Biological Research with Electronic Structure Methods

In my research I use electronic structure methods (density functional theory *and ab initio* methods) to study molecules of biological interest. In this presentation I focus on three different topics; (1) a small dipeptide, the study of which started off as a search for the most stable conformer, but turned into an investigation of methodological accuracy; (2) stacking of DNA bases, either isolated or as part of nucleotides; and (3) halogen bonding, a special case of intermolecular interaction.