Abstract

Drug design is a complex optimization process for which a universal model of action has not yet been developed. The productivity of the pharmaceutical industry appears to be declining; thus, over the past 20 years, pharmaceutical R&D has been unable to develop a sufficient number of drugs to supplant those with expiring patents.

The aim of the study was to analyze selected strategies and parameters used to evaluate the drug's potential.

In our research, we explored databases and FDA documentation available online to search for compounds with desired properties. In the analyzes we used common chemoinformatics tools and programming methods.

An important stage of our research was to analyze whether the list of bestselling drugs, which model the ideal medications, can reflect or shed light on current trends in pharma. We used the top 100 bestselling prescribed drugs in the US market as a model, which enabled us to compare the data with the FDA approval statistics. We defined a new parameter (drug age) quantifying drug innovation. Drug age analysis shows that the drugs are getting older. Productivity in the pharmaceutical industry is decreasing.

In reaserch we also explained the chemical meaning of the ligand efficiency (LE) metrics. Although there is a controversy in the literature regarding both the mathematical validity and the performance of LE, it is in common use as an early estimator for drug optimization.