

## Daftar Pustaka

- [1] M. F. Aditya, A. Aditsania, and I. Kurniawan, 'Implementation of the Grey Wolf Algorithm in Optimization of Artificial Neural Network Method for Fingerprint-Based Toxicity Prediction', in *2023 6th International Conference of Computer and Informatics Engineering (IC2IE)*, Sep. 2023, pp. 109–114. doi: 10.1109/IC2IE60547.2023.10331599.
- [2] E. S. Rumaseuw, Y. Iskandar, E. Halimah, and A. Zuhrotun, 'Characterization And Acute Toxicity Test Of Black Garlic Ethanol Extract Based On OECD', *Interest J. Ilmu Kesehatan.*, pp. 215–224, Jan. 2022, doi: 10.37341/interest.v0i0.379.
- [3] B. Sharma *et al.*, 'Accurate clinical toxicity prediction using multi-task deep neural nets and contrastive molecular explanations', *Sci. Rep.*, vol. 13, no. 1, p. 4908, Mar. 2023, doi: 10.1038/s41598-023-31169-8.
- [4] T. Unterthiner, 'Multi-Target Deep Neural Networks for Toxicity Prediction / Author Thomas Unterthiner, MSc', Sep. 2016. Accessed: Apr. 04, 2024. [Online]. Available: <https://www.semanticscholar.org/paper/Multi-Target-Deep-Neural-Networks-for-Toxicity-MSc-Unterthiner/508e38f8e984bf0ecbb41d20b8b951f75afe5>
- [5] B. Shaker, S. Ahmad, J. Lee, C. Jung, and D. Na, 'In silico methods and tools for drug discovery', *Comput. Biol. Med.*, vol. 137, p. 104851, Oct. 2021, doi: 10.1016/j.combiomed.2021.104851.
- [6] W. Chen, X. Liu, S. Zhang, and S. Chen, 'Artificial intelligence for drug discovery: Resources, methods, and applications', *Mol. Ther. Nucleic Acids*, vol. 31, pp. 691–702, Feb. 2023, doi: 10.1016/j.omtn.2023.02.019.
- [7] 'In Silico Approach for Predicting Toxicity of Peptides and Proteins | PLOS ONE'. Accessed: Apr. 24, 2024. [Online]. Available: <https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0073957>
- [8] 'Cuckoo search optimisation for feature selection in cancer classification: a new approach - PubMed'. Accessed: Feb. 09, 2025. [Online]. Available: <https://pubmed.ncbi.nlm.nih.gov/26547979/>
- [9] E. Kim and H. Nam, 'Prediction models for drug-induced hepatotoxicity by using weighted molecular fingerprints', *BMC Bioinformatics*, vol. 18, no. Suppl 7, p. 227, May 2017, doi: 10.1186/s12859-017-1638-4.
- [10] L. Pu, M. Naderi, T. Liu, H.-C. Wu, S. Mukhopadhyay, and M. Brylinski, 'eToxPred: a machine learning-based approach to estimate the toxicity of drug candidates', *BMC Pharmacol. Toxicol.*, vol. 20, no. 1, p. 2, Jan. 2019, doi: 10.1186/s40360-018-0282-6.
- [11] 'Cuckoo Search-Driven Optimization of Artificial Neural Networks for Accurate Fingerprint-Based Toxicity Prediction | IEEE Conference Publication | IEEE Xplore'. Accessed: Apr. 28, 2024. [Online]. Available: <https://ieeexplore.ieee.org/document/10390946>
- [12] F. Siddique *et al.*, 'Revisiting methotrexate and phototrexate Zinc15 library-based derivatives using deep learning in-silico drug design approach', *Front. Chem.*, vol. 12, p. 1380266, 2024, doi: 10.3389/fchem.2024.1380266.
- [13] Y. Zhou *et al.*, 'In silico prediction of ocular toxicity of compounds using explainable machine learning and deep learning approaches', *J. Appl. Toxicol.*, vol. n/a, no. n/a, doi: 10.1002/jat.4586.
- [14] F. Mostafa, V. Howle, and M. Chen, 'Machine Learning to Predict Drug-Induced Liver Injury and its Validation on Failed Drug Candidates in Development', Mar. 20, 2024. doi: 10.21203/rs.3.rs-3951806/v1.
- [15] 'MolToxPred: small molecule toxicity prediction using machine learning approach - RSC Advances (RSC Publishing)'. Accessed: Apr. 24, 2024. [Online]. Available: <https://pubs.rsc.org/en/content/articlelanding/2024/ra/d3ra07322j>
- [16] X.-S. Yang and S. Deb, 'Cuckoo Search via Lévy flights', in *2009 World Congress on Nature & Biologically Inspired Computing (NaBIC)*, Dec. 2009, pp. 210–214. doi: 10.1109/NABIC.2009.5393690.
- [17] D. Opitz and R. Maclin, 'Popular Ensemble Methods: An Empirical Study', *J. Artif. Intell. Res.*, vol. 11, pp. 169–198, Aug. 1999, doi: 10.1613/jair.614.
- [18] L. Breiman, 'Random Forests', *Mach. Learn.*, vol. 45, no. 1, pp. 5–32, Oct. 2001, doi: 10.1023/A:1010933404324.
- [19] A. J. Ferreira and M. A. T. Figueiredo, 'Boosting Algorithms: A Review of Methods, Theory, and Applications', in *Ensemble Machine Learning: Methods and Applications*, C. Zhang and Y. Ma, Eds., New York, NY: Springer, 2012, pp. 35–85. doi: 10.1007/978-1-4419-9326-7\_2.
- [20] '(PDF) A Survey of Ensemble Learning: Concepts, Algorithms, Applications, and Prospects'. Accessed: Dec. 14, 2024. [Online]. Available: [https://www.researchgate.net/publication/363621267\\_A\\_Survey\\_of\\_Ensemble\\_Learning\\_Concepts\\_Algorithms\\_Applications\\_and\\_Prospects](https://www.researchgate.net/publication/363621267_A_Survey_of_Ensemble_Learning_Concepts_Algorithms_Applications_and_Prospects)
- [21] 'Confusion Matrices: A Unified Theory | IEEE Journals & Magazine | IEEE Xplore'. Accessed: Feb. 10, 2025. [Online]. Available: <https://ieeexplore.ieee.org/document/10769075>
- [22] 'Papers with Code - ClinTox Dataset'. Accessed: Dec. 07, 2024. [Online]. Available: <https://paperswithcode.com/dataset/clintox>