Hybrid Quantum Neural Network Approaches to Protein—Ligand Binding Affinity Prediction

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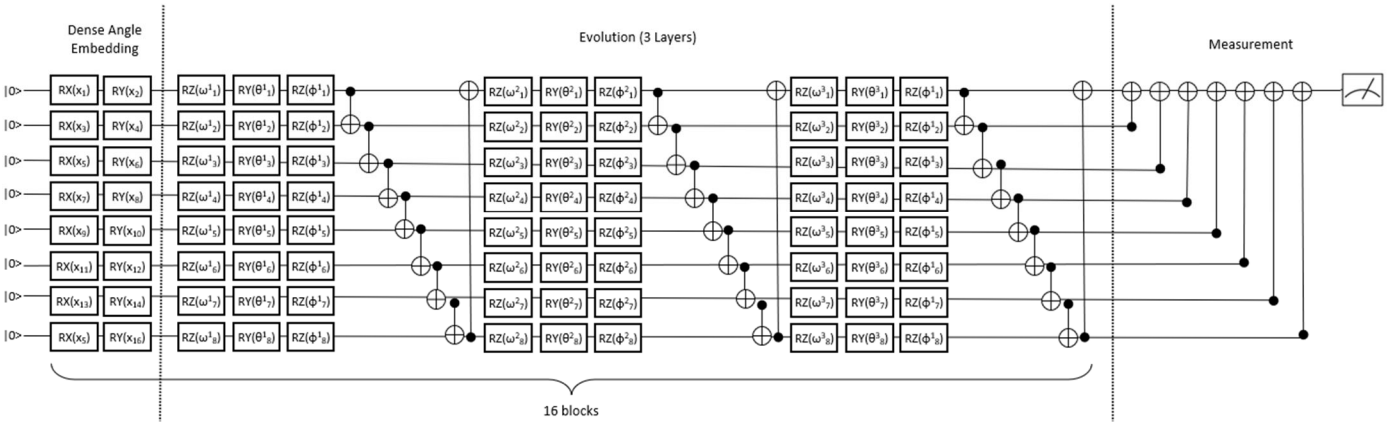
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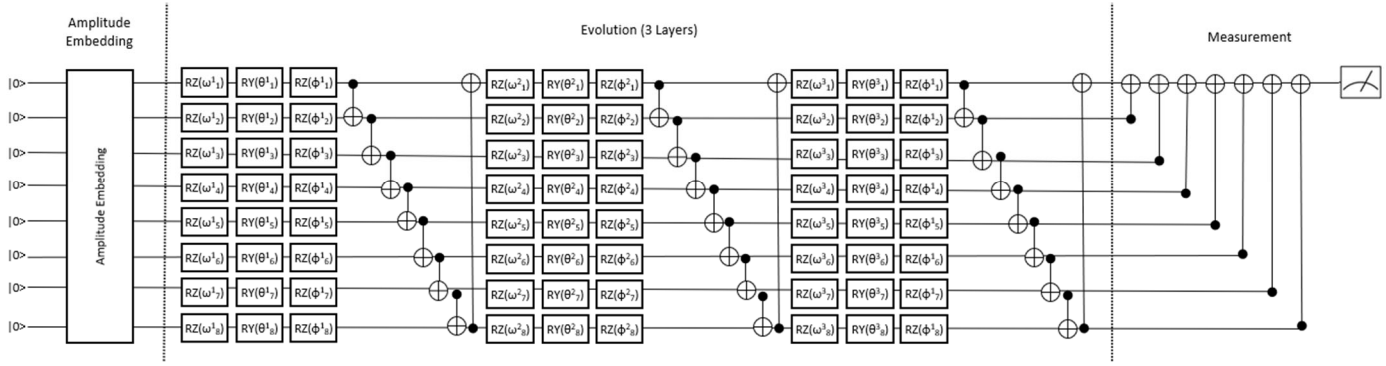
Supplementary Table S1. Smiles Character Set

"A": 1, "C": 2, "D": 3, "E": 4, "F": 5,"G": 6, "H": 7, "I": 8, "K": 9, "L": 10, "M": 11,"N": 12,"P": 13, "Q": 14, "R": 15, "S": 16, "T": 17, "V": 18, "W": 19,"Y": 20, "X": 21

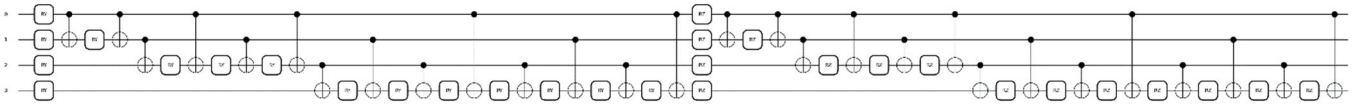
Supplementary Table S2. Protein Sequence Character Set



Supplementary Figure S1. Prediction module (VQR) with dense angle embedding.



Supplementary Figure S2. Prediction module (VQR) with amplitude embedding.



