EDITORIAL

New Computational Approaches Aimed at the Prediction of More Selective and Active Drugs

Development of new and more selective drugs is a main objective in medicinal chemistry. In fact, most drugs interact with unintended, often unknown, biological targets and these off-target interactions may lead to clinical toxic events and less efficacy. In this contest, computational approaches may play a relevant role while looking for new and more selective drugs against a specific target. Several computational approaches have been developed in the recent years with proven efficacy.

This special issue of the Current Topics in Medicinal Chemistry is aimed at illustrating new developments and recent findings in the field of computational approaches aimed at predicting new and selective drugs against specific targets.

The first paper by Garcia-Hernandez et al., focuses on the use of optimization techniques in order to learn the edit costs used when comparing graphs by means of the graph edit distance. This distance might provide useful structure-activity information for future drug design efforts. Overall, this paper shows that the graph edit distance along with learned edit costs is useful to identify bioactivity similarities in a structurally diverse group of molecules [1].

The second paper by Concu et al., shows the application of an innovative machine learning approach to predict the selectivity of new drugs against a specific target, in this case one of the two isoforms of the monoamine oxidase [2].

The third paper has been developed by Kumar et al., and present A Multi-layered Variable Selection Strategy for QSAR Modeling of Butyrylcholinesterase Inhibitors. Variable selection is a relevant field in QSAR in order to develop robust and reliable models [3].

The fourth paper by Gómez-Ganau et al., presents an in silico and in vitro study of the development of new epidermal growth factor receptor inhibitors. This receptor is a major target in medicinal chemistry since its dysregulation is involved in several types of cancers, such as breast, lung, gastric, etc. [4].

The last paper developed by Pei et al., reports an interesting review on the relationships between HRV signals and the personalized drug response in different diseases and patients since there is still a great variability and the mechanisms are complex and remain unclear [5].

REFERENCES


Dr. Riccardo Concu  
(Guest Editor)  
Current Topics in Medicinal Chemistry  
Investigator  
Requimte/Faculdade de Ciências da Universidade Do Porto  
Rua do Campo Alegre, s/n  
4169-007 Porto  
Portugal  
E-mails: ric.concu@gmail.com; riccardo.concu@fc.up.pt

1873-4294/20 $65.00+.00 © 2020 Bentham Science Publishers