Modern drug discovery is a long, multifaceted process, that encompasses the ‘classical’ chemical entities (the so called ‘small molecules’) as well as new technologies, such as peptides, ribonucleic acids (RNAs) and therapeutic antibodies. Despite the considerable interest of pharma industry in those alternative drug modalities, the ‘classical’ drug-discovery approaches initiated by screening sets of small-molecular compounds for their activity against the specific disease still bring a large share of new drugs to the market. There is a large number of factors that drive successful drug development. This research proposal focuses on those that relate to the technologies that give access to the new, more ‘sophisticated’ chemical space and to the intensive research on novel functional groups that improve the characteristics of the investigative agents.

In this project, it will be attempted to address these two factors by expanding yet largely unexplored chemical space of drug-like sulfoximine class and by widening scope of multicomponent reactions (MCRs) which are important tools in modern drug discovery. MCRs are chemical reactions where more than two starting materials react to form a single, complex product which essentially contains all the atoms of used reagents. As they proceed with high atom economy and use simple, one-pot procedures, which makes them suitable for time- and cost-efficient tools for generating investigative new compounds for drug discovery. In this project, in this project it will be demonstrated for the first time, that sulfoximines are versatile reagents in MCRs and that their reactions lead to biologically important molecules that are non-accessible by other means. To do that, three important types of MCRs will be examined and optimized. To demonstrate the usefulness of this technology, a suitable subset of drug-like reaction products (the so-called ‘compound library’) will be obtained. More, the sulfoximino- analogs of several known drugs, biomolecules and clinical candidates are to be created and their biological activities will be evaluated. The results of this investigations can potentially find applications in pharmaceutical industry and academic researchers working in the multidisciplinary field of drug discovery. Finally, as one of the investigated MCRs, the Ugi reaction has an interesting course, we will investigate its mechanism when sulfoximides are employed as the starting reagents. This would not only be interesting from scientific point of view, but may also lead to new technologies for efficient and cheap manufacturing of active pharmaceutical ingredients.