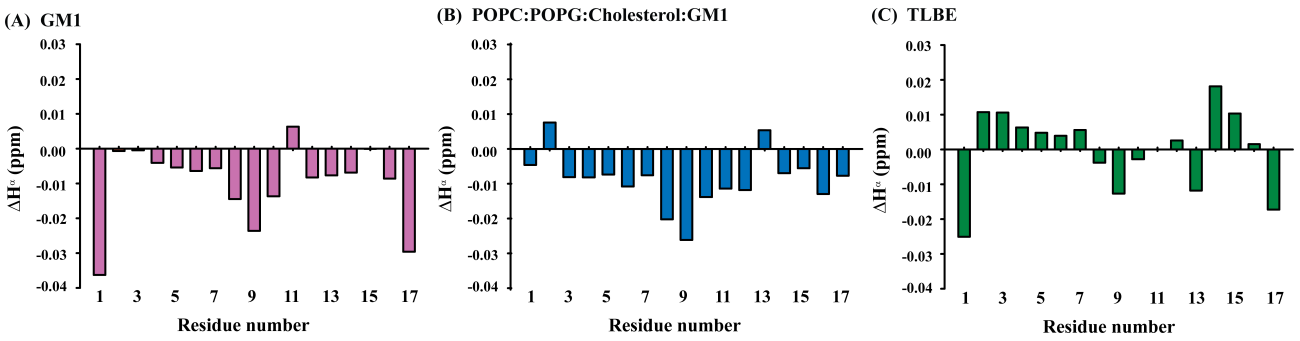

Figure S3: Bar diagram representing the chemical shift deviation for the CαH resonances of each residue of DK17 from their random coil values, obtained in the *trNOESY* spectra of DK17 (in 10 mM Na_2HPO_4 buffer of pH 4.5) in the presence of various LUVs.

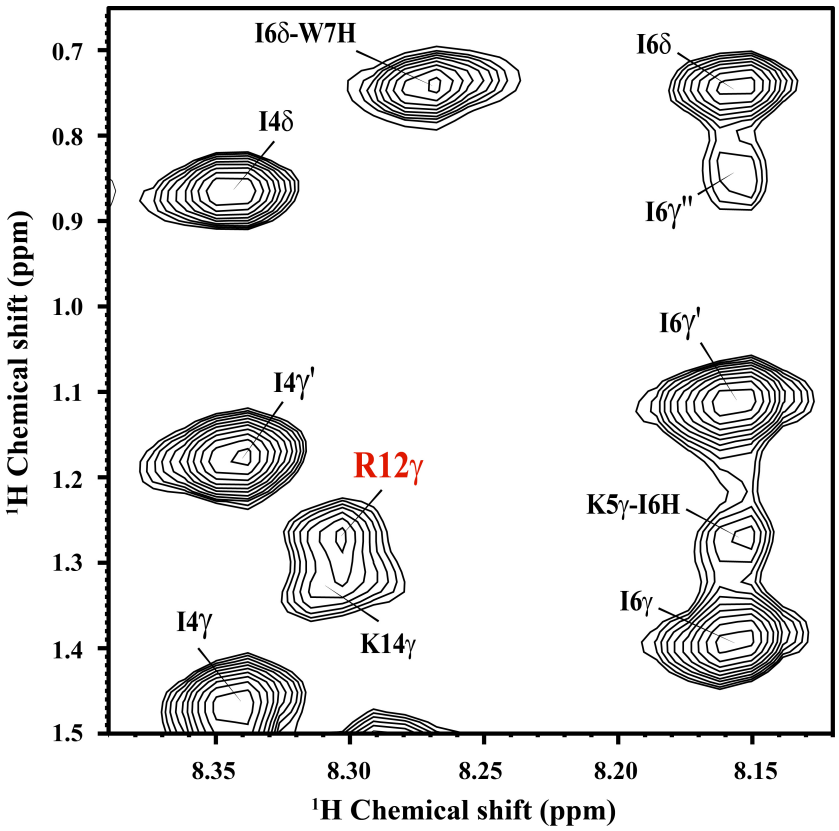

Figure S4: The trNOESY spectra of the aliphatic side chains of DK17 (in 10 mM Na2HPO4 buffer of pH 4.5) in the presence of GM1 LUVs showing up field shift of CγH2 protons of Arg12 residue (R12γ) due to its sandwiched orientation between the aromatic ring protons of Phe8 and Trp15.

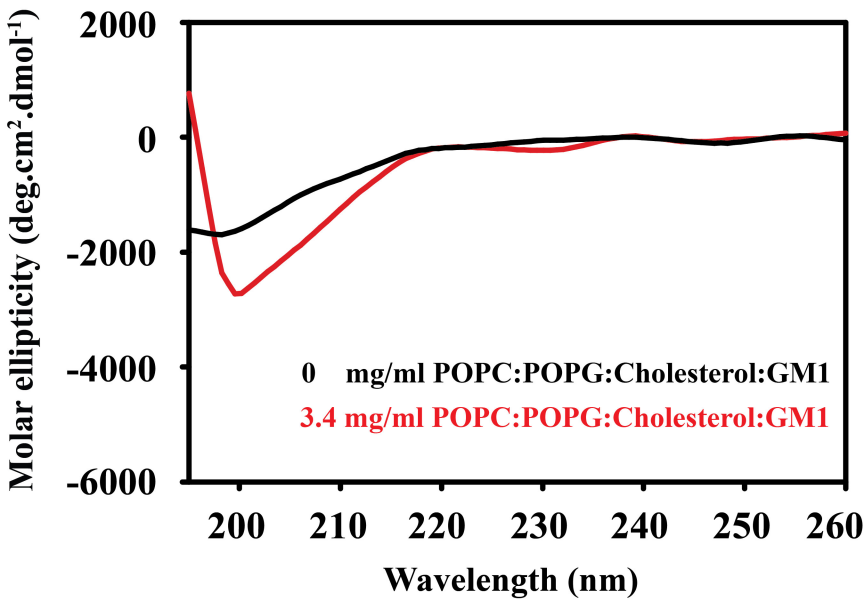

Figure S5: Secondary structure changes of mutated DK17 in aqueous solution (0 mg/ml) or upon interaction with lipids, POPC:POPG:cholesterol:GM1 LUVs (3.4 mg/ml).