

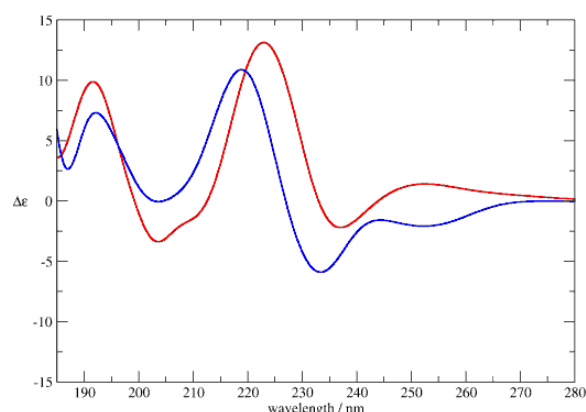
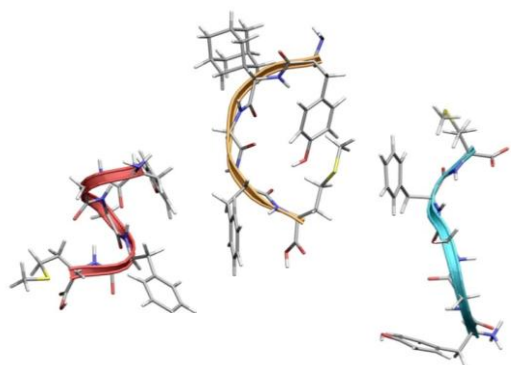
CONFORMATIONAL STUDY OF SMALL PEPTIDES AND ITS RELATION TO CIRCULAR DICHROISM SPECTROSCOPY

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Opioid peptides are known to be associated with many physiological features such as pain mediation, opiate dependence, and euphoria. [1] They are also known to possess affinity for several distinct receptors, implying an ability to assume different shapes for different purposes. Particularly important in this respect is the anti-cancer activity of Opioid Growth Factor (OGF). Improved effects have been seen for its unnatural analogues, which have been proposed to have a structural origin. [2] Using replica exchange molecular dynamics, we have investigated the structural preferences of these peptides. The simulations were performed in explicit trifluoroethanol, as a prototypical low polarity environment. In order to provide a direct link with experiment, circular dichroism spectra of the peptides were calculated using a QM/MM approach in which the peptide was treated quantum mechanically, while the effect of the solvent was included classically.

[1] K. Y. Sanbonmatsu, A. E. Garcia, *Proteins*, **2002**, *46*, 225-234.

[2] M. Gredičak, F. Supek, M. Kralj, Z. Majer, M. Hollosi, T. Šmuc, K. Mlinarić-Majerski, Š. Horvat, *Amino Acids*, **2009**, *38*, 1185-1191.