\( \pi \)-stacking interaction between heterocyclic rings in a reaction field of biological system

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Reaction fields in biological systems are given by surrounding structures where various interactions such as hydrogen bonding interaction, van der Waals interaction, and \( \pi \)-stacking interaction can be seen. However, there is no experimental method to determine the interaction energy values. Recently, computational techniques have been used as a standard in order to estimate the values or to verify the experimental results. Here, we are focusing on the \( \pi \)-electrons, \( \pi \)-orbitals, and conjugate systems in relation to the \( \pi \)-stacking interaction between heterocyclic rings in the reaction field: the active site of human carbonic anhydrase II [1-3]. The electron density difference was calculated on the basis of the Moller-Plesset perturbation theory on the NEC SX9 machine equipped with Gaussian 09 program package. The interaction was treated by the harmonic oscillator equation to obtain the spring constant (kcal mol\(^{-1}\) rad\(^{-2}\)). Consequently, determining the interaction profile is mandatory to explain the transfer of proton between molecules in the reaction.

Keywords: \( \pi \)-stacking interaction, Moller-Plesset perturbation theory, harmonic oscillator equation, electron density difference, human carbonic anhydrase II