Due to the wide range of properties, heterocycles find their applications in medical, pharmaceutical and other fields of chemistry. Nucleic acid bases are one of the most important heterocycles. However, according to our knowledge, there is no systematic investigation concerning substituent effect on their properties. It should be stressed that substituent may influence not only properties of a given system but also its tautomeric preferences. Additionally, substituents incorporated in different positions of molecules may serve as an effective tool for the modification of various characteristics and physicochemical properties of the systems.

Adenine is a derivative of purine and one of five π-electron heterocyclic components of DNA and RNA. Its derivatives with a 5-membered sugar are known as nucleosides, whereas further connections with phosphate groups constitute nucleotides – the building blocks of nucleic acids. Moreover, adenine interaction with cisplatine (an important medicine in some forms of cancer diseases) leads to a mutation of a helix. Therefore, it is very important to know an impact of well-defined factors with specified electron donating/accepting properties – i.e. a substituent – on changes in the electronic structure of adenine.

The aim of this project is to study the substituent effect on properties of adenine, obtained for its four the most stable tautomers. A choice of adenine as the object of this investigation also results from the possibility of applying the widest set of parameters characterizing an effect of the substituent on properties of particular fragments of this molecule. The substituent effect will be demonstrated by both the classical and some modern approaches. Their application allows to evaluate quantitatively and reliably what are the electron-donating or electron-accepting properties of individual positions in adenine. Thus, it should give information of possible positions where the interaction with the reagent may take place, and what properties should represent the reagent (electrophilic or nucleophilic) in order to lead them to interact with adenine, consequently resulting in the DNA mutation.