In silico prediction of Anti-infective properties of therapeutic chemicals at Medicinal Plants

F. Nobakht*, H. Mohabatkar, M. Behbahani
Department of Microbial Biotechnology, University of Isfahan, Isfahan, Iran
*Farzanehnobakht.93@gmail.com

Abstract: Infectious disease is the leading cause of death worldwide, and billions of dollars are invested every year in developing anti-infective drugs. Many of these drugs are useless due to resistant bacteria. The urgent need to treat the resistant bacterial infections lead to discovering new drugs from medicinal plant beyond their traditional use. Natural products as standardized plant extracts provide unlimited opportunities for designing new drugs, because of the unmatched availability of chemical diversity.
In this study, we used the results of phytochemical analysis of 20 medicinal plants for our preliminary data and then used bioinformatics tools to *in silico* screening of these compounds for anti-infective activity. For this purpose, we used iATC-mISF web server to predict the therapeutic classes of our 518 compounds. This web server only recognizes SMILES format of compounds. To achieve this format, PubChem compound database available at NCBI was used. Then, we used Swiss Target Prediction webserver to make sure that these compounds have no target in Homo sapiens, therefore can be used in human as drugs without any side effects.The results of drug discovery show that only four compounds belonged to class seven, which had anti-infective activity, and only one of these compounds, that belongs to *Dorema ammoniacum*, had no target in human and could pass through all screening methods. The use of in silico methods for drug discovery in natural products has increased during the last decade. The appearance of new bioinformatics methods, along with a growing range of data on phytochemical structures has opened vast perspectives in the study of the pharmacological activity of plant preparations.

Keywords: Bioinformatics; Medicinal plants; Anti-infective activity; Drug Discovery; Screening

References

[1] X Cheng, SG Zhao, X Xiao, KC Chou, "iATC-mISF: a multi-label classifier for predicting the classes of anatomical therapeutic chemicals." J. Bioinformatics (Oxford, England), 33 (2017) 341–346

[2] D Gfeller, A Grosdidier, M Wirth, A Daina, O Michielin, V Zoete; "SwissTargetPrediction: a web server for target prediction of bioactive small molecules," Nucleic Acids Research, 42 (2014) 32–38

[3] M.R. Delnavazi; S. Tavakoli; A. Rustaie; H. Batooli; N. Yassa, "Antioxidant and antibacterial activities of the essential oils and extracts of Dorema ammoniacum roots and aerial parts" Department of Pharmacognosy, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran. Vol. 1, 2014, pp 11-18