Supplementary Material (ESI) for PCCP

Autonomous folding in the membrane proximal HIV peptide gp41$_{659-671}$: pH tuneability at micelle interfaces. - Supplementary Information

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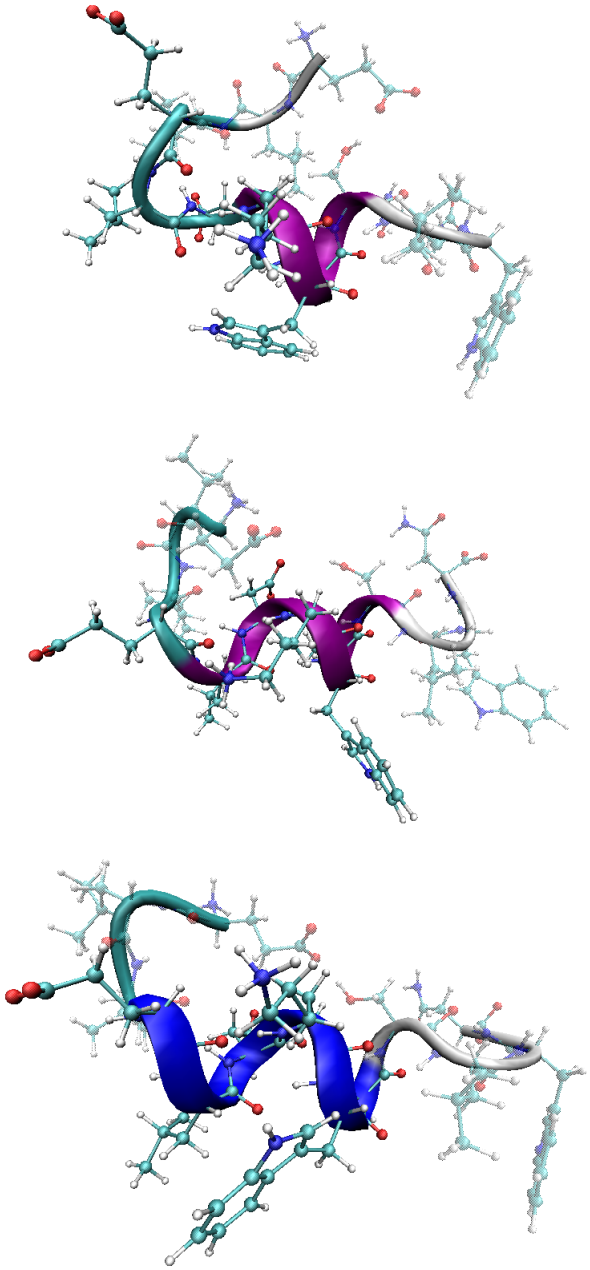

Figure 1: Secondary Structure of gp41 after equilibration: CHARMM (top), AMBER-ff03 (middle), AMBER-ff99SB (bottom).

