Leveraging computational chemistry to optimise Machine Learning Models in Drug Discovery

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This is discussed in Mayr et al. 2018

References

Mayr, Andreas et al. (June 20, 2018). "Large-Scale Comparison of Machine Learning Methods for Drug Target Prediction on ChEMBL". In: *Chemical Science* 9.24, pp. 5441–5451. ISSN: 2041-6539. DOI: 10.1039/C8SC00148K. URL: https://pubs.rsc.org/en/content/articlelanding/2018/sc/c8sc00148k (visited on 08/19/2025).