WEB-RESOURSES FOR PREDICTION OF BIOLOGICAL ACTIVITY OF ORGANIC COMPOUNDS

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Chemistry and chemical technology are among the largest producers of diverse and complex information about the properties of organic compounds, the most important of which is biological activity. Pleiotropic action of the majority of organic compounds requires a comprehensive assessment of their biological activity spectra[1]. Experimental testing of dozens/hundreds millions of compounds on thousands biological activities is not feasible; the rational approach is based on the use of computational methods for assessment. Computational estimates can be obtained using information technologies and resources that contain information about the structure and biological activity of organic compounds (PubChem, ChEMBL, etc.). Most of the developed methods are based on the calculation of structural similarity of organic compounds and extrapolation to the novel compounds biological activity of known analogues. Earlier[2], we compared the quality of prediction provided by some web-resources for the 36 drugs approved by FDA in 2014, and showed the advantages of machine learning methods[3] in comparison with the similarity estimates. In this work, we have carried out a prediction of biological activity profiles for 171 drug substances from the list of Top200 Drugs and compared the predictive accuracy of the web-resources including ChemProt, PharmMapper, SEA, SuperPred, Target Hunter, SwissTargetPrediction and PASS Online. The opportunities for utilization of the created set as the "Benchmarking Set", the quality of the prediction of biological activity using different web-resources, and the possibility of their application in medicinal chemistry are discussed.

References

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