QUANTUM-ENHANCED DEEP LEARNING FOR PREDICTING PCSK9/NARC-1 INHIBITOR BIOACTIVITY: A NOVEL APPROACH TOWARDS CORONARY ARTERY DISEASE THERAPY

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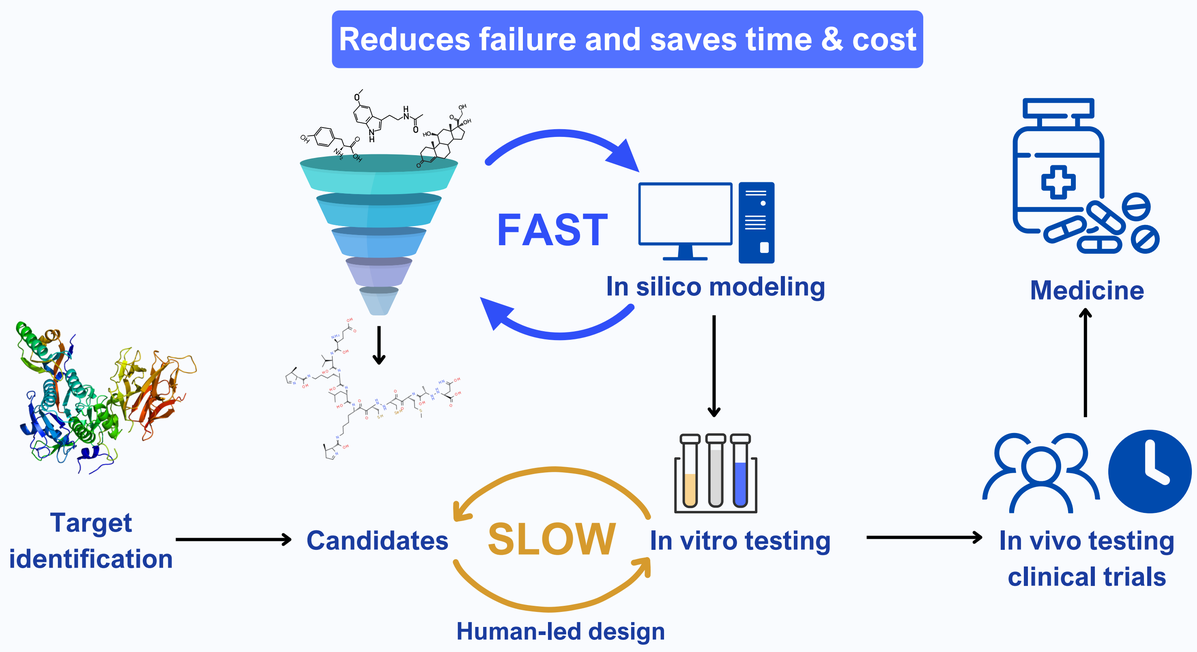
PROBLEM

