Supporting Information

Structural Insights of a Self-Assembling, 9-Residue Peptide from the C-terminal tail of the SARS Corona Virus E-protein in DPC and SDS Micelles: A Combined High and Low Resolution Spectroscopic Study

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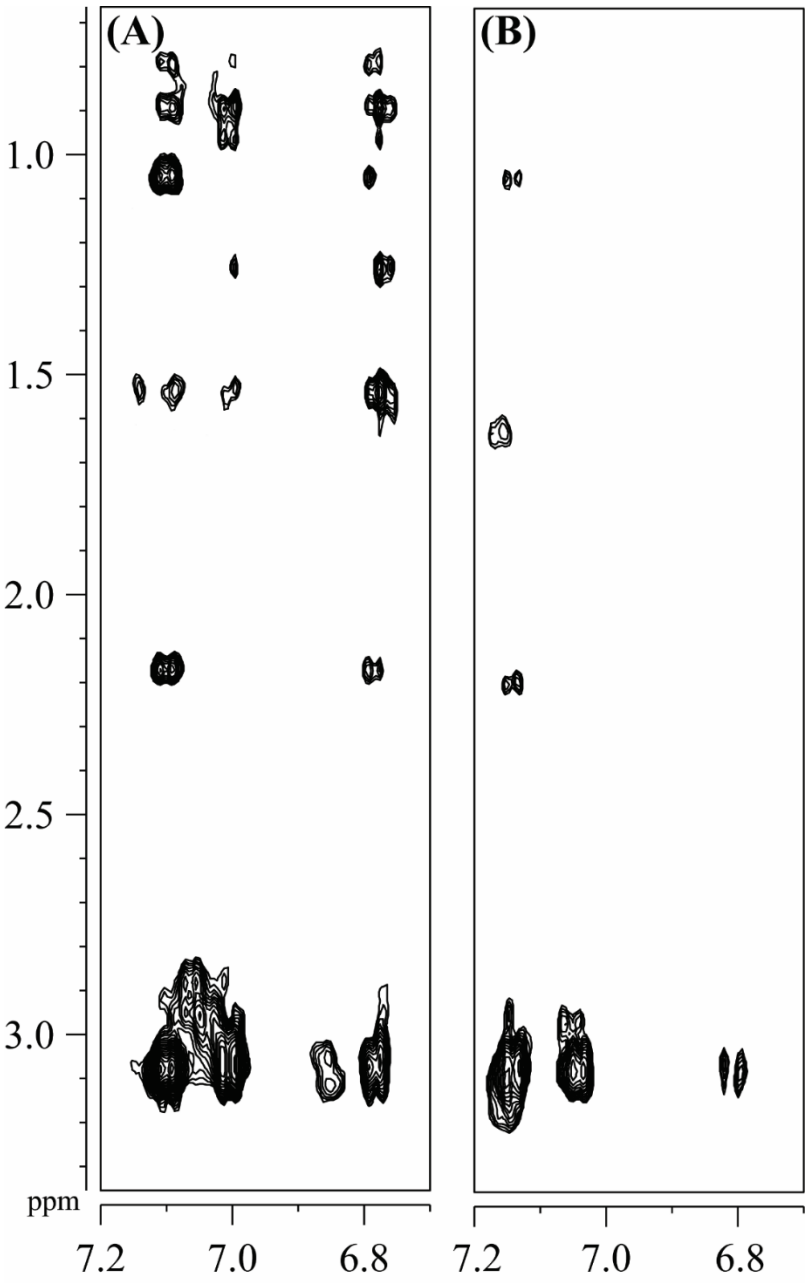

Figure S1. Aromatic region of the NOESY spectra (150 ms mixing time) of TK9 in (A) DPC and (B) SDS micelle. The experiments were performed in Bruker 500 MHz spectrometer at 310 K. The concentrations of peptide and micelles were 1mM, 125 mM, and 200 mM respectively in aqueous solution (pH~ 4.6) at 310 K.

