Quantum Innovation Challenge 2025

Quantum Neural Network-enhanced Residual Multi-Layer Perceptron Mixture-of-Experts (QNN-enhanced ResMLP_MoE)

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1. Dataset & Task

- Task: 1) PK/PD modelling, 2) Dose optimization

Patient Data

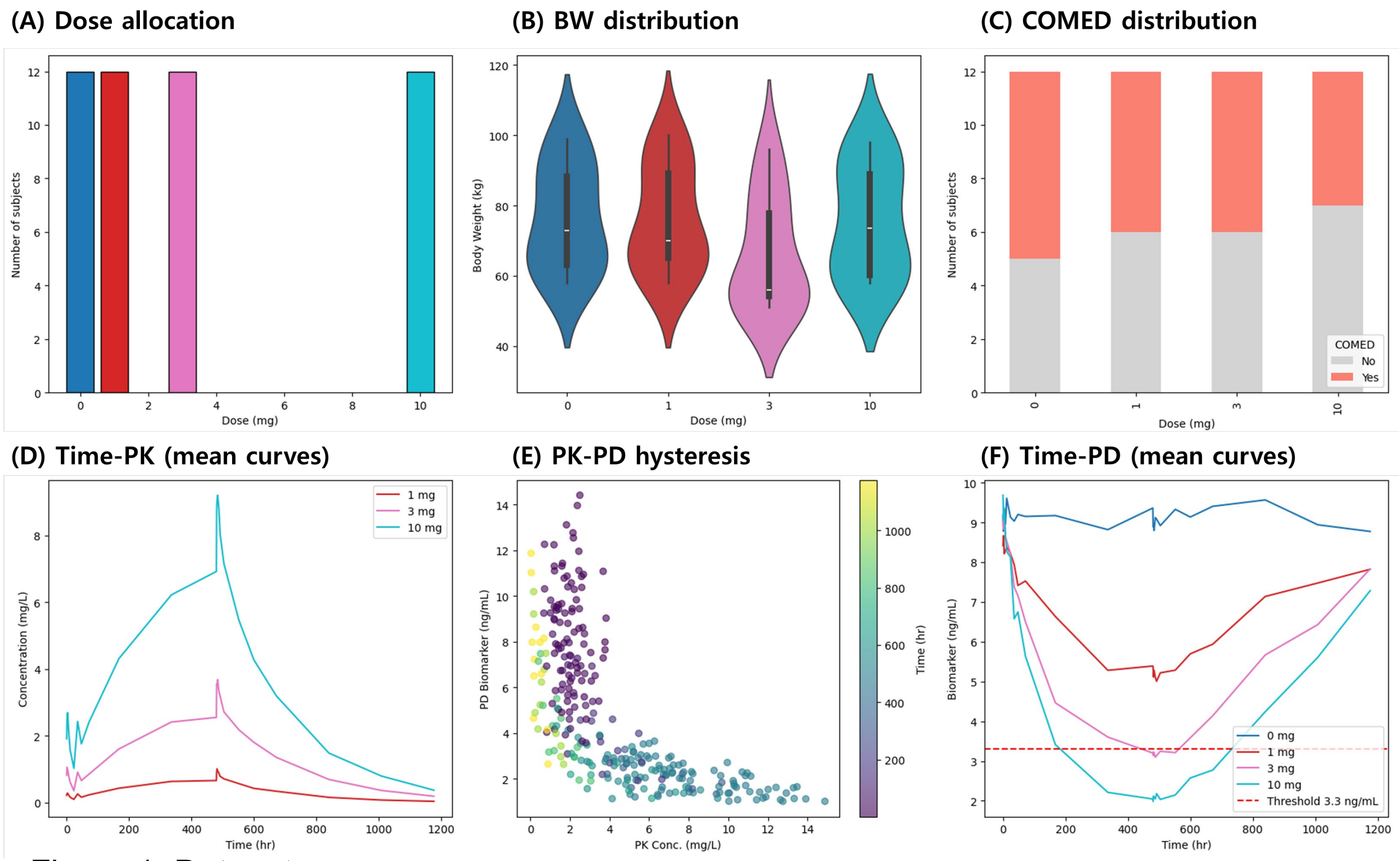


Figure 1: Dataset.

