



Machine Learning for Molecular Modelling in Drug Design

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Message from the Guest Editor

Machine Learning (ML) has become a crucial component of early drug discovery. This research area has been fuelled by two main factors. The first one is the fast-growing availability of bioactivities between molecules of known chemical structure and non-molecular and molecular targets. This trend has been catalysed by the development of community resources (e.g., ChEMBL, PubChem or PDB) that facilitate re-using these data sets for predictive modelling. The second factor is the easy access to high-quality implementations in R or Python of a range of ML algorithms, along with the continuous introduction of new advances (e.g., XGBoost, deep learning or conformal prediction). As a result, an increasing number of data-driven ML models are being proposed and found advantageous in some way to identify new starting points for the drug discovery process.

We invite scientists working on this area to submit their original research or review articles for publication in this Special Issue. Topics of interest include (but are not limited to) docking, QSAR, target prediction, virtual screening or lead optimization. Both application and methodology research studies are welcome.





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