Leveraging computational chemistry to optimise Machine Learning Models in Drug Discovery

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This is discussed in Baptista et al. 2025

References

Baptista, Delora et al. (2025). "Evaluating Molecular Representations in Machine Learning Models for Drug Response Prediction and Interpretability". In: *Journal of Integrative Bioinformatics* 19.3 (), p. 20220006. ISSN: 1613-4516. DOI: 10.1515/jib-2022-0006. PMID: 36017668. URL: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9521826/ (visited on 08/19/2025).