Supporting Information to the article: Secondary structure of alanine-rich peptide AKA_2 in a reverse micelle and in bulk water: capped and zwitterionic

Anna Victoria Martinez, Edyta Małolepsza, Laura Domínguez, Qing Lu, and John E. Straub[a)]
Department of Chemistry, Boston University, Boston, MA 02215

[a)] Author to whom correspondence should be addressed. Electronic mail: straub@bu.edu

I. GROMOS FIGURES

A. Secondary structure

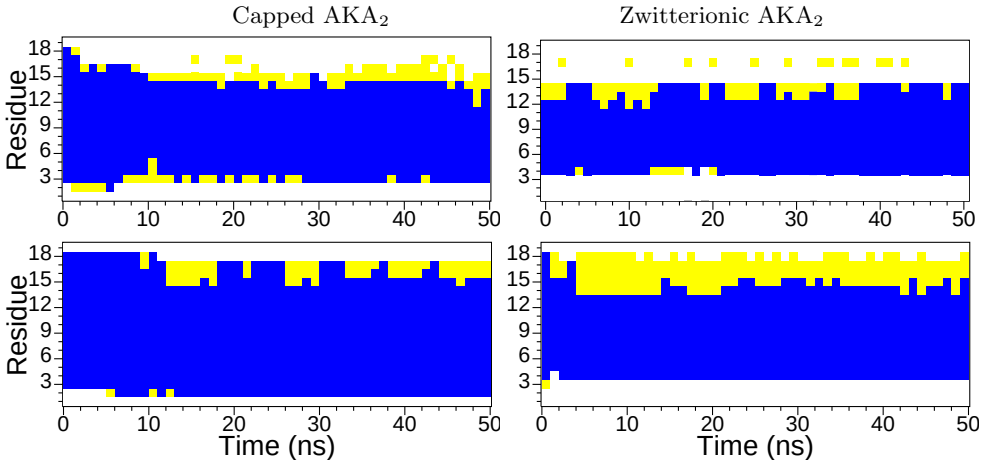

FIG. 1. Secondary structure progress with respect to time of AKA_2 peptides, in unrestrained (top) and spherically restrained (bottom) reverse micelles for the GROMOS systems - capped AKA_2 (left) and zwitterionic AKA_2 (right). The secondary structure is colored as follows: Helix – blue, Turn – yellow, Coil – white. The structure of the terminal residues of all four peptides fluctuates, but the core residues of the capped peptides maintain more helical character than the zwitterionic peptides.

B. Peptide interactions with RM environment

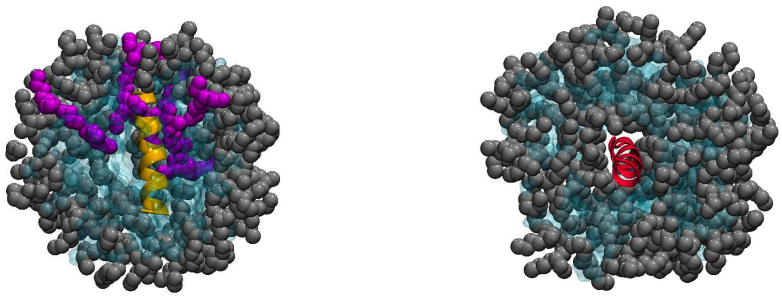

FIG. 2. GROMOS capped AKA_2 in restrained RM (left) and unrestrained RM (right). The snapshot on the left is a cross-section of the restrained reverse micelle. The AOT tails colored in purple are in the water pool. The rest of the AOT tails are represented in gray. The snapshot on the right is a cross-section of the unrestrained RM showing how the AOT tails surround the peptide, which is in the center of a "donut" of AOT molecules. In the GROMOS systems the AKA_2 peptides are less hydrated than those for the CHARMM systems. There are AOT tail groups in the interior of the RMs closer to the peptides displacing water molecules.

