Chemical compounds have often a tendency to form different crystalline structures, which differ in mutual arrangement of molecules. Such phenomenon is called polymorphism and has great influence on the physicochemical properties of a chemical substance. Sometimes one polymorphic form can be decidedly different from another one in terms of its hardness, stability or water solubility. This is especially important in the case of chemicals used as medicines, as polymorphism can influence the outcome of the pharmacological therapy. Currently available computational chemistry methods more and more often allow for predicting a tendency of a molecule to form polymorphs, as well as predicting how these polymorphs can look like. Unfortunately, molecular structure of compounds important for pharmaceutical sciences is often very complicated, which seriously limits the applicability of such predictions. This project is aimed at the methodological development of a joint use of crystal structure prediction (CSP) and solid-state nuclear magnetic resonance (NMR), which will allow for the determination of crystal structures of yet undescribed polymorphic forms. In addition, this development, as well as experiments and calculations planned in this project will result in a deeper understanding of preferences seen for certain molecules to crystallize in a specific way. Sometimes molecules with very similar chemical structure can have decidedly different preferences to align themselves in a crystal lattice, and therefore they have different tendencies to form polymorphs. For example, for two molecules differing only to a very small extent by slightly different arrangement of atoms in their structure, it is possible that one of them will form a variety of different polymorphs, whereas the other will have only one form (will be monomorphic). One of the aims of this project is to get closer to an answer to a question why this is happening. Such an understanding will help to develop a field called crystal engineering, which tries to design crystalline forms with desired physicochemical properties. One of the expected outcome of this project is also a discovery of new, yet undescribed polymorphic forms of the selected anti-inflammatory agents: meloxicam, apremilast and roflumilast.