Medicinal chemistry has undergone significant changes in recent years due to the large-scale introduction of combinatorial chemistry techniques and the design of drugs based on their structure. Thanks to these tools, it is easier to identify the leading molecule and synthesize their analogs to maximize the chance of finding compounds with the desired biological activity.

One of the critical aspects when evaluating potential drug candidates is determining their physicochemical properties, such as lipophilicity, solubility in the aqueous environment, and affinity for phospholipids and plasma proteins. It should be remembered that each drug substance must reach the target site in the appropriate concentration and remain in a bioactive form long enough for the expected pharmacological effect to occur. Current research indicates that inadequate pharmacokinetic properties, including absorption, distribution, metabolism, and elimination (ADME), are one of the main reasons for failure in developing new drugs. It is estimated that 6 out of 7 tested candidates fail during the clinical trials since they have inadequate pharmacokinetic properties.

Currently, numerous mathematical models and programs are available to assess lipophilicity and affinity to plasma proteins. However, there are no tools to predict phospholipid affinity. The project aims to fill this gap and develop an approach that will enable the estimation of affinity for phospholipids based on the molecule's structure. It should be emphasized that the affinity to phospholipids is a more biosimilar measure of the lipophilicity of medicinal substances than the currently used logP coefficient referring to the partitioning of substances between water and n-octanol.