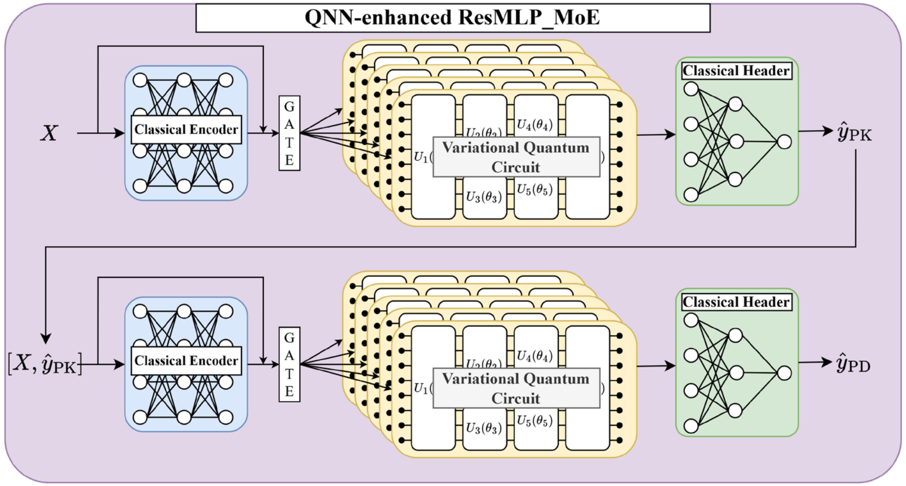
2. Quantum-enhanced ML Framework for Dose Optimization

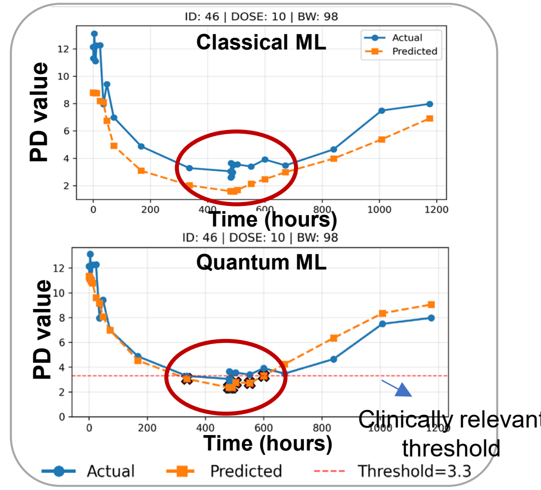
QNN-enhanced ResMLP_MoE Framework

Input Data

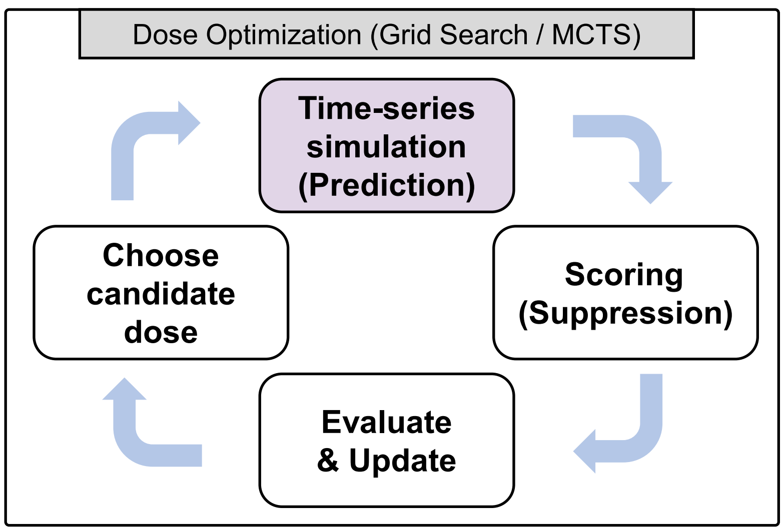
Bio information
- Patient ID
- Weight..

Drug Information
- Dose
- Start Date
- Time





Dose Optimization



Team PNU

Prof. Giltae Song

AI, Biomedical Data

Develops deep learning models for PK/PD prediction

Team Members:
Sanghun Sel, Juseong Kim, Mingyeol Kim

Prof. Won-Joo Hwang

Quantum Computing, AI

Applies quantum algorithms to PK/PD modeling

Team Members:
Seon-Geun Jeong, Le Tung Giang, Nguyen Doan Hieu, Mai Dinh Cong

Prof. In-Soo Yoon

PK/PD, Biopharmaceutics

Provides domain expertise in PK/PD and clinical pharmacology

Specialized in clinical validation and dose optimization strategies

3. Model Search

- Cascade + ResMLP+MoE achieves the best performance in terms of PK/PD RMSE.