II. ENVIRONMENTAL FUNDAMENTAL FREQUENCY SHIFT CONTRIBUTIONS

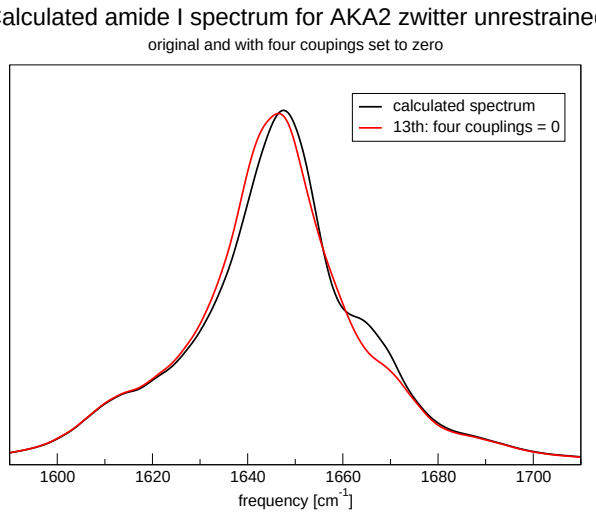

FIG. 3. Comparison of calculated spectrum for AKA_2 in unrestrained RM (black) and spectrum calculated after setting four couplings of 13-th peptide bond to zero to prove that these couplings cause small peak appearance.

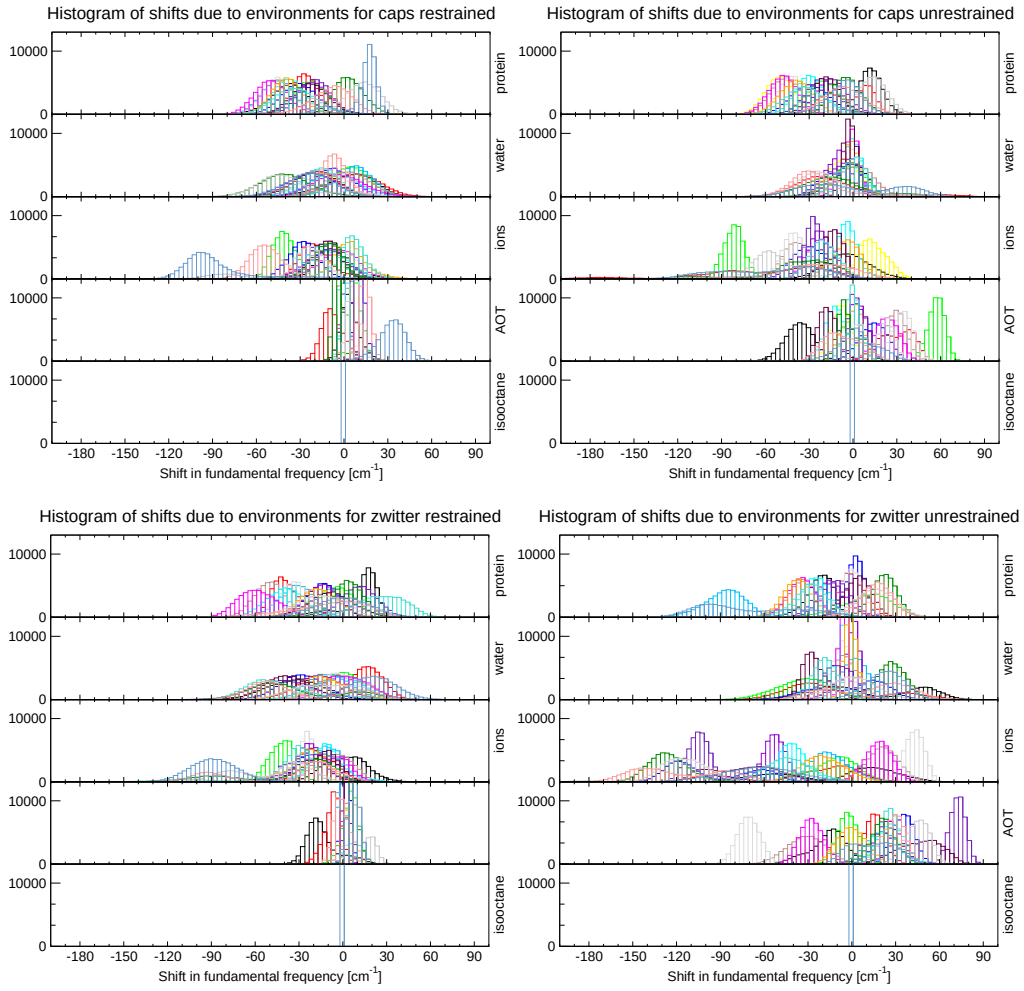

FIG. 4. Comparison of histograms of fundamental frequency shifts caused by protein, water, counterions and AOT molecules.