ABSTRACT

There is a need for reliable rules of thumb for various applications in the area of biochemistry, supramolecular chemistry and material sciences. Simultaneously, the amount of information, which we can gather from X-ray crystal geometries about the nature of recognition processes, is limited. Deeper insight into the noncovalent interactions playing the most important role is needed in order to revise these universal rules governing any recognition process. In this thesis, systematic development and study of the accuracy of the computational chemistry methods followed by their applications in protein•DNA and host•guest systems, are presented.

The non-empirical quantum mechanical tools (DFT-D, MP2.5, CCSD(T) *etc*. methods) were utilized in several projects. We found and confirmed unique low lying interaction energies distinct from the rest of the distributions in several amino acid−base pairs opening a way toward universal rules governing the selective binding of any DNA sequence. Further, the predictions and examination of changes of Gibbs energies (ΔG) and its subcomponents have been made in several cases and carefully compared with experiments. We determined that the choline (Ch+) guest is bound 2.8 kcal/mol stronger (calculated ΔG) than acetylcholine (ACh+) to self-assembled triple helicate rigid cage, corresponding a K(Ch+)/K(ACh+) = 109 that is in fairly good correlation with the experimental value of 20. Finally, excellent correlation between theoretical and experimental ΔG has been reported (ρ^2 = 0.84) for cucurbit[n]uril (CB[n]) host•guest systems. Here, prediction has been made that binding in CB[7]•Diam-4,9-di(NMe$_2$propanoNH$_3$) complex could become next world record in the world of noncovalent interactions. This diamantane derivate is now being synthetized. Clearly, these findings demonstrate that the computational chemistry has a solid position as the complementary source of information to the data obtained from the experiments.