Simulating Quantum-Coherence Dynamics in ALS Neuronal Ion Channels via Lindblad Master Equation: A Computational Biophysics Approach

Zahran, Zainab (School: Galal Official Language School)

The incurable nature of Amyotrophic Lateral Sclerosis (ALS) is compounded by a diagnostic lag, where symptoms emerge only after irreversible motor neuron attrition. Rather than viewing ALS solely through biochemical breakdown, this research explores quantum signaling disruptions preceding cellular decay. This work investigates the SOD1-G93A mutation by modeling quantum decoherence within neuronal ion channel selectivity filters using the Lindblad master equation. The methodology integrates four stages: (1) structural noise profiles were quantified from Protein Data Bank (PDB) data; (2) quantum simulations modeled coherence loss via a stochastic dipole-coupling framework; (3) results were translated into electrophysiological predictions of Distal Motor Latency (DML); and (4) a gradient boosting classifier validated biophysical marker separability across a synthetic 10,000-sample population. The model predicts SOD1-G93A accelerates decoherence by 300% (4.00×) versus wild-type conditions, causing ~30% coherence loss (?C). This disruption produces a predicted DML delay of 0.30–0.32 ms, aligning with borderline abnormal values in early-stage nerve conduction studies. The classifier achieved an AUC-ROC of 0.94, confirming quantum structural markers form statistically separable distributions between WT and ALS environments—validating feature design over clinical classification performance. To translate these findings, a diagnostic framework—the Quantum Decoherence Score (QDS)—was developed and validated across a 16+ variant SOD1 panel. Unlike biomarkers detecting downstream damage, the QDS provides a physics-layer signal upstream of cell death, establishing a computational framework for pre-symptomatic detection grounded in quantum biophysics.

Awards Won:
Third Award of $1,200