Abstract

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The postulates of quantum mechanics have become the basis for the development of advanced computational methods of quantum chemistry, which are not only complementary to other research methodologies, but even allow to replace the laboratory experiment in many respects. In the following dissertation thesis, we present the results of works in the field of application of molecular modeling methods to biologically significant structures, as well as in the field of theoretical approach to the solution of the Schrödinger equation for specific types of Hamiltonians. We can thus divide the five objectives of the thesis into two groups.

The first group of goals is represented by the results of using non-perturbative, variational methods for finding eigenvalues and eigenfunctions of Hamiltonians. We relied primarily on Heisenberg's matrix mechanics, which uses the representation of the position and momentum operators in matrix form, and thus became a computationally feasible variant for searching for the spectra of the Hamiltonian, even not only fermion - boson interaction.

The second group of objectives summarizes the results from density functional method (DFT) optimization and molecular dynamics simulations of aptamer-ligand interactions. It also describes the structural variability of the protein receptor in the

environment of an explicit water solvent by analyzing the trajectory from dynamic simulation. Finally, we analyze the physico-chemical properties and reactivity of the potential drug through calculations at the DFT level, which made it possible to predict vibrational, UV-VIS spectra and examine the distribution of electron density and orbitals. Additional ADME in silico analysis provided insight into the biodistribution of the conjugate of dithranol with salicylic acid as a potential drug for supportive treatment of psoriasis.

Key words: Variational method, Hamiltonian, molecular modeling, DFT