Chiral molecules have the same chemical composition and identical distances between atoms, but on the molecular level they differ by the position of functional groups, so that it is impossible to superimpose the molecule and its mirror image. These molecules are ubiquitous in our environment. They comprise building blocks of living organisms (proteins and carbohydrates), as well as numerous exogenic substances, such as drugs and food additives. There are many examples of compounds which, depending on their enantiomeric form, can taste or smell differently, or even worse, may exert various effects on our bodies, what is crucial for chiral drugs in particular. There is a long list of examples, where one enantiomer possesses a required pharmaceutical activity, whereas another one is at best nonactive. Sometimes the second enantiomer can be even toxic or can provoke serious side effects.

Because of the same stoichiometry and connectivity, the enantiomers have exactly the same physical and chemical properties. They can be differentiated only by their optical activity – they rotate the plane of polarized light in opposite directions. The chemical differentiation of enantiomers is possible only when they interact with other chiral molecules. The resulting diastereoisomeric complexes exhibit different stability depending on the type of enantiomers of which they are made. This stereoisomer's property is widely used in the analytical and preparative methods, which aim to separate a mixture of two enantiomers. Among such methods one can name chiral chromatography and chromatographic separation with addition of a chiral selector.

In the field of chiral chromatography there is the common recognition of the requirement for the existence of a sufficiently large differences in strength and orientation-specific intermolecular interactions in diastereoisomeric complexes. On contrary, there is a lack of comprehensive theoretical studies which would systematize this practical knowledge and allow for a qualitative analysis of the performance and limitations of chiral chromatography and related methods. There exist several theoretical approaches which may permit for systematic examination of stabilization energy and potential energy of interaction taking into account the differences characteristic for diastereoisomeric complexes.

The proposed new method of analyzing the components of the interaction energy between the enantiomer with its chiral partner should fill the existing gap in the applications of theory of intermolecular interactions. The completion of the planned research will lead to the formulation of a new set of rules with a firm theoretical background, allowing to forecast the stability of diastereoisomeric complexes. The developed model could then be applied to predict *in silico* the selectivity of separation of the mixture of enantiomers and to propose better chiral selectors. Due to the fact that in living organisms the majority of complex molecules are chiral, the accurate insight into the nature of the interaction between chiral partners will be crucial for practical applications in the future. The method which is to be developed within the current proposal will be tested on selected case studies of diastereoisomeric complexes popular in chiral chromatography.