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Computational Chemistry as a Tool for Studying Complex Molecular Systems

In the last twenty years or so we have witnessed tremendous advances in the field of computer technology as well as the development of very efficient algorithms for electronic structure calculations. As a result, a variety of computational quantum chemistry methods are now applicable to complex molecular systems made of several hundred atoms which in the past could be tackled only by using force-field methods (e.g. molecular mechanics). The advantage of this approach is that important chemical events such as bond breaking, bond formation, electronic charge polarization and delocalization, can be modeled with a high degree of accuracy. Hence, computational chemistry represents a powerful tool in the hand of researchers that can nicely complement experiments.

In this talk I will discuss the results of recent computational studies carried out on three different molecular systems: 1) yatakemycin, a potent antitumor agent of natural origin which operates in-vivo by alkylating DNA, 2) human erythropoietin (HuEPO), a small polypeptide which controls the delivery of oxygen to tissues, and 3) bis-allylpalladium, an organometallic complex that acts as a catalyst in the allylation of aldehydes to yield homoallyl alcohols.