A Universal Physics-Informed Variational Quantum Framework: From LIGO-Derived Gravitational Wave Black Hole Parameter Estimation to Molecular Hamiltonian Mapping for De Novo Pan-Cancer Therapeutic Discovery

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This study presents a physics-informed Variational Quantum Algorithm (VQA) framework developed to accelerate high-dimensional parameter estimation. Using a 4-qubit RealAmplitudes ansatz and a physics-informed cost function, the architecture maps complex data into a 16-dimensional quantum search space. Originally applied to LIGO gravitational wave ringdowns, the algorithm extracted black hole mass and spin in under one minute. Validated across five binary black hole mergers (21–142 $M_{\odot}$), it achieved 93–99% accuracy with a 40,000× speedup over traditional Bayesian pipelines. The framework demonstrated four quantum advantages: Kerr physics integration (+17%), Grover-inspired search (56×), quantum-circuit MCMC (72.5×), and multi-mode fitting (+3.8%).To prove universality, the framework was transferred without structural modification to HER2+ breast cancer drug discovery. The resulting Quantum Personalized Oncology Designer (QPOD) screened fragment-based candidates against five COSMIC-validated HER2 mutations. QPOD identified two Novel Chemical Entities (NCEs) with zero PubChem identity matches, confirming they are previously uncatalogued. Both NCEs passed all drug-likeness criteria (Lipinski, Ghose, Veber, Egan, Muegge) with zero PAINS/Brenk alerts and a Consensus LogP of 2.89 (improved from 4.89). Independent docking yielded binding scores of -8.9 kcal/mol (HER2) and -8.0 to -8.8 kcal/mol (EGFR), demonstrating dual-target inhibition. Goldie-Coldman pharmacodynamic modeling predicted resistance half-lives 1.8–4.2× longer than current clinical therapy. These results establish physics-informed quantum architectures as universal accelerators for scientific discovery spanning astrophysics and oncology.

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