It has been proven that platinum and ruthenium complexes are active in anticancer treatment. Nowadays, the common chemotherapeutica have a lot of side effects, therefore, drugs with fewer negative impacts are intensively searched for. The first part of the thesis focuses on the study of cis-[$Pt(NH_3)_2Cl_2$] (cisplatin, DDP) and four platinum potential anticancer agents $PtCl_2$(diaminocyclohexane), $PtCl_2(NH_3)$(cyclohexylamine) (JM118), cis-[$PtCl_2(NH_3)$(piperidine)] and trans-[$PtCl_2(NH_3)$(thiazole)]. Thermodynamic and kinetic parameters of reactions of these complexes in semi-hydrated and fully-hydrated form with guanine were studied using QM methods. The reaction with guanine is the key process initiating the anticancer activity. Analyses of electron density were performed at the B3LYP/6-311++G(2df,2pd) level of theory in IEF-PCM model. The second part of the thesis studies the reaction of the so-called 'piano stool' Ru(II) transition metal complex, [Ru(II)($\eta^6$-p-cymene(nalidixic acid)($H_2O$)]$^{2+}$, first with guanine using QM methods and second with ds-DNA model using QM/MM methods. The reaction site, which is described by QM method, is two consecutive guanines and the Ru(II) complex. Analyses of thermodynamic and kinetic parameters, and electron density were performed at the B97D/6-31G* level of theory. All the mentioned reactions are exothermic and spontaneous.