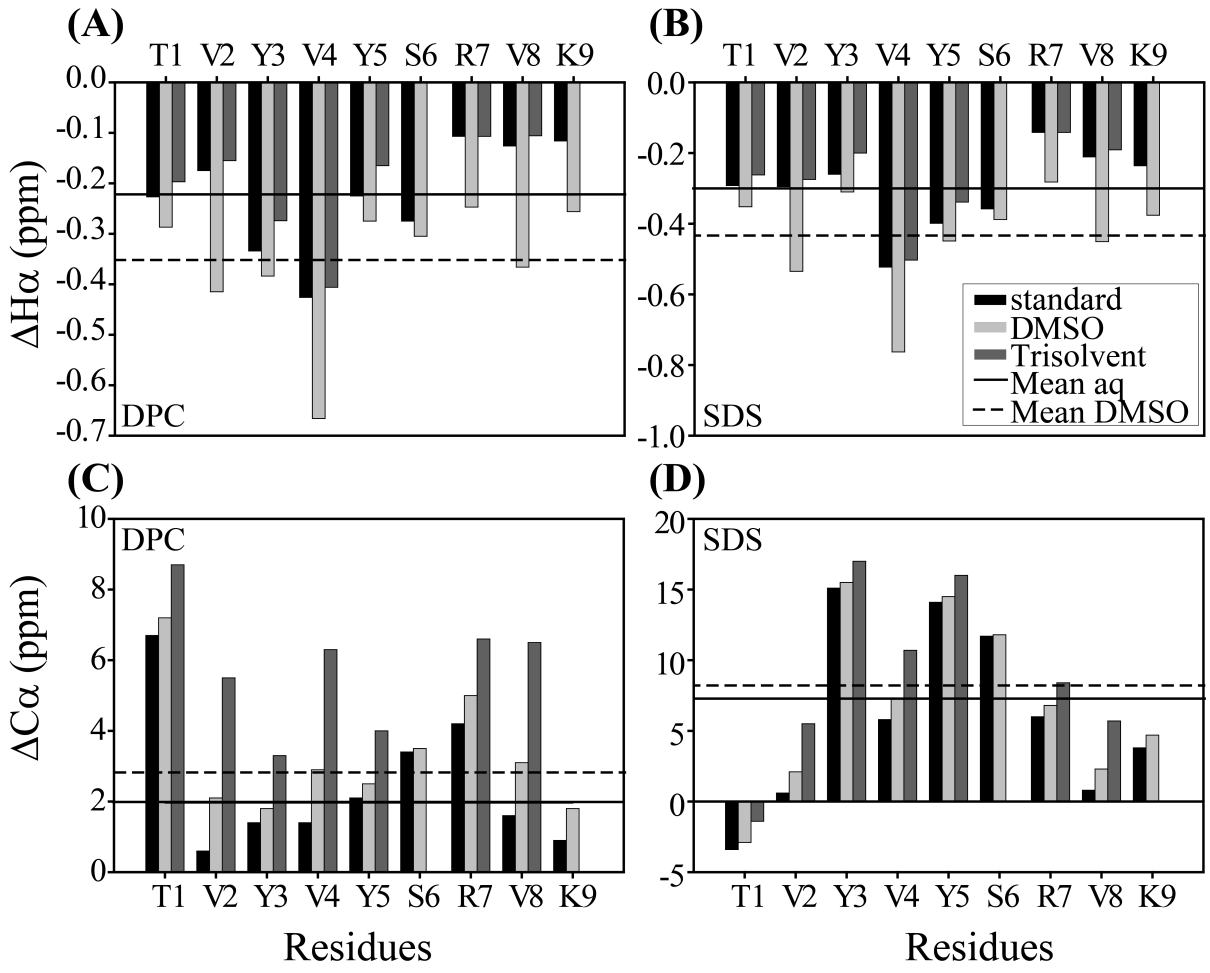

Figure S2. Comparison of the Chemical shift deviations in standard solution, DMSO and trisolvent for TK9 structural conformation in DPC and SDS micelle. (Upper Panel) The chemical shift deviation for H^{α} resonances of each residue of TK9 from the standard random coil values in an aqueous solution, DMSO and the tri-solvent (chloroform, methanol, and water (4:4:1 by v/v)), either in (A) DPC micelle or in (B) SDS micelle. (Lower Panel) The chemical shift deviation for $^{13}C^{\alpha}$ resonances of each residue of TK9 from the standard random coil values either in (C) DPC micelle or in (D) SDS micelle. The black line represents mean standard chemical shift deviation and the dotted line refers to the mean deviation in DMSO.