Coronary Artery Disease (CAD) was the cause of

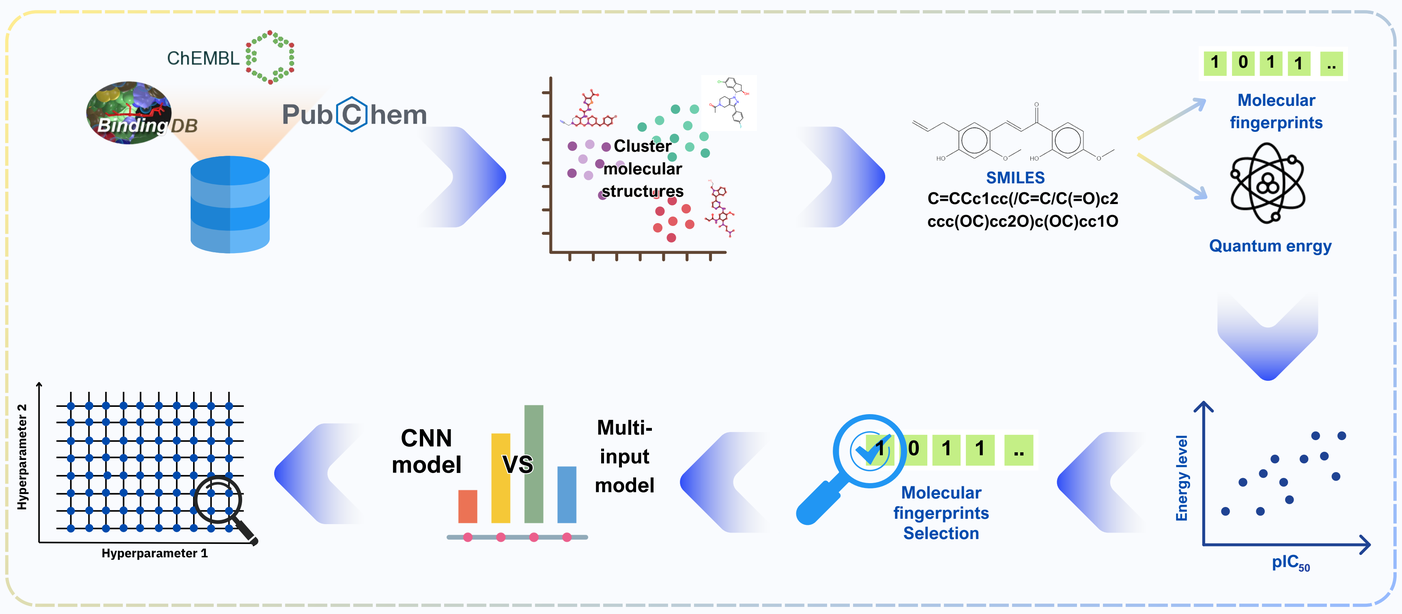
1 in 3 Deaths

3 GOOD HEALTH AND WELL-BEING

The role of computational in the early-stage drug discovery process



FRAMEWORK



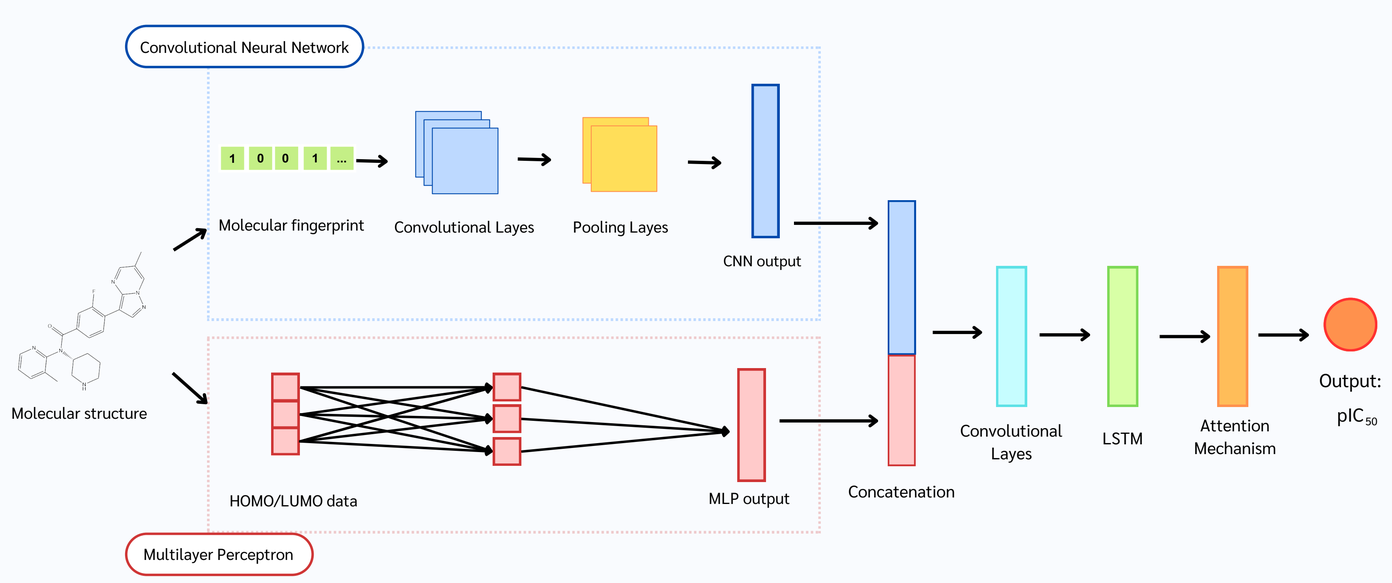


Fig. 1. Multi-input model architecture

FINDING

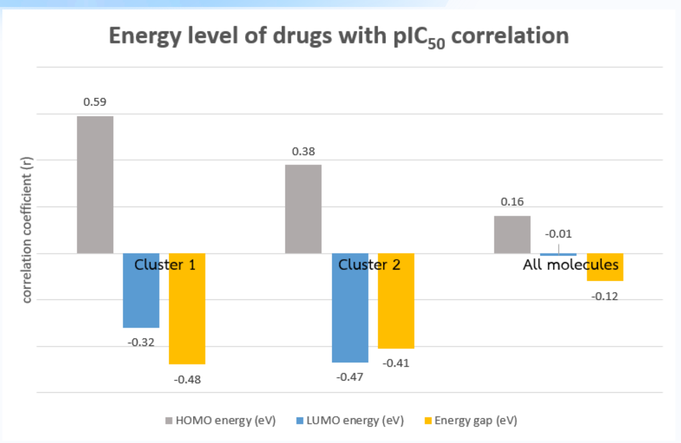


Fig. 2. Correlation between energy level and pIC_{50} of molecules in each cluster