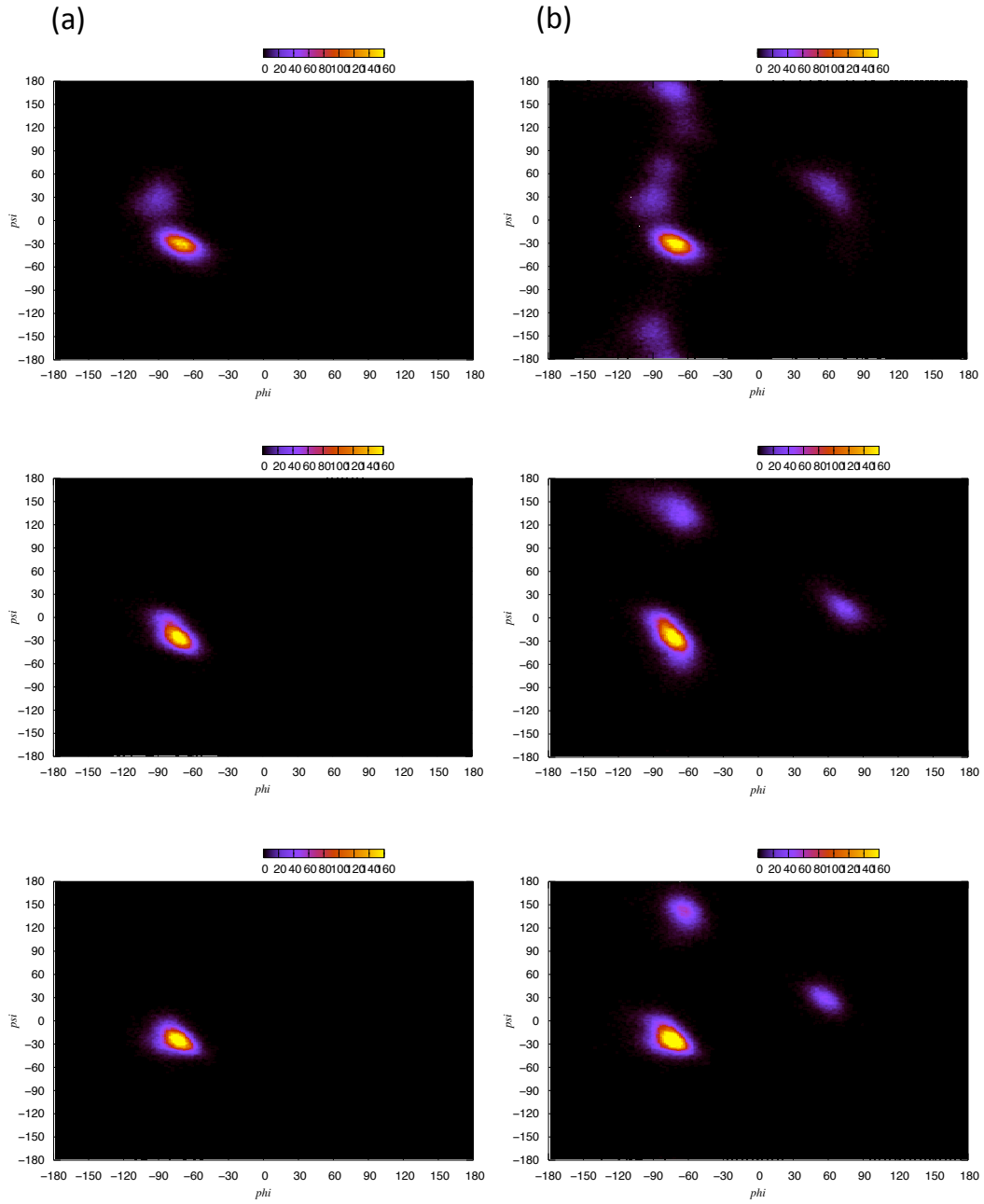

Figure 2: Ramachandran plots of the (a) epitope and (b) full sequence over the initial 1ns: CHARMM (top), AMBER-ff03 (middle), AMBER-ff99SB (bottom)

