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Editorial: Machine Learning in Bio-cheminformatics

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In recent years, the application of machine learning (ML), including deep learning (DL), has experienced exponential growth, which has promoted data-driven discovery in diverse fields, particularly in bioinformatics and cheminformatics. ML identifies the hidden patterns from large amounts of biological/chemical data to make predictions or decisions. Specifically, ML-based frameworks have been successfully applied to different bioinformatics domains, such as the prediction of protein structures, the identification of binding sites for protein−protein interactions, and the discovery of new therapeutic targets. Additionally, ML is frequently adopted in a variety of cheminformatics investigations to enhance the efficiency of drug design, determine the optimal pathway for an effective synthesis of compounds, and predict the physicochemical characteristics of key molecules. To foster the further application of ML to diverse fields in bio-cheminformatics, we introduce a collection of 65 papers selected from 233 submissions. Geographically, the selected papers originate from various countries, including United States, China, Italy, Belgium, Brazil, India, Japan, South Korea, and United Kingdom. We believe that these articles represent the latest progress of ML in bio-cheminformatics.

Revealing of the molecular mechanism remains a key focus of ML-based bioinformatic studies with many interesting papers in this collection. Paul et al.[1] collectively applied both XGBoost and Shapley values to offer an effective prediction of bacterial promoter with enhanced interpretability. Xin et al.[2] employed a domain-based attention mechanism to identify DNA N4-methylcytosine sites. Yang et al.[3] discovered human miRNA target sites by learning the interaction patterns between miRNAs and mRNA fragments. Li et al.[4] used adaptive feature representation learning to predict plant miRNA-encoded peptides. Wang et al.[5] enabled the identification of plant-secreted peptides using contrastive learning and feature-correction strategies. He et al.[6] designed an information network to consensually predict the associations between miRNA/lncRNA and diseases. Godinez et al.[7] introduced a new method for predicting compound activity by incorporating a dose-dependent transcriptomic profile and activity transformer model. Vani et al. and Bouvier[8,9] explored protein analogue conformations using AlphaFold2-RAVE and free energy landscapes learning, respectively.

The ***analysis of sophisticated biological data*** is another popular direction for the application of ML to bioinformatic studies. A total of four papers analyzing the complicated biological data are included in this collection. Zhou et al.[10] developed a deep neural network-based framework for identifying differentially expressed genes based on RNA sequencing data. Hozumi et al.[11] processed the single-cell RNA sequencing data using their correlation clustering and projection (CCP) method. Zhang et al.[12] introduced a multiomics integration framework with information enhancement and image representation. Cottrell et al.[13] proposed persistent *Laplacian*-enhanced principal component analysis (PCA) to improve the performance of the classic PCA model for single-cell RNA data.

The ***processing and optimization of chemical data*** is one of the most popular directions for ML-based cheminformatic studies. Khashei et al.[14] offered a chemometric classification method based on intelligent discrete deep learning. Duan et al.[15] constructed a perturbation-based variable selection method for near-infrared spectroscopy analysis. Whitehead et al.[16] quantified the advantages of quantitative interpolation over QSAR methods in toxicological data modeling. He et al.[17] conducted a systematic ML study on Kokumi analysis and launched a web platform for online predictions. Goldman et al.[18] inferred metabolites using a spectral transformer for chemical formula prediction. Flanagan et al.[19] analyzed data synthesis techniques to enhance Raman spectroscopy classification.

Many papers on ***diverse directions*** are also gathered into this collection to describe the application of ML in cheminformatic studies. A series of articles in this collection focused on the prediction of the physicochemical characteristics of chemical compounds, and these characteristics included: temperature-dependent viscosity, solvation Gibbs energies, p*Ka*, metal coordination geometry, binding energy, and electronic property.[20−25] Another set of papers focused on molecular generation and design by introducing software/tool,[26,27] developing transformer-based new algorithms,[28] and optimizing molecule via molecular scaffold decoration.[29] The remaining tested the performance of ChatGPT in chemical generation and similarity indexing.[30]

Recently, ML has been simultaneously utilized by both bioinformatic and cheminformatic studies, which is then integrated to cope with complicated bio-cheminformatic problems. In this collection, three major types of studies were reported. (*a*) ***protein structure prediction and functional annotation***. A variety of intelligent frameworks were introduced for predicting the structures of blood-brain

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barrier-penetrating peptide, antimicrobial peptide, and intrinsically disordered protein.[31−34] Elia Venanzi et al.[35] applied a machine learning method that integrated protein structure, sequence, and dynamics to predict the enzymatic activity of bovine intestinal kinase variants. Zachary Smith et al.[66] identified druggable binding sites of protein target using graph neural networks with attention. (*b*) ***virtual screening and drug design***. Some methods, algorithms, and functional tools were constructed to facilitate the application or improve the performance of the classic virtual screening strategy.[36−39] Machine learning methods were also adopted in this collection to identify new hit compounds, discover promising leads for cholestasis, interpret QSAR models, and learn molecular representations.[40−43] DiStefano et al.[44] and Mao et al.[45] conducted research on toxicity prediction and antiviral drug design, respectively. Moreover, ML was also applied to explore the pharmaceutical properties of diverse drug candidates.[46−51] A novel knowledge base for nonalcoholic fatty liver disease was developed.[52] Heyndrickx et al.[53] adopted cross-pharma federated learning to unleash the benefit of QSAR. Fatemeh Rafiei et al.[67] combined feature-based and similarity-based methods for predicting drug synergy. (*c*) ***ligand−receptor docking***. Ligand−receptor interactions were predicted by Fang et al.,[54] Mqawass et al.,[55] Zhang et al.,[56] Gorantla et al.,[57] and Wang et al.[58] using XGBoost, fusion graph neural network, multiobjective graph neural network, decoding deep learning, and meta-learning in a large-scale dynamic graph, respectively. Qu et al.[59] applied a water network-enhanced bistate model to predict protein−ligand affinities. Li et al.[60] employed a capsule-based integrated deep learning network to predict the interactions between ncRNA and proteins. Various ML methods are also used to study drug-target interaction, drug−drug interaction, introducing protein−ligand database with complex structure models.[61−65]

Bio-cheminformatics has been a hot topic in chemical and biomedical research and is a welcome area for the *Journal of Chemical Information and Modeling* (JCIM). We hope the papers showcased in this special issue highlight some of the exciting advances in ML-driven bio-cheminformatics studies.

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Notes

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