Autonomous folding in the membrane proximal HIV peptide gp41\textsubscript{659–671} : pH tuneability at micelle interfaces. -

Supplementary Information

Gregor et al
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 20 mM 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.