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The impact of molecular docking programs and virtual screening in modern drug design

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Modern drug design heavily relies on computer-based methods. With the aid of computational methods, it is possible to predict the properties of compounds quickly and accurately, by calculating a large number of constants and coefficients. It is possible to predict the physical, chemical, and biological properties of compounds using computer methods, as well as their potential interactions with various receptors and enzymes.

The wide range of implemented software products enables users to choose one that allows them to extract the necessary information according to the problem to be solved and the most suitable for the specific technical and professional skills of the scientist [1, 2]. An overview of the most commonly used molecular docking and virtual screening programs, as well as the opportunities they offer for drug development, is presented in this work.

Keywords: computer-aided drafting and design, molecular docking, virtual screening, drug design, scoring functions, ligand-receptor interactions

References

[1] F. Sapundzhi, T. Dzimbova, The importance of biological databases in modeling of structure-activity relationship, *Bulgarian Chemical Communications*, 54:97-102, 2022.

[2] F. Sapundzhi, Scoring Functions and Modeling of Structure-Activity Relationships for Cannabinoid Receptors, *International Journal of Online and Biomedical Engineering (iJOE)*, 15(11):139-145, 2019.