Abstract

The aim of the work was an attempt to utilize molecular descriptors, pharmacological properties, and economic data of selected series of drugs and materials, including the list of pharmacological bestsellers (TOP100 of the 2010 to 2019) and FDA approvals (from 1985 to 2019), for the analysis of the economic aspects of molecular design. The primary method of analysis was the fragmentation of the analyzed compounds. An example of fragmental analysis in drug design is the ligand efficiency (LE) method. We analyzed the changes in LE for a series of drugs registered by the FDA and proposed an alternative tool, Product Ligand Efficiency, PLE.

Economics plays a crucial role in the design of drugs and materials. Unfortunately, economic data is difficult to access. The list of bestselling drugs is an exception here. The most frequently occurring fragments in the TOP100 were compared to all FDA-approved drugs. Similar to the case of pharmacologically privileged fragments, can we identify similar structures that are significant for economics?

It is paradoxical that in materials design, a significant drawback is the lack of databases of the properties of synthesized molecular systems. We prepared a compilation of literature data for selected series of photoreagents, which will be integrated with a database currently encompassing heterogeneous methanation catalysts, Catalytic *Material Database* available at http://cmd.us.edu.pl/catalog/.