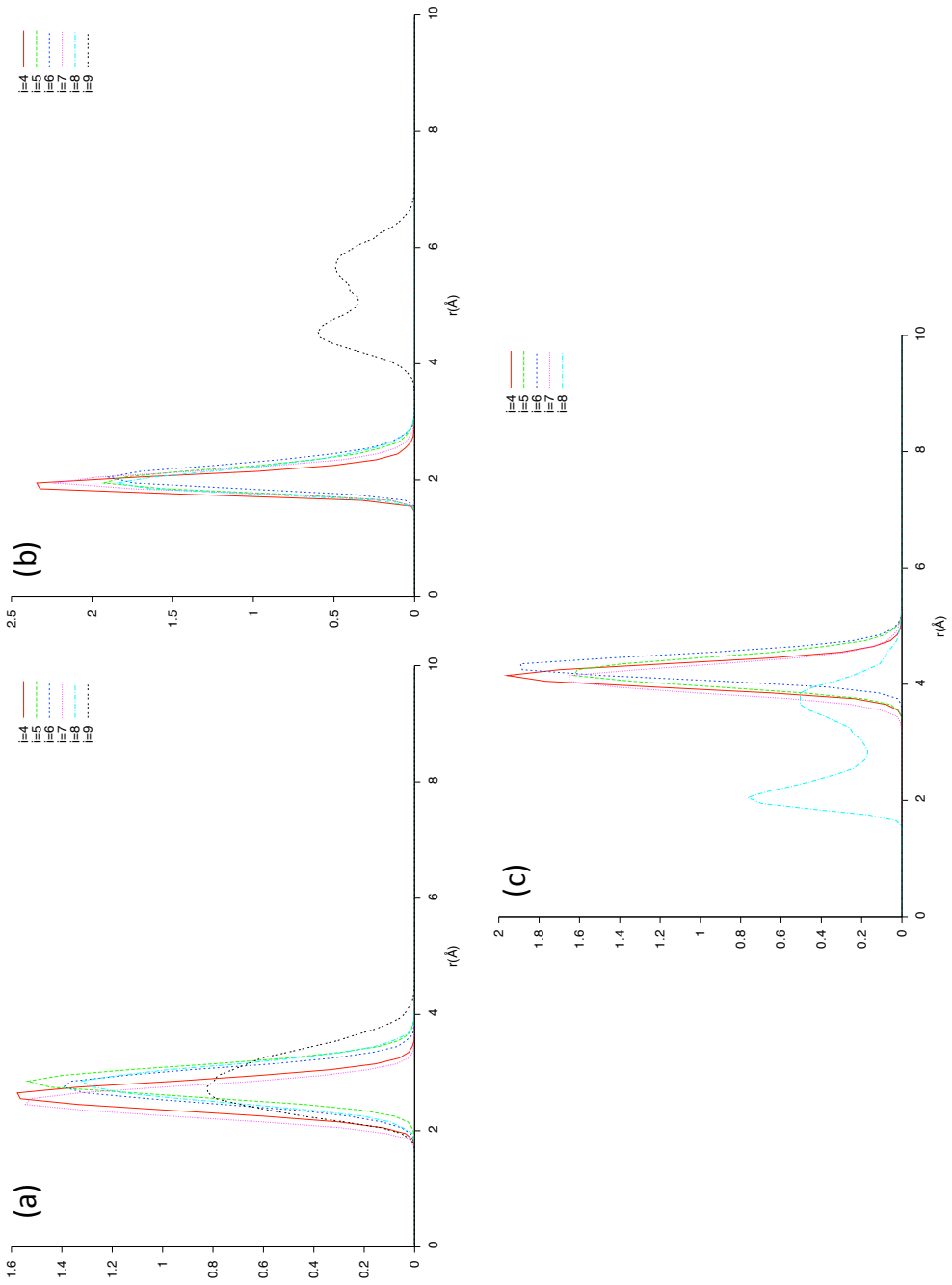

Figure 3: Bond distribution over last 5ns of simulation using CHARMM force-field: (a) i,i+3 bonding, (b) i,i+4 bonding, (c) i,i+5 bonding

