Interactions within biomolecular systems depend mostly on electrostatics. Therefore good description of this particular component is a key factor in any bio-simulations. Nowadays most of in vitro experiments are preceded by thoughtful research in silica. The accuracy of those computations is limited since physically based - quantum mechanic calculations are inapplicable here because of computational cost. They are replaced by the usage of models based on classical mechanic. By the famous quotation of Henri Theil - „Model are to be used, not believed" ones are advised to be careful with drawing conclusions from methods that have lack of physical background.

Force fields are wide range tools for biomolecular investigations. The most popular ones use the simplest models gaining speed of calculations but losing the accuracy. At the same time continuous efforts are being undertaken to find the best model. The general rule of molecular modeling development is increasing accuracy with simultaneously reducing the calculation time.

In our project we propose to enhance the versatility of a model built from the University at Buffalo DataBank (UBDB); the only model which can be successfully applied in both X-ray crystallography and molecular modeling. In the area of electrostatic interactions energy estimation we plan to perform a deep analysis of our method in order to better understand its pros and cons. Previous calculations demonstrated superiority of UBDB over other tested force fields method in accurate estimation of Ees. Proposed here research will allow us to find possible improvements of the model, or to find a new one. We will test the possible variations of UBDB and compare them to methods of quantum mechanics and to force fields.

The second part of our examinations relies on comparison to an experimental data. A newly established improved model will be used to reproduce electron densities of molecules likewise UBDB does. Such obtained densities will be compared to X-ray high resolution diffraction data.

Above studies will be carried out in order to obtain a model with wide applicability.