

References

- [5] Hewitt, M.; Cronin, M. T. D.; Enoch, S. J.; Madden, J. C.; Roberts, D. W.; Dearden, J. C. In Silico Prediction of Aqueous Solubility: The Solubility Challenge. *J. Chem. Inf. Model.* 2009, 49 (11), 2572–2587. <https://doi.org/10.1021/ci900286s>.
- [6] Lusci, A.; Pollastri, G.; Baldi, P. Deep Architectures and Deep Learning in Chemoinformatics: The Prediction of Aqueous Solubility for Drug-Like Molecules. *J. Chem. Inf. Model.* 2013, 53 (7), 1563–1575. <https://doi.org/10.1021/ci400187y>.
- [7] Tang, B.; Kramer, S. T.; Fang, M.; Qiu, Y.; Wu, Z.; Xu, D. A Self-Attention Based Message Passing Neural Network for Predicting Molecular Lipophilicity and Aqueous Solubility. *J Cheminform* 2020, 12 (1), 15. <https://doi.org/10.1186/s13321-020-0414-z>.
Figures adapted under the CC BY 4.0 license.
- [8] Schnieders, M. J.; Baltrusaitis, J.; Shi, Y.; Chattree, G.; Zheng, L.; Yang, W.; Ren, P. The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. *J. Chem. Theory Comput.* 2012, 8 (5), 1721–1736. <https://doi.org/10.1021/ct300035u>.