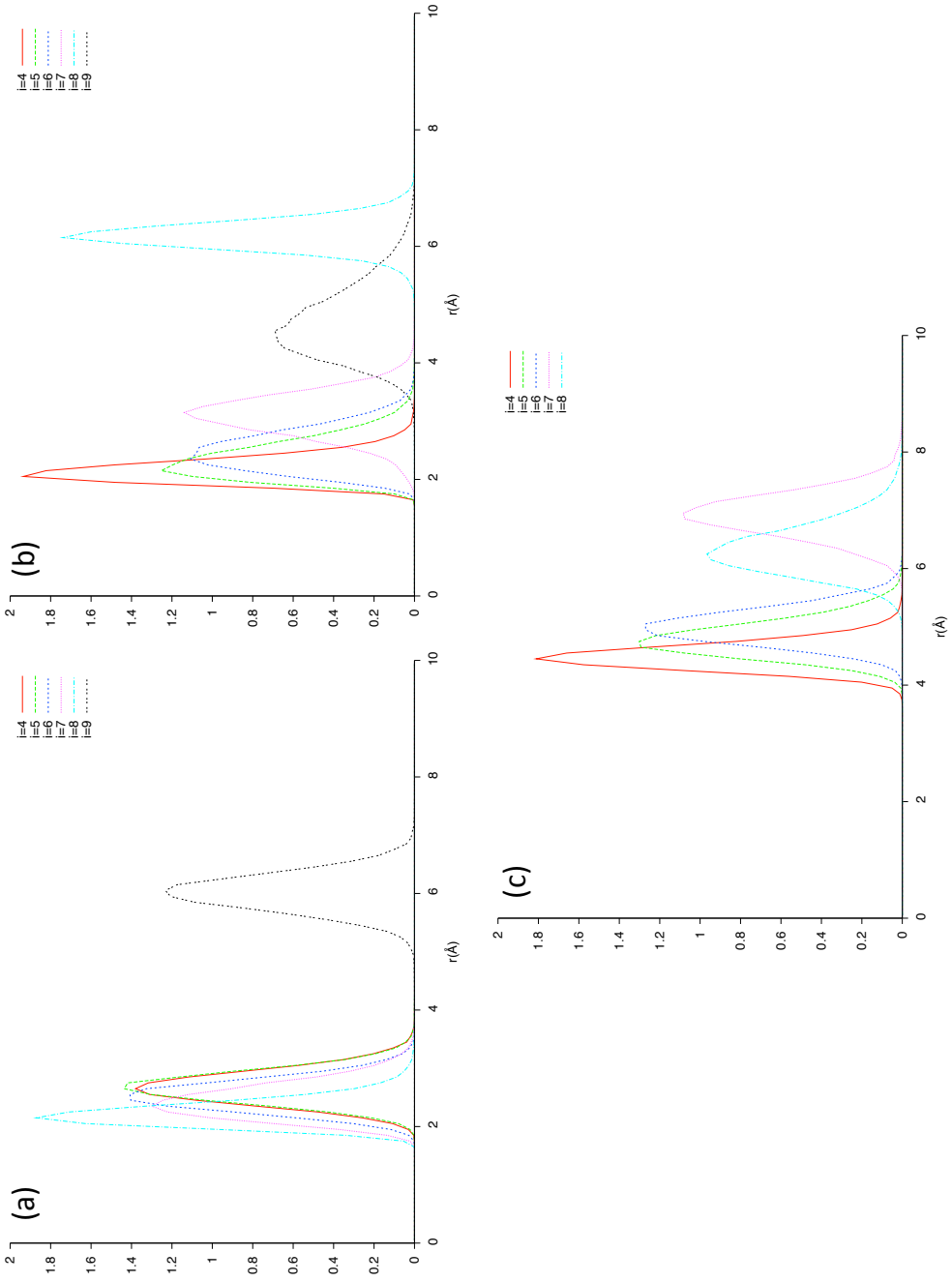

Figure 4: Bond distribution over last 5ns of simulation using AMBER-ff03 force-field: (a) i,i+3 bonding, (b) i,i+4 bonding, (c) i,i+5 bonding

