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Self-assembly of FKE8 peptides using CHARMM ABDELILLAH OUAZZANI, ABDELKADER KARA, ANIKET BHATTACHARYA, University of Central Florida — We investigate the molecular self-assembly of FKE8 peptides (with a sequence FKFEFKFE) using CHARMM. Previous studies^{1,2} of the FKE8 peptides have shown helical ribbon structures during the formation of β -sheets. In order to understand this supra-molecular structure, first we investigate the stable configuration of two FKE8 molecules as a function of the orientation of the long axis of the molecules. We find that stable configuration of these two molecules (based on energy minimization) occurs when the long axes of the two molecules are orientated at an angle $\simeq 51.5^{\circ}$ with respect to each other. This angle may be relevant to understand the pitch of the helical structure. Next we study the self-assembly of several FKE8 molecules starting with an initial configuration where two successive FKE8 molecules are oriented at an angle $\simeq 51.5^{\circ}$ with respect to each other.

¹ W. Hwang, D. Marini, R. D. Kamm, and S. Zhang, J. Chem. Phys. **118**, 389 (2003).

² S. Vauthey, S. Santoso, H. Gong, N. Watson, and S. Zhang, Proc. Natl. Acad. Sci. U.S.A. **99**, 5355 (2002).

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