

Drug research and development is extremely expensive and time-consuming process with the high risk of negative results. The key stage of this process is the discovery of novel pharmaceutical agents. Nowadays drug discovery is based on investigations of pathological mechanisms of diseases, identification of relevant pharmacological targets, findings or design of the active compounds (hits), and their further optimization to lead compounds. We will consider how the four listed above stages of drug discovery process are executed by pharmaceutical science and industry. Examples of successful medicines found either through the empirical search or created using computer-aided drug design methods will be presented (Figure 1).

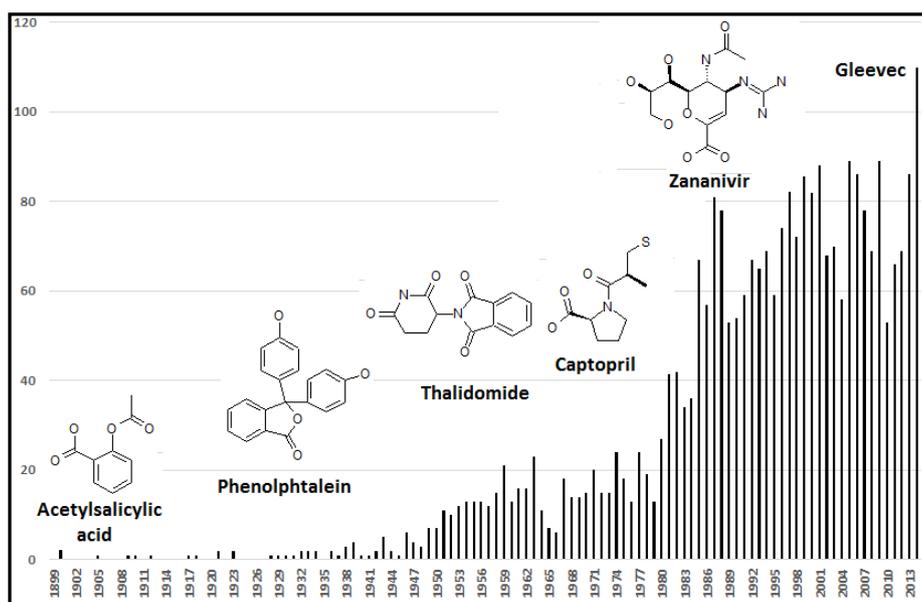


Figure 1. The number of pharmaceuticals launched in 1899-2014 (source: Thomson Reuters Integrity).

Due to the tough competition, pharmaceutical industry is an exceptionally innovative business. It should execute R & D of new pharmaceuticals based on the most recent achievements of biomedicine, biotechnology and chemistry. On the other side, a lot of biomedical and chemical studies are stimulated by the unmet medical needs.

Despite of many efforts to prove the safety of investigational drugs during the preclinical and clinical trials, some drugs have been removed from the market due to the unexpected life-threatening actions. Using such examples one may study if the application of modern cheminformatics methods [1] could help to filter out the potentially dangerous compounds at the early stages of research.

Many current drugs have been discovered due to the serendipity. Thus, some potential biological activities of such pharmaceutical agents remain unstudied. Rational application of cheminformatics methods helps to find novel biological activities of these compounds, which lead to drug repurposing. Similar approach allows to disclose the hidden pharmacological potential of natural compounds from medicinal plants directing to the most promising way of their studies [2].

1. Filimonov D.A. et al. *Chemistry of Heterocyclic Compounds*, 2014, **50**: 444-457.

2. Lagunin A.A. et al. *Natural Product Reports*, 2014, **31**: 1585-1611.