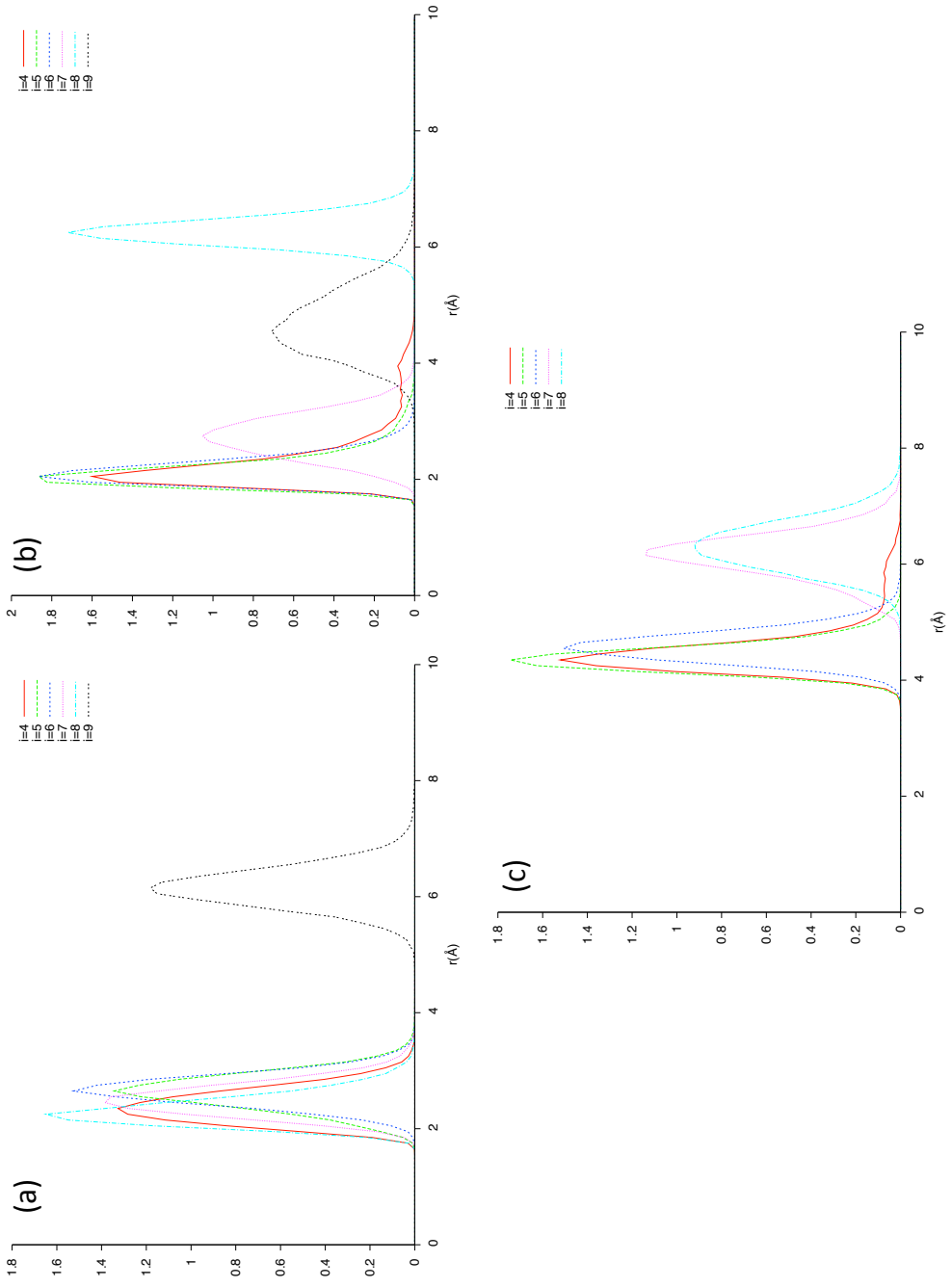

Figure 5: Bond distribution over last 5ns of simulation using AMBER-ff99SB force-field: (a) i,i+3 bonding, (b) i,i+4 bonding, (c) i,i+5 bonding

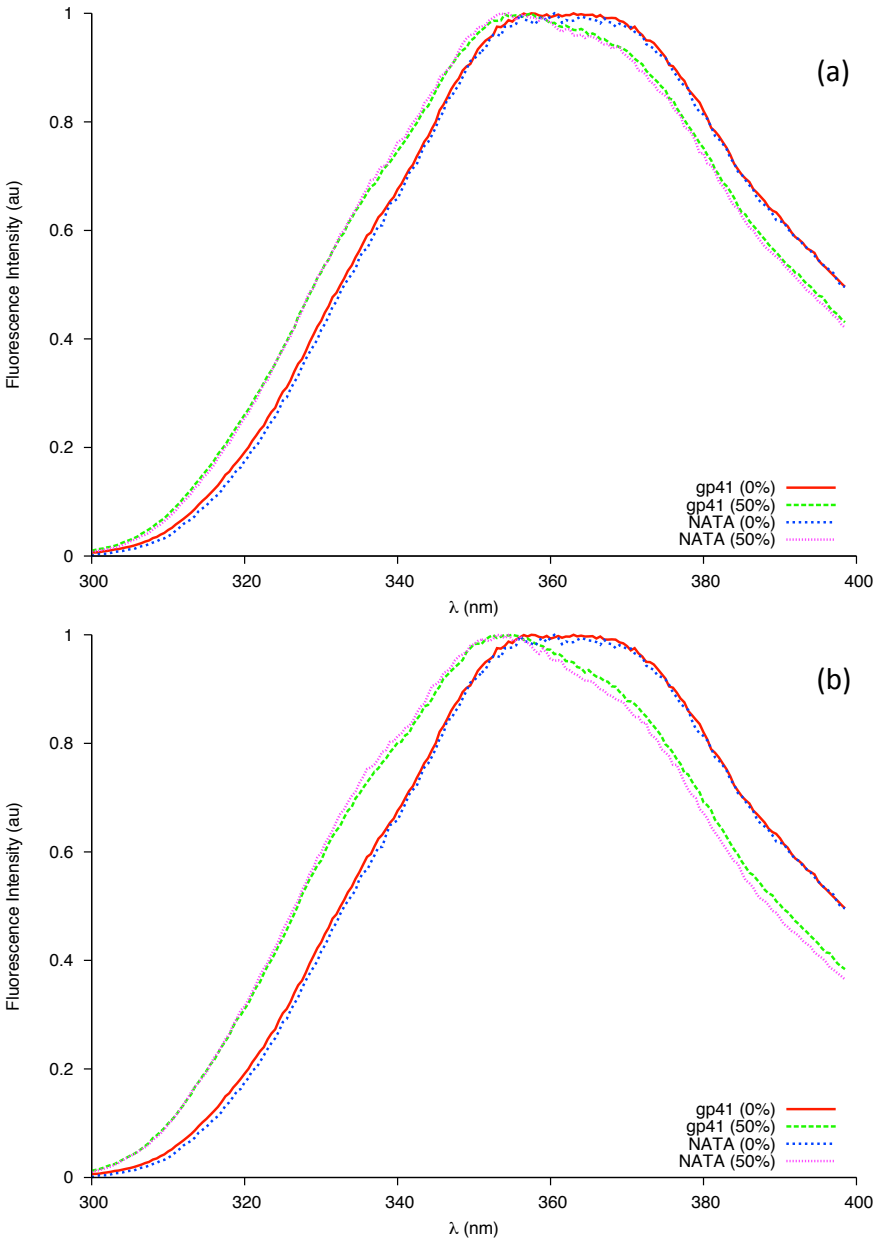

Figure 6: Changes to the intrinsic Trp fluorescence of the gp41 peptide and 10μM NATA control due to the presence of (a) 50% Methanol and (b) 50% Acetonitrile.

