The Project involves development of methods and tools to deal with the difficult problem of searching for compounds that can be new potential drugs. The leading tool of the protocol will involve the enumeration of new compounds on the basis of optimal fingerprint obtained via the application of machine learning algorithms and on the basis of the application of deep learning techniques. It starts a new path in cheminformatic approaches by combining standard ligand- and fragment-based methods and introducing optimization at different level (compounds representation). Obtained compounds will be optimized also in terms of physicochemical and pharmacokinetic properties. Additionally, a methodology for prediction of the scheme of interaction of ligand with the protein will be developed. All approaches will be applied to generation of ligands of serotonin receptor 5-HT_7. The most promising compounds will be purchased from commercial vendors and their affinity to 5-HT_7R, as well as selected physicochemical and ADMET properties will be evaluated in *in vitro* experiments. The computational strategies developed within the Project will constitute the newest cheminformatics and computer-aided drug design approaches. Application of deep learning in drug design process is still limited, despite its possibilities, and developing a deep learning-based generative methods for the formation of new potential ligands will provide a great scientific input to the discipline of computer-aided drug design. Moreover, all tools for the computational evaluation of physicochemical and pharmacokinetic properties of compounds will be made freely available in the form of online platforms, and as their optimization is crucial at some stages of development of bioactive compounds, it will be of great use for the whole scientific community from pharmacy, chemistry, cheminformatics and related fields.

The target chosen for the case study (serotonin receptor 5-HT_7) is extremely important from the social point of view, as a target for central nervous system disorders – one of the biggest problem of societies from developed countries that is predicted to be still a growing issue. The drugs currently used to treat disorders such as depression and anxiety possess long list of drawbacks, such as delay in the therapeutic effect (not mentioning the treatment-resistant patients), and adverse effects such as headache, weight gain, nausea, diarrhea, fatigue, sweating, dizziness, tremor, and dry mouth. The need for search of new drugs is not only present in the field of depression and anxiety, but disorders such as Alzheimer's disease and schizophrenia are also still waiting for their more effective treatment. For example, in schizophrenia, the currently used treatment strategies are quite effective in the controlling of the positive symptoms of this disorder, whereas the negative symptoms, such as cognitive disorders, and memory problems are not sufficiently treated by the neuroleptics used, although they are extremely important aspects from the social point of view, enabling patients coming back to professional activities and proper functioning in the society. This makes the desire for the search for novel ligands of receptors taking part in the pathophysiological mechanisms of those disorders, either as they might become a novel therapeutics in the future, or they might constitute a tool compounds for the detailed examination of 5-HT_7R functioning.