PREDIKSI INHIBITOR ANGIOTENSIN-CONVERTING-ENZYME (ACE) SEBAGAI AGEN ANTIHIPERTENSI DENGAN MENGGUNAKAN ARTIFICIAL NEURAL NETWORK YANG DIOPTIMALKAN OLEH ARTIFICIAL BEE COLONY

Atilla Fejril, Isman Kurniawan, S.Pd., M.Si., M.Sc., Ph.D.

Hypertension is a leading cause of death worldwide, requiring efficient methods for Angiotensin-Converting Enzyme (ACE) inhibitor prediction. This study combines Artificial Bee Colony (ABC) algorithm with Artificial Neural Network (ANN) using the ChEMBL dataset. The model with a population size of 10 achieved the best performance, with an R^2 of 0.683, demonstrating accurate and cost-effective prediction. These findings underscore the potential of ABC-ANN integration for combating hypertension, though further validation with larger datasets is needed.

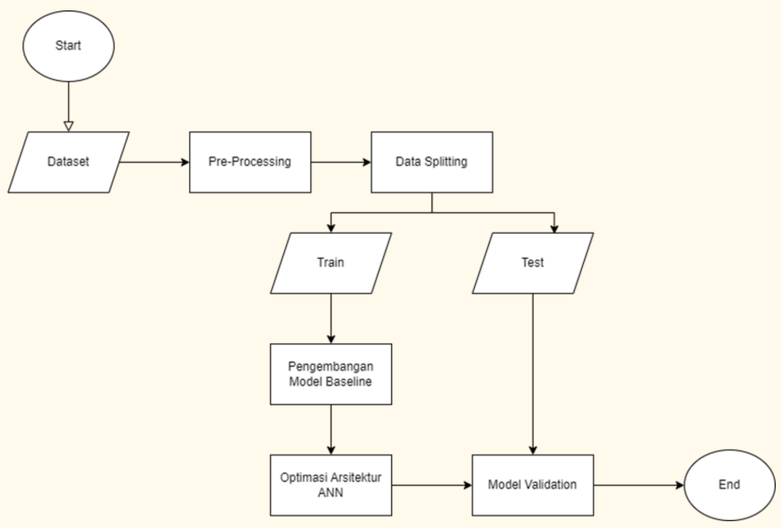
Background

- Hypertension is a leading cause of death worldwide.
- ACE inhibitors are important drugs for treating hypertension
- Traditional methods, such as wet-lab testing, are time-consuming and costly.
- Machine learning and deep learning, particularly ANN, have the potential to improve ACE inhibitor prediction.
- Hyperparameter optimization of ANN using the ABC algorithm can enhance model performance.

Topic and Limitation

- Predicting ACE inhibitor activity with ANN optimized by the ABC algorithm.
- Evaluation of model performance
- Limited to the ChEMBL dataset; results may not generalize to larger datasets.
- Based on a single ANN model; further validation is needed.

Methodology



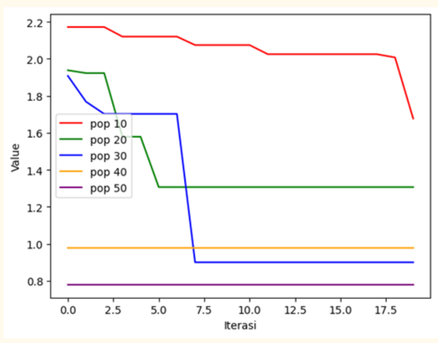
Evaluation

Model	R^2	k	r_m^2	Δr_m^2
pop10	0.763	0.870	0.671	0.176
pop20	0.702	0.832	0.620	0.106
pop30	0.740	0.866	0.652	0.193
pop40	0.661	0.730	0.557	0.239
pop50	0.771	0.850	0.537	0.146

Comparison results using training data from each model created based on optimisation

Model	R^2	k	r_m^2	Δr_m^2
pop10	0.683	0.921	0.568	0.233
pop20	0.529	0.825	0.407	0.131
pop30	0.652	0.851	0.521	0.252
pop40	0.668	0.754	0.522	0.251
pop50	0.684	0.880	0.537	0.244

Comparison results using test data from each model created based on optimisation



convergent plot generated from each model created

Conclusion

This study shows that an ANN optimized with the ABC algorithm effectively predicts ACE inhibitor activity. The pop10 model excels locally, while pop50 captures overall data patterns best. ABC-ANN offers a more efficient, cost-effective alternative to traditional methods in drug discovery.

References

[1] M. H. Strauss, A. S. Hall, and K. Narkiewicz, "The Combination of Beta-Blockers and ACE Inhibitors Across the Spectrum of Cardiovascular Diseases," Cardiovascular Drugs and Therapy, vol.
[2] M. Thorat, S. Pandit, and S. Balote, "Artificial Neural Network: A brief study," Asian Journal of Convergence in Technology, vol. 8, no. 3, pp. 12–16, 2022, doi: 10.33130/ajct.2022v08i03.003.

Telkom University

Fakultas Informatika