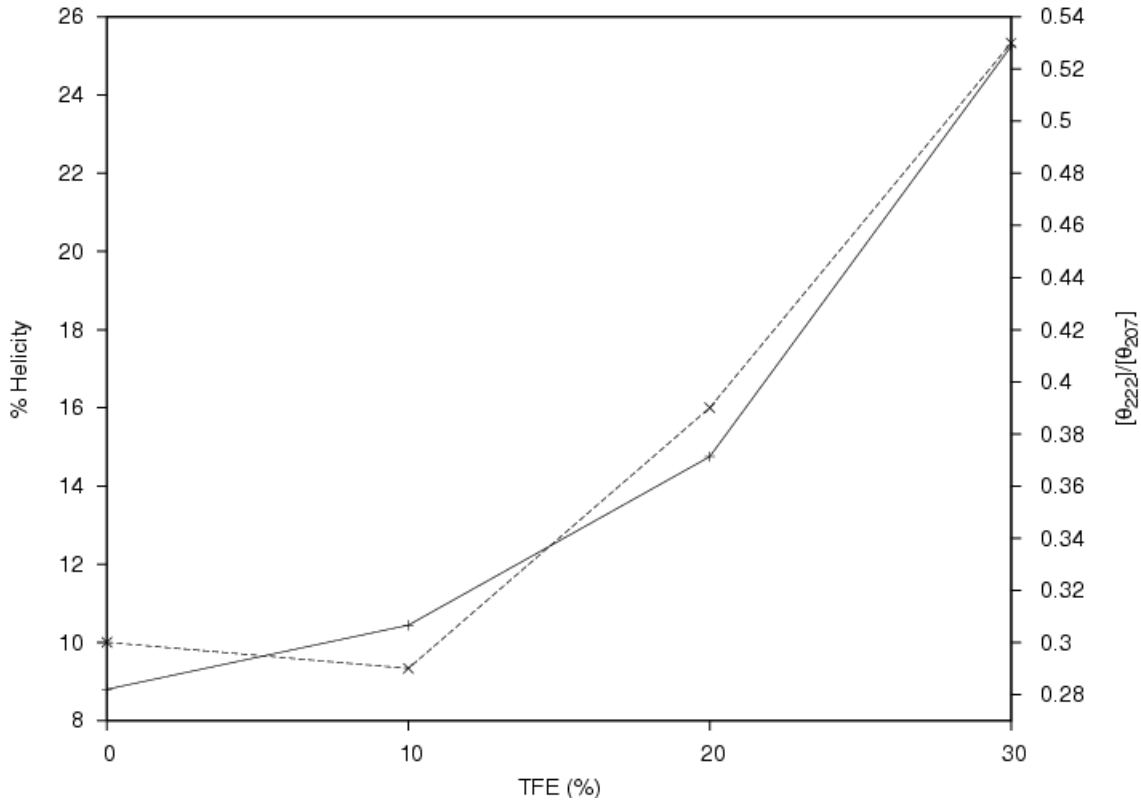

Figure 7: Helical content (solid line) and ratio of $[\theta_{222}]/[\theta_{207}]$ (dotted line) of 0.04mM $gp41_{659-671}$ over various concentrations of TFE.

