

Mechanochemistry is one of the most dynamically developing research directions, which opens new possibilities and perspectives in the synthesis of new materials. With this approach a wide variety of chemicals can be obtained, including organic and inorganic compounds, metal complexes and drug molecules. The chemical reactions, which are carried out in ball mills in a solid phase usually are clean and having high yields. An undoubted advantage of mechanochemical processes is their ecological aspect, which is a result of elimination of significant amounts of solvents, used in classic organic chemistry reactions.

Our attention during carrying out this project will be focused on the optimization of mechanosynthetic reactions conditions, preparation of short- and long-chain peptides, and pharmaceutical co-crystals of two drug molecules (apremilast and linezolid). The main objective of our research project is to simplify methodology used for the formation of the above-mentioned systems, which when performed in accordance with classic approaches are often time-consuming and having low yields.

Advanced instrumental and computational techniques will be used to study both types of processes scheduled in the current project (i.e. peptide syntheses and pharmaceutical co-crystals formation). Our aim is to recognize at a molecular level the mechanisms, which decide on the course of these chemical processes in a solid phase, as well as to describe the factors that influence the route of the reactions and their final outcome. Such a deep understanding of the studied processes will be a fundament for the development of new methodological solutions, which will expand the applicability of mechanochemistry in a condensed matter. The main analytical technique, which will be used in this project, is solid-state NMR (SS NMR) spectroscopy, enhanced by other techniques, such as single-crystal and powder diffractometry, thermal analyses and computer modeling. Another aim of the project, besides the elaboration of new methods of synthesis in solid state, is to obtain new crystal forms of the above-mentioned drugs, which will have better physicochemical properties, than the existing ones. Additionally our project has an educational aspect. During its realization we will create a research team, in which members will use our “know how” in solid-state NMR spectroscopy and learn the secrets of the method in such a way, that after finishing the project they will be able to apply and develop this methodology in other laboratories in Poland and worldwide.