JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

pubs.acs.org/jcim Editorial

Editorial: Machine Learning in Bio-cheminformatics

Cite This: *J. Chem. Inf. Model.* 2023, 63, 1−1 Read Online

ACCESS | Metrics & More | Article Recommendations

Recent years have witnessed exponential growth in machine learning (ML), including deep learning (DL), studies. ML has facilitated data-driven discoveries in a wide variety of scientific fields and disciplines, especially bio-cheminformatics. It identifies hidden patterns from extensive biological/chemical data and then makes predictions/decisions based on such patterns. Particularly, ML-based frameworks have been successfully adopted by various *bioinformatic* studies to enable the accurate prediction of protein structures,[1] discover the binding sites of protein−protein interactions,[2] and accelerate the identification of therapeutic targets.[3] Moreover, ML has been frequently employed in diverse *cheminformatic* research to improve the efficiency of drug design,[4] identify the best route for synthesizing chemicals,[5] and predict the physicochemical properties of critical molecules.[6] All in all, the unprecedented ability of ML to tackle biological and chemical data challenges has led to tremendous breakthroughs in various research directions, including bio-cheminformatics. Future growth in bio-cheminformatics will be fueled by the further development of new ML algorithms, the advances in experimental technologies which generate chemical and biological data, the identification of significant problems in chemistry and biology, the availability of high-performance computers and the application of innovative mathematical tools.

The *Journal of Chemical Information and Modeling* (JCIM) aims to continue its role as a publishing hub for state-of-the-art interdisciplinary studies integrating biological/chemical research with information and mathematical sciences. To foster further applications of ML to diverse topics in chemistry and chemical biology (including but not limited to the prediction of molecular structures/interactions/properties, the discovery of drugs/targets, and the planning of retrosynthetic routes), JCIM is announcing the publication of a special issue on **Machine Learning in Bio-cheminformatics**.

We invite submissions from researchers and scientists worldwide to report on new approaches and/or important applications in the field of Machine Learning in Bio-cheminformatics. We welcome all types of manuscript that fit the scope of JCIM, such as articles, perspectives, viewpoints, reviews, letters, and application notes. Please find more information on manuscript types at JCIM's official site and our earlier Editorial on ML. We are requesting interested authors to submit their manuscripts by August 1 2023, with the expected publication date being December 2023. We look forward to your contributions.

Kenneth M. Merz
Guo-Wei Wei
Feng Zhu orcid.org/0000-0001-8069-0053

AUTHOR INFORMATION

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jcim.2c01496

Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

REFERENCES

(1) Jumper, J.; Evans, R.; Pritzel, A.; Green, T.; Figurnov, M.; Ronneberger, O.; Tunyasuvunakool, K.; Bates, R.; Zidek, A.; Potapenko, A.; Bridgland, A.; Meyer, C.; Kohl, S. A. A.; Ballard, A. J.; Cowie, A.; Romera-Paredes, B.; Nikolov, S.; Jain, R.; Adler, J.; Back, T.; Petersen, S.; Reiman, D.; Clancy, E.; Zielinski, M.; Steinegger, M.; Pacholska, M.; Berghammer, T.; Bodenstein, S.; Silver, D.; Vinyals, O.; Senior, A. W.; Kavukcuoglu, K.; Kohli, P.; Hassabis, D. Highly accurate protein structure prediction with AlphaFold. *Nature* **2021**, *596* (7873), 583−589.

(2) Gainza, P.; Sverrisson, F.; Monti, F.; Rodola, E.; Boscaini, D.; Bronstein, M. M.; Correia, B. E. Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning. *Nat. Methods* **2020**, *17* (2), 184−192.

(3) Piazza, I.; Beaton, N.; Bruderer, R.; Knobloch, T.; Barbisan, C.; Chandat, L.; Sudau, A.; Siepe, I.; Rinner, O.; de Souza, N.; Picotti, P.; Reiter, L. A machine learning-based chemoproteomic approach to identify drug targets and binding sites in complex proteomes. *Nat. Commun.* **2020**, *11* (1), 4200.

(4) Zhavoronkov, A.; Ivanenkov, Y. A.; Aliper, A.; Veselov, M. S.; Aladinskiy, V. A.; Aladinskaya, A. V.; Terentiev, V. A.; Polykovskiy, D. A.; Kuznetsov, M. D.; Asadulaev, A.; Volkov, Y.; Zholus, A.; Shayakhmetov, R. R.; Zhebrak, A.; Minaeva, L. I.; Zagribelnyy, B. A.; Lee, L. H.; Soll, R.; Madge, D.; Xing, L.; Guo, T.; Aspuru-Guzik, A. Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nat. Biotechnol.* **2019**, *37* (9), 1038−1040.

(5) Fortunato, M. E.; Coley, C. W.; Barnes, B. C.; Jensen, K. F. Data augmentation and pretraining for template-based retrosynthetic prediction in computer-aided synthesis planning. *J. Chem. Inf Model* **2020**, *60* (7), 3398−3407.

(6) Zhou, G.; Lubbers, N.; Barros, K.; Tretiak, S.; Nebgen, B. Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. *Proc. Natl. Acad. Sci. U.S.A.* **2022**, *119* (27), No. e2120333119.

Published: January 9, 2023