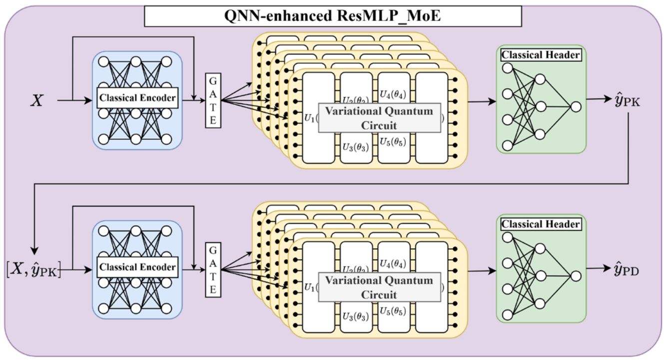
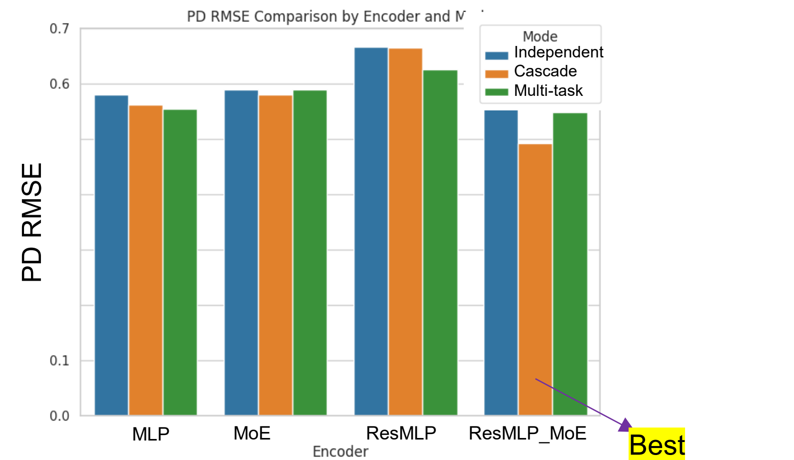


Figure 3: QNN-enhanced ResMLP_MoE.



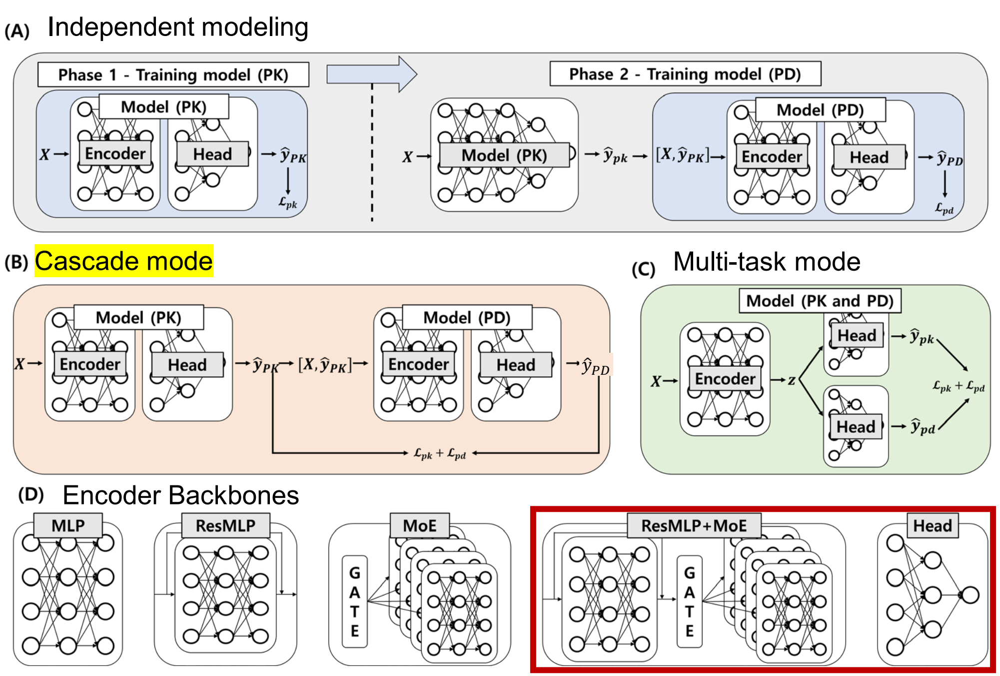


Figure 4: Overview of modeling frameworks.