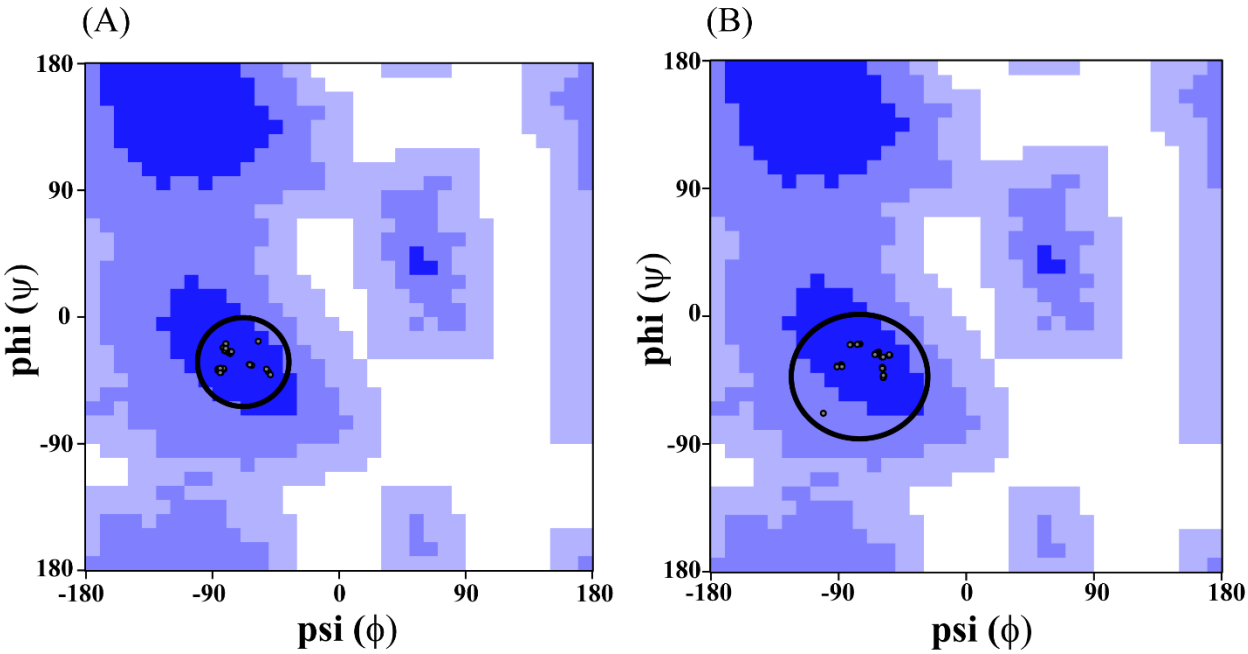

Figure S3. Ramachandran plot displaying the distribution of Phi (Φ) and Psi (Ψ) angles of representative NMR derived conformations of TK9 in (A) DPC and (B) SDS.

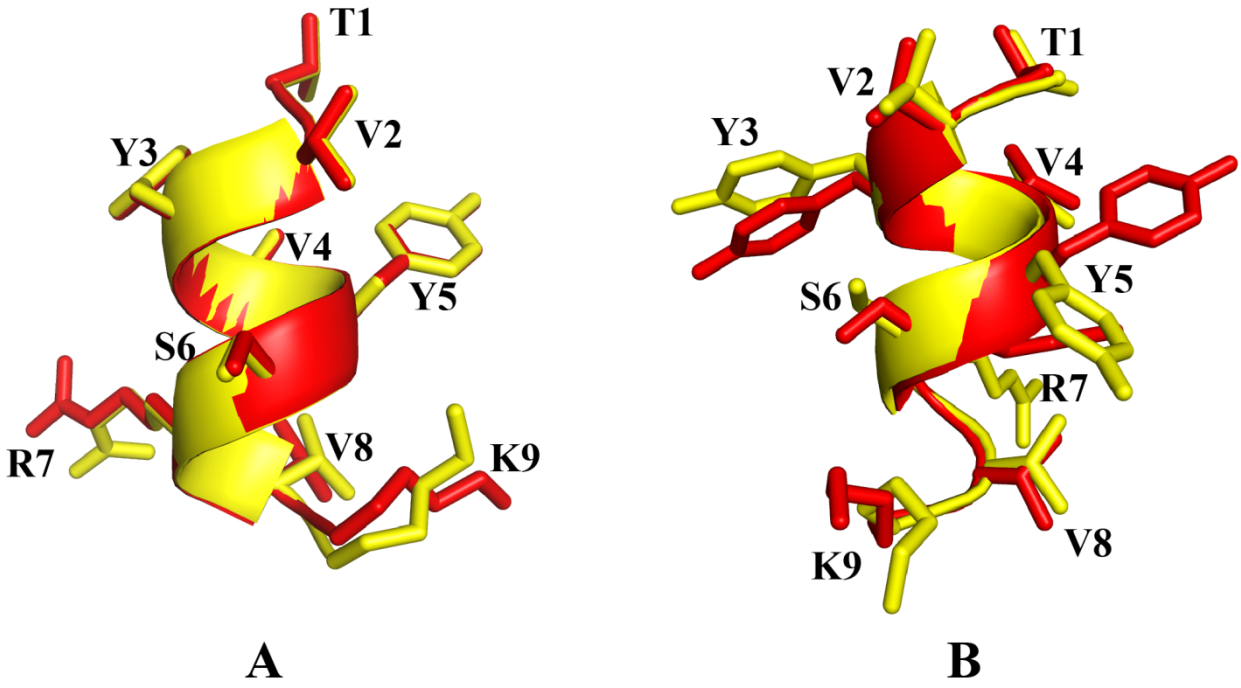

Figure S4. Comparison of the three-dimensional solution structure of TK9 in the absence (ϕ= -30 to -120) (red colour) and presence of torsional angle constraints (yellow), obtained from PREDITOR for (A) DPC and (B) SDS micelles. The structures agreed well with each other in either micellar environments with the overall RMSD values being ~0.18 Å in case of DPC and ~0.51 Å in SDS micellar conditions.

