Summary of doctoral thesis

Database exploration in search of novel drug designing rules

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The pharmaceutical industry has been one of the most lucrative business areas of all time. However, faced with numerous problems in recent years, it appears to be declining. Despite the use of the latest technology, there has been no significant improvement which would result in the implementation of new, better, and more innovative pharmaceutical drugs.

The aim of this study was to explore databases and to analyse current trends in pharma R&D, as well as to propose strategies for facilitating the process of drug development. This study shows the synergy between the numerous research methods in several scientific fields, such as chemistry, computer science, economics and pharmacy. Thus, the calculated chemical descriptors and economic parameters were used in statistical analysis. Comparison of the university and pharma R&D reveals a number of similarities. Accordingly, comparative analysis of trends and developments, both in science and the pharmaceutical industry, has been performed. Thus, an effort was made to explain the role of and impact of the market on the trends in pharma which could encourage changes in the drug structure. A population of FDA drugs were collected, characterized by drug-like and drug-age properties, and an additional implementation of the fragmentation algorithms helped to understand the topology of the investigated drug population.

In summary, the analysis revealed many interesting trends in drug development in recent years. The study shed new light on the known methods for the design of active compounds.