EDITORIAL

New Experimental and Computational Tools for Drug Discovery. Part – XII

This special issue is the number XI of the series “New experimental and computational tools for drug discovery”. The series also has its own project page on Researchgate [CTMC Drug Discov. Series] (see this website for details, project log, and further information). The papers included in this issue follow the same line and can be summarized as follows.

Shahrukh et al. delineate Mantle cell lymphoma (MCL), characterized by the mutation and overexpression of the cyclin D1 protein. The study identifies potential inhibitors of MMP9, such as Proteasome, BTK, and TAK1 to determine an effective protein target for the MCL. These inhibitors show good affinity and interaction profile of compound over the most effectively established inhibitor SB-3CT. Also, the pharmacophore study reveals its high efficacy based on various interactions. Based on the ADMET profile, the compound (PubChem ID: 102173753) was found to be non-toxic and could be a potent drug for MCL treatment [1].

Dieguez et al. emphasizes on the importance of the verification of the accuracy of Metabolic Reaction Networks (MRNs) models towards their use for target discovery in Medicinal Chemistry. Complex Checking of the connectivity (structure) of complex MRNs models proposed for new microorganisms with promising properties is an important goal for chemical biology. In principle, we can perform a hand-on checking (Manual Curation). However, this is a hard task due to the high number of combinations of pairs of nodes (possible metabolic reactions). In this work, we used Combinatorial, Perturbation Theory, and Machine Learning, techniques to seek a CPTML model for MRNs >40 organisms compiled by Barabasis’ group. First, we quantified the local structure of a very large set of nodes in each MRN using a new class of node index called Markov linear indices f_k. Next, we calculated CPT operators for 150000 combinations of query and reference nodes of MRNs. Last, we used these CPT operators as inputs of different ML algorithms. The present work opens a door to the study of MRNs of multiple organisms using PTML models [2].

Santana et al. called our attention over the implications of regulatory aspects of nanotechnology and computational sciences in EU related to the development of new nanotechnology, medicinal chemistry, and related products. Machine Learning (ML) has experienced an increasing use given the possibilities to expand the scientific knowledge of different disciplines, such as nanotechnology. This has allowed the creation of Cheminformatic models, capable of predicting biological activity and physicochemical characteristics of new components with high success rates in training and test partitions. Given the current gaps of scientific knowledge and the need of efficient application of medicines products law, this paper analyzes the position of regulators for marketing medicinal nanoproducts in European Union and the role of ML in the authorization process. For this, a dogmatic study of the European regulation and the guidelines of the European Medicine Agency on the use of predictive models for nanomaterials was carried out. It is concluded that there is a favorable and flexible position for the development of the use of predictive models to complement the applicant’s information [3].

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