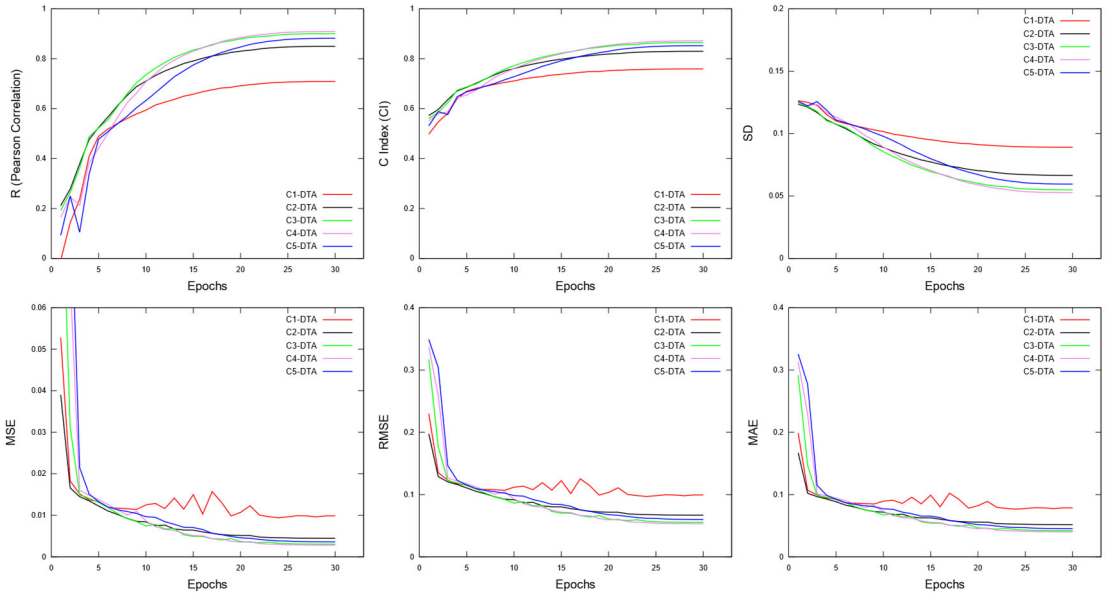
Supplementary Figure S3. Amplitude embedding with 4 qubits.

Hardware and software	Experimental environment
Operating System	Linux (Ubuntu) wp2 5.15.0-89-generic
CPU	GenuineIntel Common KVM processor (3599.996MHZ 4 Cores)
RAM	16 GB
Python version	Python 3.9.19
PyTorch version	PyTorch 2.2.2
PennyLane version	PennyLane 0.35.1

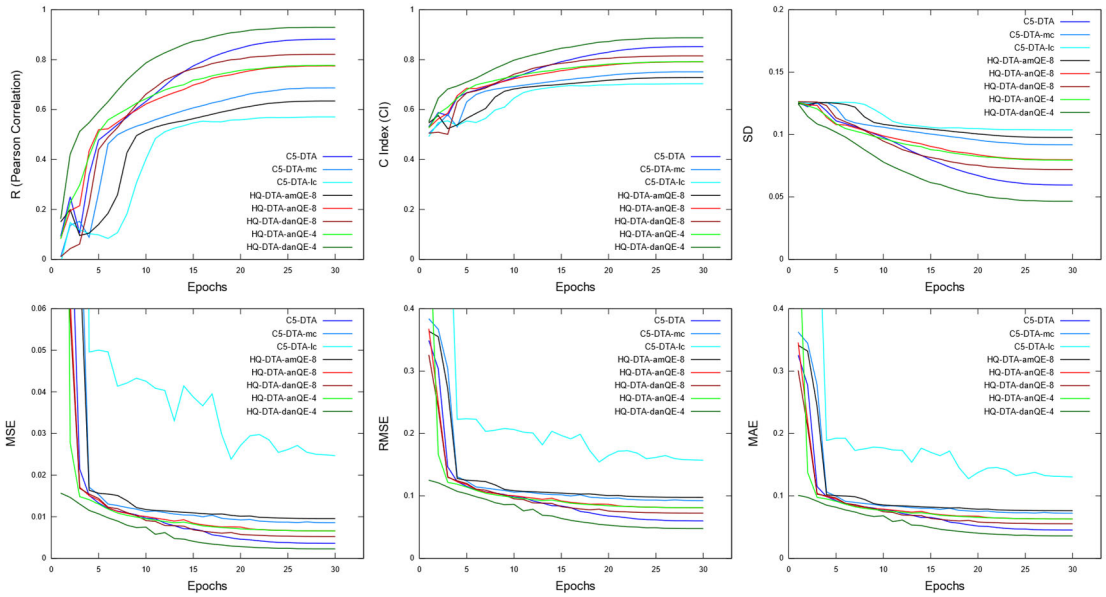
Supplementary Table S3. The experimental environment

	Type	Parameters	Values
		Optimizer	AdamW
		Learning rate	0.0001
		Batch size	256
		Epoch	30
		Loss function	MSE
		SMILES length	160
		Protein sequence length	1000
		Embedding dim	128
1D dilated CNN		Filter size	128
		Kernel size	3
		Stride	1
		Padding	[1, 2, 4, 8, 16]
		Dilated size	[1, 2, 4, 8, 16]
Regression Prediction	Classical	Linear layers	3
		Neurons	C5-DTA [256,512,256,1] C5-DTA-mc [256,128,64,1] C5-DTA-lc [256,16,8,1]
		dropout	0.2
	Quantum	Qubits	8/4
		Device	default.qubit

Supplementary Table S4. The parameters for all experiments



Supplementary Figure S4. Evaluation metrics of classical C1-DTA, C2-DTA, C3-DTA, C4-DTA and C5-DTA on training dataset.



Supplementary Figure S5. Evaluation metrics of classical (C5-DTA, C5-DTA-mc, C5-DTA-lc) and hybrid (HQ-DTA-amQE-8, HQ-DTA-anQE-8, HQ-DTA-danQE-8, HQ-DTA-anQE-4, HQ-DTA-danQE-4) models on training dataset.