The principal task of chemistry is the transformation of substances easily obtainable from abundant sources, such as oil, minerals, and biomass, into useful compounds, characterized with desired properties. These can range from simple products – fertilizers, dyes, fuels to the most sophisticated – advanced materials and new pharmaceuticals. The job of chemists is to improve the existing and to develop novel methods for carrying out these transformations in a possibly efficient but environmentally benign manner. An equally important aspect of chemical research is expanding the general knowledge, on one hand, motivated by the human kind desire to better understand the surrounding world, and on the other, to enable further practical applications making our life easier.

The proposed research project is in line with both of the above points of view. Its major objective is to develop an array of novel chemical reactions, tools for the transformation of substances, possessing broad applicability mainly in the pharmaceutical and fine chemicals industries. Importantly, the planned research is not directed toward the preparation of specific chemical compounds, quite on the contrary, the devised new processes are characterized by a high level of generality and they may find various applications in different contexts. The project carries also high significance from the scientific perspective. It envisions the investigation of yet unexplored combination of the intriguing reactivity of a special class of so-called hypervalent iodine compounds with the opportunities offered by nucleophilic catalysis.

A key feature that is directly related to both the efficiency and environmental friendliness of a chemical reaction is selectivity. The reactions that proceed in high yields and in selective fashion convert most of the starting material into the desired product and thus do not generate large amounts of waste. There is also another important issue regarding the selectivity. The majority of complex compounds may exists as two mirror images (so-called enantiomers). Due to the "handedness" of the molecules of life (peptides, DNA/RNA, carbohydrates, etc.), the opposite enantiomers of a single substance often display quite different biological activities. This results in a need to selectively generate compounds, especially pharmaceuticals, in an enantiopure form. The proposed novel reactions will provide such possibility, thanks to the usage of efficient asymmetric catalysts, that is, substances which accelerate the formation of one of the two possible enantiomers of the product, so that the other is obtained in a negligible amount.

What makes the project really innovative is the application of hypervalent iodine compounds. The presence of a highly reactive iodine atom at a high oxidation state in these molecules will enable selective reactions leading to a dramatic increase in molecular complexity. This means that the reactions will transform simple starting materials directly into complex products, containing molecular motifs encountered in natural products and pharmacologically important compounds.

Importantly, hypervalent iodine species represent non-toxic alternatives to heavy-meatal oxidants commonly used in the chemical industry. This feature constitutes a huge advantage, especially in the context of the synthesis of therapeutics. Unfortunately, the inherent flaw of the hypervalent iodine compounds is their complexity resulting in a relatively high cost. Therefore, in order to counter this issue and increase the potential of industrial applicability of the developed reactions, already at the early stage it is planned to immobilize the iodine-containing catalysts on a solid support and to use them in a heterogonous form. This will allow for an easy recycling of the catalysts and for reusing them again, or alternatively for conducting the reactions in a continuous flow setup.

The development of new chemical transformations, in particular the highly innovative ones, based on frontier areas of knowledge, usually requires the application of a trial and error technique in order to optimize the reaction conditions. However, within this project it is intended to use computational methods to aid the design of the structures of the catalysts. Current quantum-chemical theory and the application of supercomputers enables simulation of chemical reactions *in silico*, and they will provide indispensable aid in the development of the new efficient and selective synthetic methods. Additionally, complementary experimental and computational approaches will be jointly used to study the mechanisms of the investigated transformations, detailed step-by-step sequences of molecular events occurring in the course of a chemical process, providing good understanding of the underlying basic chemistry.

In summary, the realization of this scientific project will facilitate the preparation of complex chemical substances, in particular pharmaceuticals (both new and existing). The project has highly interdisciplinary character, its implementation will constitute a major step forward in chemistry and it will inspire new exciting research directions.