Methods of computational chemistry represent an important tool in development of novel materials or drugs. In this thesis, they are used for investigation of Pt anticancer drugs. Interaction of five hydrated Pt(II) complexes with guanine as a small model of DNA is studied at the DFT level. Several Pt(IV) complexes exhibit less side effects and overcome some resistances of cisplatin, nevertheless they must be reduced to their Pt(II) analogues to obtain anticancer activity due to their high kinetic inertness. Therefore, reduction potentials for eleven Pt(IV) complexes are determined using DFT and post-Hartree-Fock methods. The kinetics of reduction play more important role. Thus, we study reaction mechanisms for reduction of tetraplatin by deoxyguanosine monophosphate and satraplatin by ascorbic acid. In both mechanisms the kinetic model for side reactions is employed since reducing agents occur in different protonation states.

From the perspective of interaction of metals with thymine, proton transfer is of great importance. It is shown that the presence of hydrated metal cations - Mg\(^{2+}\), Zn\(^{2+}\), Hg\(^{2+}\) leads to a significant decrease of activation barriers for the N3\(\leftrightarrow\)O3 proton transfer. The QM/MM umbrella sampling MD method is employed in a study of binding of the hydrated mercury cation to the N3 position in order to see dynamic effects. The obtained results are compared with DFT calculations. The bonding and Lennard-Jones parameters consistent with General Amber Force Field for all the first row transition metal, Ru, Rh, Pt, and Hg cations are also estimated.