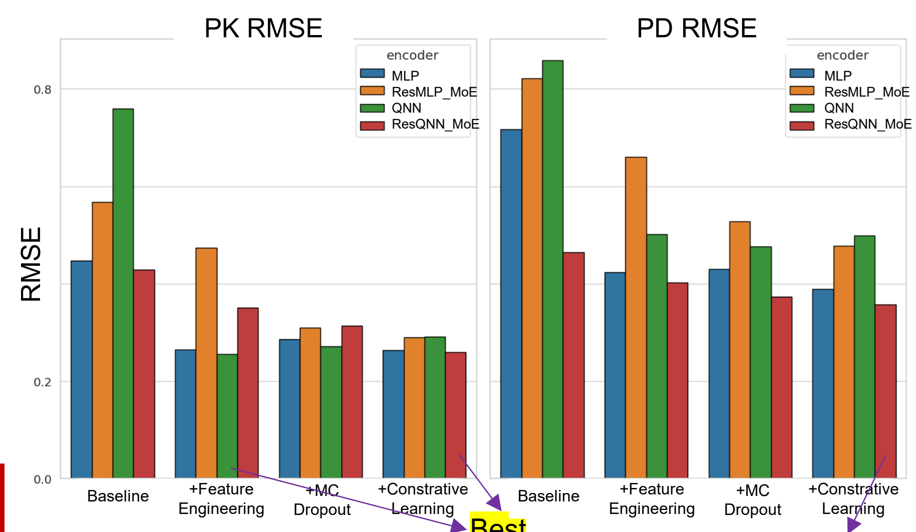


Figure 5: Empirical evaluation results.

Best

3. Quantum Model (Qubits, Layers, Advantage)

- Technical Feasibility: Based on IBM quantum systems, the quantum volume reflects the maximum circuit size with widith ≈ depth. State-of-the-arts $QV = 512 \Rightarrow T \leq 9$. That is, (9 qubits and 9 depth)

Table 1: The up-to-date IBM Quantum's quantum computers

No.	System	Qubits	QV	EPLG[a]	CLOPS[b]	T1 (μs)[c]	T2 (μs)[c]	QPU[d]	Processor
1	ibm_fez	156	512	0.8%	3.8K	136.52	78.58	us-east	Heron r1
2	ibm_toronto	133	512	1.0%	3.8K	158.27	122.18	us-east	Heron r1

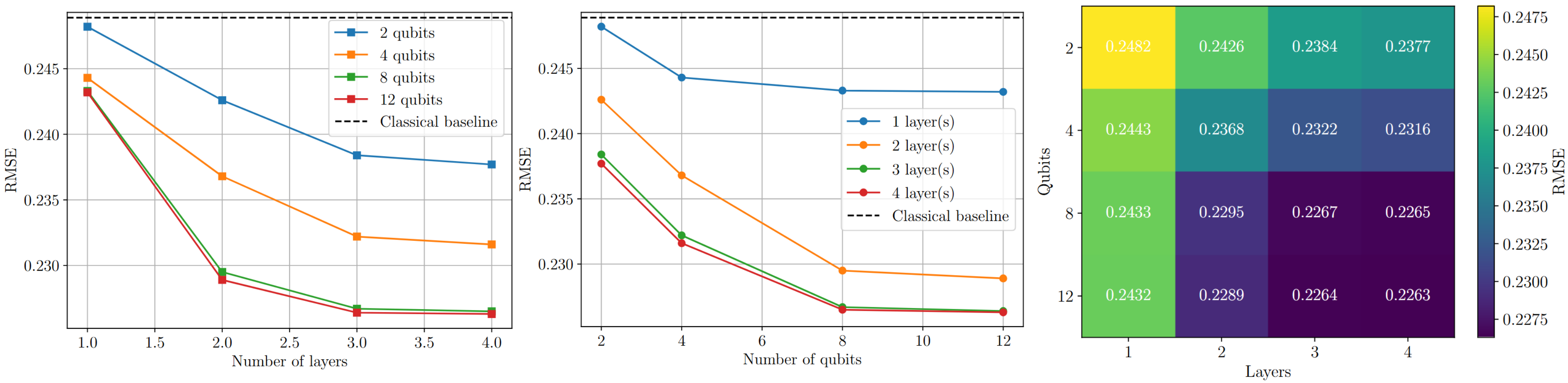
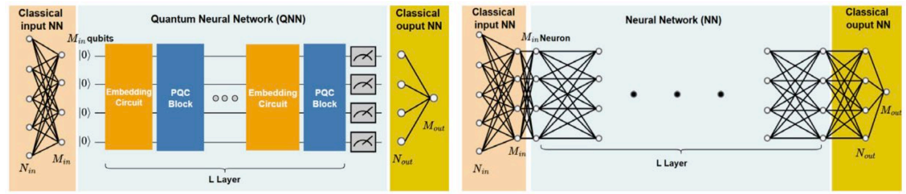