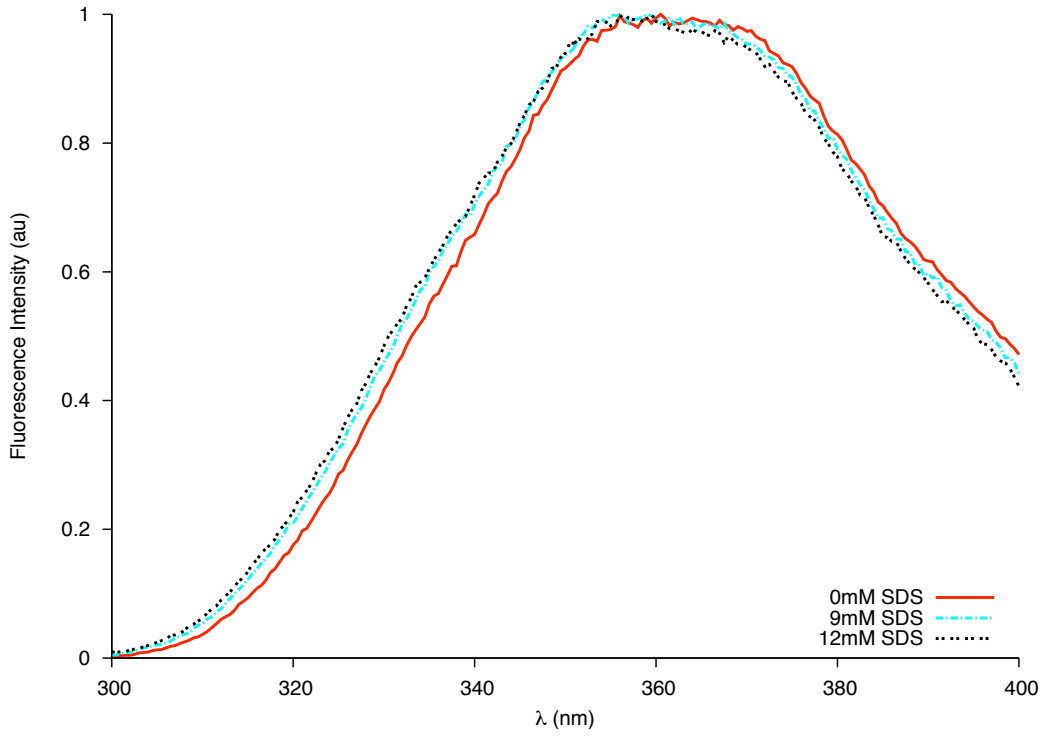

Figure 8: Intrinsic Trp fluorescence of 10μM NATA in the presence of different concentrations of SDS below (3mM) and above (6, 9, 12 mM) the cmc.

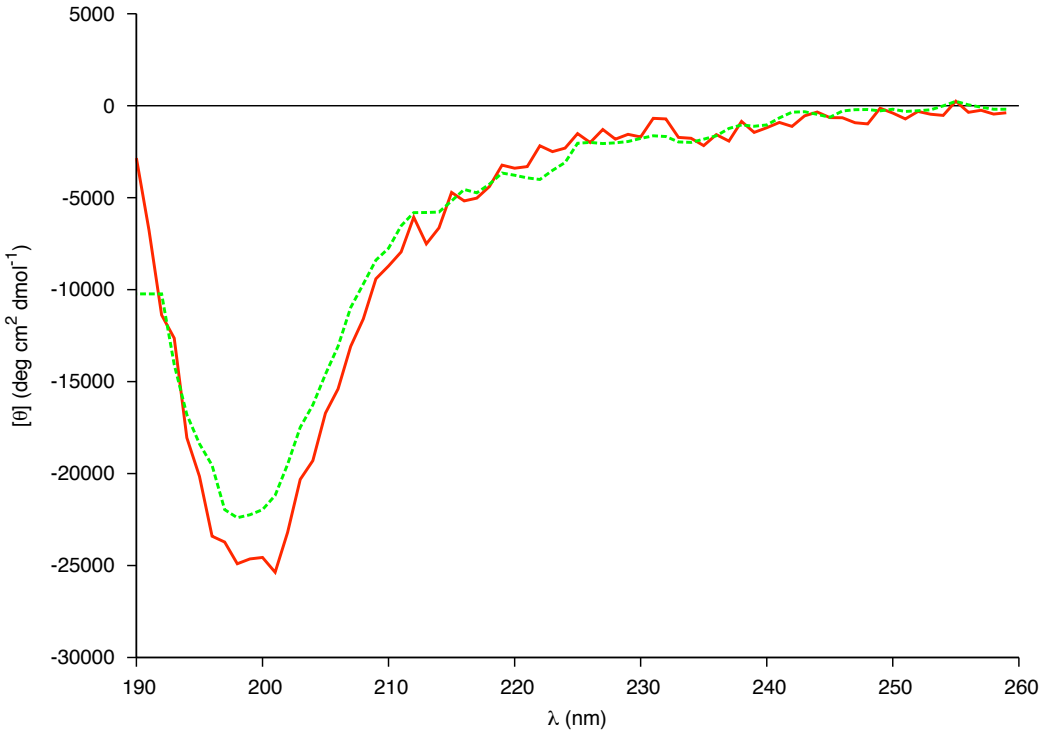

Figure 9: Changes in the far-UV CD spectra of 0.04 mM peptide in 20mM Phosphate buffer at pH 6.83 (solid line) and pH 2.14 (dashed line).

