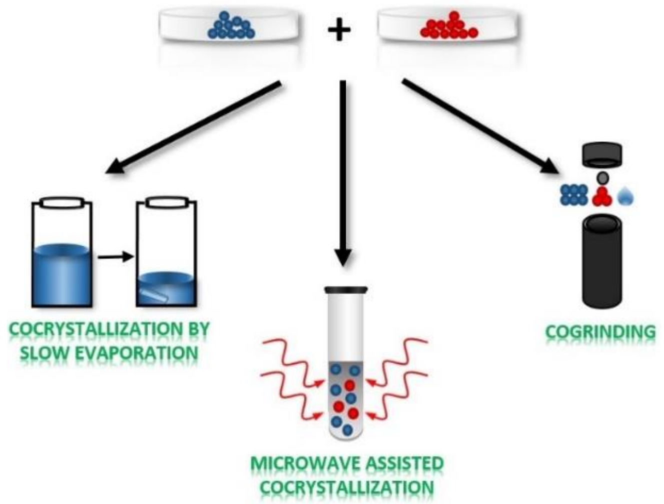

The challenge of modern pharmacy is not only to search for new medicinal substances, but also for their forms that will have a specific spectrum of physicochemical properties. In addition to their pharmacological action, these compounds must meet several other conditions, i.e. good solubility, environmental stability, tabletability, permeability or bioavailability. Most of the discovered pharmaceutical compounds do not show the desired properties, which means that they must be modified with an appropriate method to improve them.

One of the methods, **cocrystallization**, consists of introducing an excipient, called a **coformer**, into the crystal lattice of a pharmacological substance. Its careful selection through the **synthon approach** by adjusting the functional groups present in it and drug and subsequent selective non-covalent bonding of molecules into larger **supramolecular aggregates** leads to the formation of compounds with **unique physicochemical properties**, which are a function of the crystal lattice. Understanding the processes of self-organization, determining the frequency and conditions of the formation of characteristic supramolecular units in cocrystals of biologically active compounds will open the way to greater control in the design of this type of complexes with the desired physicochemical properties.

The aim of the project is to obtain and fully characterize **purine alkaloids cocrystals** with appropriate coformers, as well as to optimize the conditions for their production using **microwave radiation**.

Microwave-assisted organic synthesis is of great interest and is often used to carry out numerous organic reactions that would take very long or not take place under standard conditions. An unquestionable advantage of conducting cocrystallization in **a microwave reactor** is the possibility of very fast, selective obtaining of a pure form of a given cocrystal, and also efficient analysis and phase identification based on powder measurements (**PXRD**) of the obtained solids. The use of the microwave method, in parallel with the solution and mechanochemical methods, also gives a greater chance of obtaining forms that cannot be produced by other methods, especially polymorphic forms with unique physicochemical properties, the formation of which in most cases cannot be predicted.

The cocrystallization conditions optimizations will allow us to determine not only how they will affect reactants conversion, but also the type of phase formed, which in the future will contribute to the faster and easier design of this type of reaction. The above research will also open the way to discovering many new compounds with interesting physicochemical properties (determined by techniques such as **TGA**, **DSC**, **UV-Vis**, **FT-IR**). Determination of their crystal structure by X-ray methods (**SCXRD**) will allow indicating the interactions conditioning good cocrystallization of the studied class of compounds with selected coformers and will allow to associate it with these properties. In addition, the use of **high-resolution X-ray crystallography** for the appropriate quality of single crystals will enable the analysis of the electron density distribution in cocrystals, which will allow an in-depth analysis of intermolecular interactions.

One of the objectives of this project is to demonstrate **the potential of the microwave-assisted cocrystallization method** as a fast and economical method of obtaining co-crystals. In addition, the results of the conducted research will undoubtedly influence **the development of crystal engineering** in the area of the chemistry of cocrystals of biologically active compounds as **materials with unique physicochemical properties**.