Figure 6: Results of QNN-enhanced ResMLP_MoE

[1] Jeong, Seon-Geun, Kyeong-Hwan Moon, and Won-Joo Hwang. "Hybrid quantum neural networks for efficient protein-ligand binding affinity prediction." *EPJ Quantum Technology* 12.1 (2025): 1-36.

4. Conclusion

- Quantum advantages [1]:
- 1) Model complexity reduction

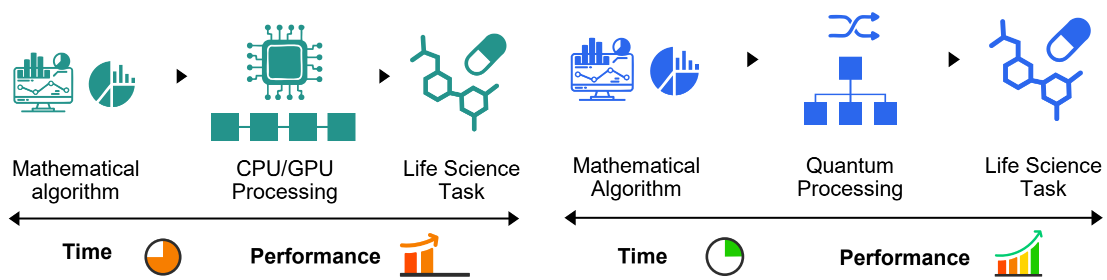


(a) Architecture of HQNN (b) Architecture of NN

- 2) approximation performance (Neural Network $F(x)$, Quantum Neural Network $Q(x)$, continuous function $f(x)$)
  $|f(x) - F(x)|dx < \varepsilon$, $|f(x) - Q(x)|dx < \delta$.   ($\varepsilon > \delta$) in the same number of parameters.

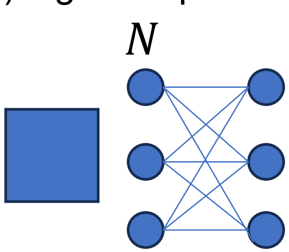
- 3) model convergence speed (Training time)

- 4) inference time (Faster than NN)

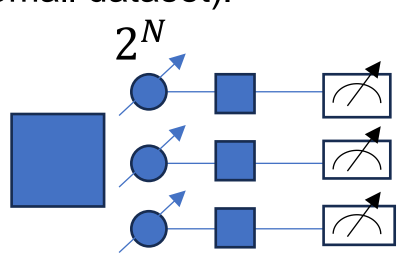


Model	# Qubit	# C params	# Q params	# Operation time
Classical NN	–	$(N_{in}+M_{out})M_{in}+M_{in}^2(L_{nn}+2)$	–	$O((N_{in}+M_{out})M_{in}+M_{in}^2(L_{nn}+2))\mathrm{CPU}_{time}$
HQNN	M_{in}	$(N_{in}+M_{out})M_{in}$	$3M_{in}L_{qnn}$	$O((N_{in}+M_{out})M_{in})\mathrm{CPU}_{time}+O(4L_{qnn})\mathrm{QPU}_{single}+O(M_{in}L_{qnn})\mathrm{QPU}_{two}$

- 5) higher expressivity (Small dataset).



Classical representation Space



Quantum Hilbert representation Space

[1] Jeong, Seon-Geun, Kyeong-Hwan Moon, and Won-Joo Hwang. "Hybrid quantum neural networks for efficient protein-ligand binding affinity prediction." *EPJ Quantum Technology* 12.1 (2025): 1-36.

Thank you!