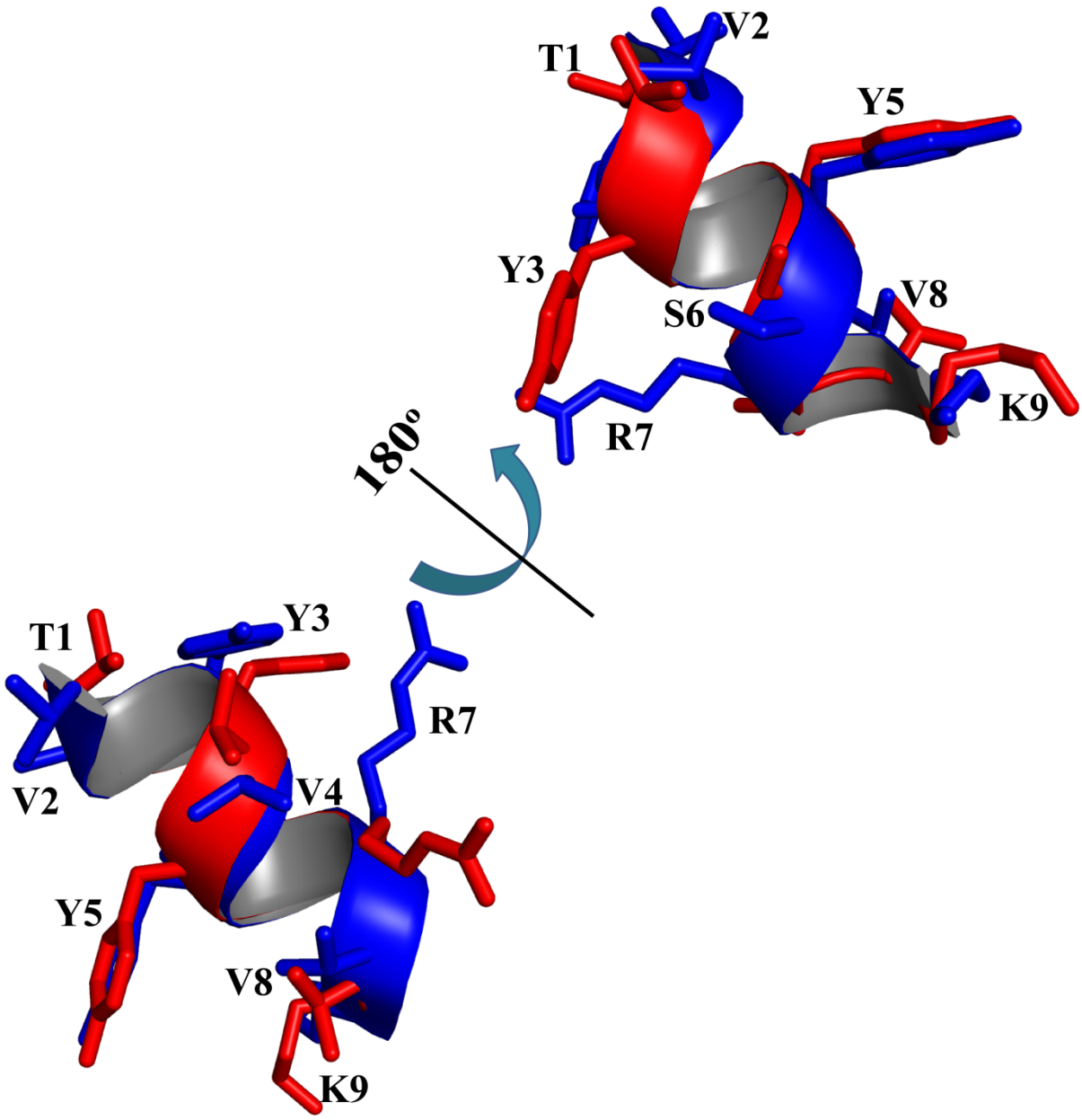

Figure S5. Overlaid conformations of TK9 determined in SDS micelle (red) with the T^{55}VYVYSRVK^{63} segment from the full-length SARS CoV E-protein in SDS micelle (RCSB PDB id: 2MM4). The overall helical segment (Thr1-Lys9) superimposed reasonably with a backbone RMSD of 0.94 Å.