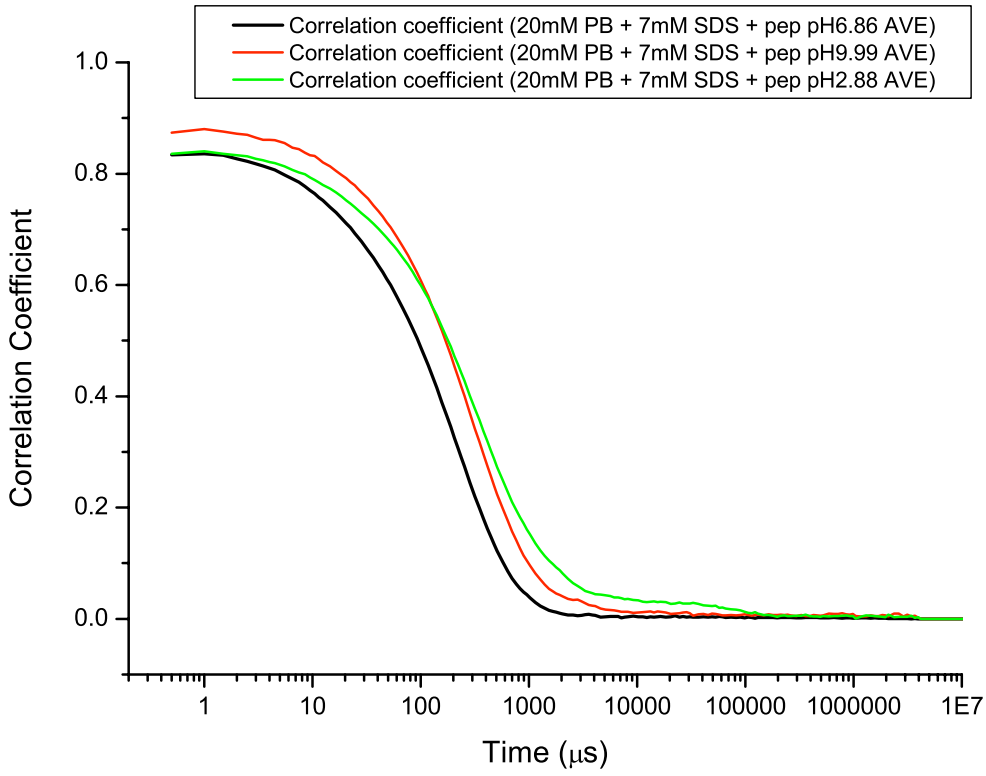

Figure 10: Correlogram of a solution of 7mM SDS in 20mM PB at different pH: demonstrating that under all conditions they are above the cmc

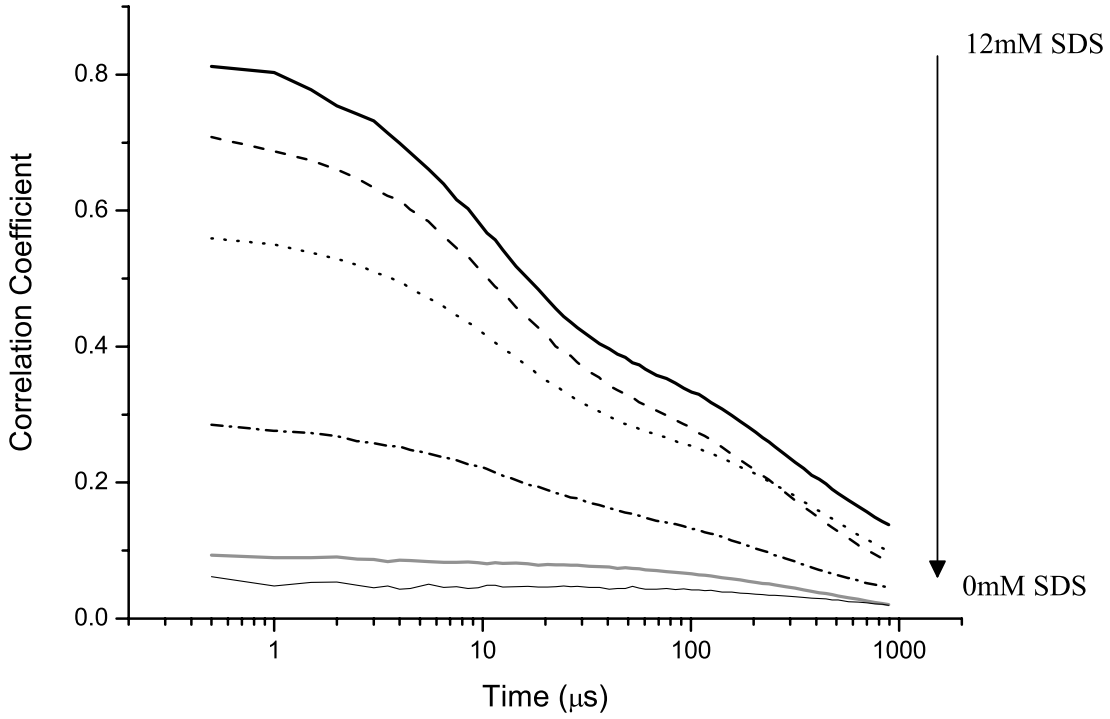

Figure 11: Correlograms of solutions at different SDS concentrations.