

## Structure-Activity Analysis of Neuropeptide FF using Replica Exchange Molecular Dynamics

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We are predicting the most stable conformations of Neuropeptide FF (NPFF) using Replica Exchange Molecular Dynamics (REMD). NPFF has been implicated in pain modulation in mammals through the opioid system.<sup>1</sup> A lack of a crystal structure for this short peptide has greatly hindered our understanding of ligand-receptor interactions for this system; its flexibility makes REMD an appropriate method for structural analyses.<sup>2</sup> We identify correlations among the three most stable conformations and compare the results to an experimental binding affinity assay.

(1) Roumy, M. and Zajac, J. Neuropeptide FF, pain and analgesia, *European Journal of Pharmacology*, 1998, **345**, 1-11.

(2) Vyas, N. et al. Structure-activity relationships of neuropeptide FF and related peptidic and non-peptidic derivatives, *Peptides*, 2006, **27**, 990-996.