

- [24] QHwan Kim, Joon-Hyuk Ko, Sunghoon Kim, Nojun Park, and Wonho Jhe. Bayesian Neural Network with Pretrained Protein Embedding Enhances Prediction Accuracy of Drug-Protein Interaction. *Bioinformatics*, 37(20): 3428–3435, 2021.
- [25] Dingyan Wang et al. A Hybrid Framework for Improving Uncertainty Quantification in Deep Learning-Based QSAR Regression Modeling. *Journal of Cheminformatics*, 13(1):1–17, 2021.
- [26] Thomas-Martin Dutschmann, Lennart Kinzel, Antonius Ter Laak, and Knut Baumann. Large-Scale Evaluation of k-Fold Cross-Validation Ensembles for Uncertainty Estimation. *Journal of Cheminformatics*, 15(1):49, 2023.
- [27] Tianzhixi Yin, Gihan Panapitiya, Elizabeth D Coda, and Emily G Saldanha. Evaluating Uncertainty-Based Active Learning for Accelerating the Generalization of Molecular Property Prediction. *Journal of Cheminformatics*, 15(1):105, 2023.
- [28] Jie Yu, Dingyan Wang, and Mingyue Zheng. Uncertainty Quantification: Can We Trust Artificial Intelligence in Drug Discovery? *iScience*, 25(8):104814, 2022.
- [29] Eelke B Lenselink et al. Beyond the Hype: Deep Neural Networks Outperform Established Methods Using a ChEMBL Bioactivity Benchmark Set. *Journal of Cheminformatics*, 9(1):1–14, 2017.
- [30] Robert P Sheridan. Time-Split Cross-Validation as a Method for Estimating the Goodness of Prospective Prediction. *Journal of Chemical Information and Modeling*, 53(4):783–790, 2013.
- [31] Hannah Rosa Friesacher, Emma Svensson, Adam Arany, Lewis Mervin, and Ola Engkvist. Towards Reliable Uncertainty Estimates for Drug Discovery: A Large-scale Temporal Study of Probability Calibration. In *ICML 2024 AI for Science Workshop*, 2024. URL <https://openreview.net/forum?id=5B8tsitI5s>.
- [32] Myles Hollander, Frank Proschan, and James Sconing. Measuring Information in Right-Censored Models. *Naval Research Logistics (NRL)*, 34(5):669–681, 1987.
- [33] Frederik Boe Hüttel, Christoffer Riis, Filipe Rodrigues, and Francisco Câmara Pereira. Bayesian Active Learning for Censored Regression. *arXiv preprint arXiv:2402.11973*, 2024.
- [34] Tim Pearce, Jong-Hyeon Jeong, Yichen Jia, and Jun Zhu. Censored Quantile Regression Neural Networks for Distribution-Free Survival Analysis. In *Advances in Neural Information Processing Systems*, volume 35, pages 7450–7461. Curran Associates, Inc., 2022.
- [35] Adam Arany, Jaak Simm, Martijn Oldenhof, and Yves Moreau. SparseChem: Fast and Accurate Machine Learning Model for Small Molecules. *arXiv preprint arXiv:2203.04676*, 2022.
- [36] Wouter Heyndrickx et al. MELLODDY: Cross-pharma Federated Learning at Unprecedented Scale Unlocks Benefits in QSAR without Compromising Proprietary Information. *Journal of Chemical Information and Modeling*, 2023.
- [37] Greg Landrum. RDKit: Open-Source Cheminformatics, 2006. URL <http://www.rdkit.org>.
- [38] David Weininger. SMILES, a Chemical Language and Information System. 1. Introduction to Methodology and Encoding Rules. *Journal of Chemical Information and Computer Sciences*, 28(1):31–36, 1988.
- [39] Harry L Morgan. The Generation of a Unique Machine Description for Chemical Structures – A Technique Developed at Chemical Abstracts Service. *Journal of Chemical Documentation*, 5(2):107–113, 1965.
- [40] Robin Winter, Floriane Montanari, Frank Noé, and Djork-Arné Clevert. Learning Continuous and Data-Driven Molecular Descriptors by Translating Equivalent Chemical Representations. *Chemical Science*, 10(6):1692–1701, 2019.
- [41] Andreas Mayr et al. Large-Scale Comparison of Machine Learning Methods for Drug Target Prediction on ChEMBL. *Chemical Science*, 9(24):5441–5451, 2018.
- [42] Derek Van Tilborg, Alisa Alenicheva, and Francesca Grisoni. Exposing the Limitations of Molecular Machine Learning with Activity Cliffs. *Journal of Chemical Information and Modeling*, 62(23):5938–5951, 2022.
- [43] James L Powell. Censored Regression Quantiles. *Journal of Econometrics*, 32(1):143–155, 1986.
- [44] F. Pedregosa et al. Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, 12: 2825–2830, 2011.
- [45] Igor V Tetko et al. Critical Assessment of QSAR Models of Environmental Toxicity Against Tetrahymena Pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. *Journal of Chemical Information and Modeling*, 48(9):1733–1746, 2008.
- [46] Adam Paszke et al. PyTorch: An Imperative Style, High-Performance Deep Learning Library. In *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.