Table 1. Comparing *R-squared* value and *MSE* value of each model

Model	*R-squared*	*MSE*
Multi-Input model (After Tuning)	0.8105	0.4629
Multi-Input model (Before Tuning)	0.5598	0.9116
Random Forest Regressor	0.5197	1.0853
CNN	0.3995	1.3913

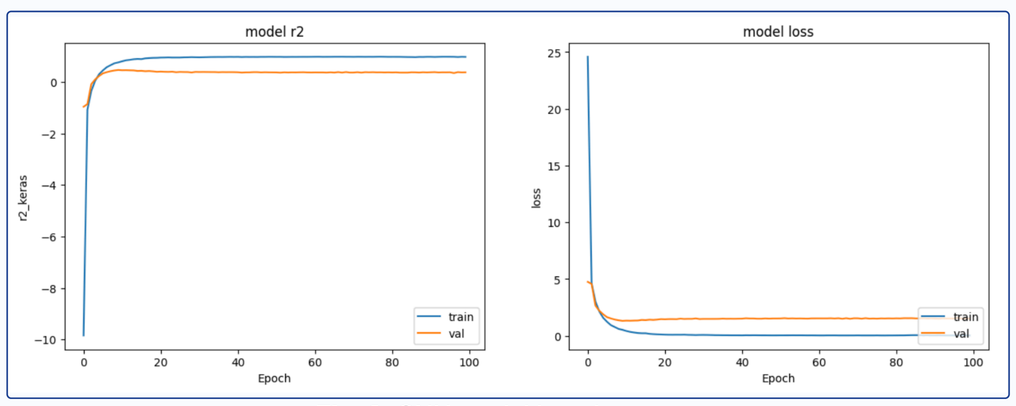


Fig. 3. CNN model learning curve

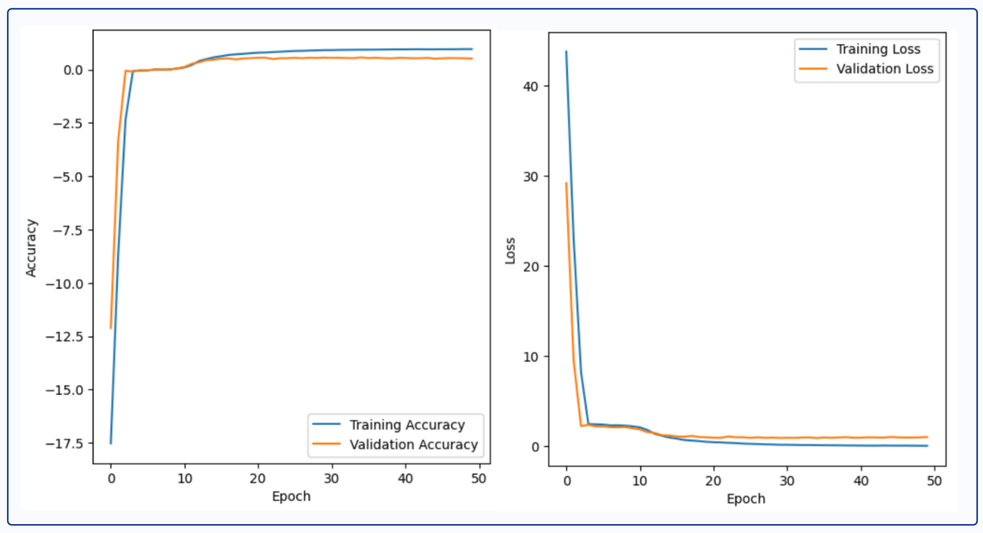


Fig. 4. Multi-Input model (After Tuning) learning curve

INTERPRETATION AND CONCLUSION

MulquaCAD

The multi-input model has evolved into a user-friendly website.

High efficiency in predicting the drug's bioactivity
compared to a normal model
with *R-squared* = 0.8105 and *MSE* = 0.4629

Reduce the time spent on finding the bioactivity of new drugs that target proteins.

REFERENCE

[1] Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. Drug Discovery Today, 23(6), 1241-1250. doi: 10.1016/j.drudis.2018.01.039.
[2] Chattaraj, P. K., Giri, S., & Duley, S. (2011). Reactivity descriptors from chemical hardness, chemical potential, and electrophilicity viewpoint. Physical Chemistry Chemical Physics, 13(42), 17407-17418. doi: 10.1039/C1CP21824B.