The Virtual Cell: Revolutionizing Personalized Cancer Treatment Through AI-Powered Simulation

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In vitro drug sensitivity testing is critical for identifying effective cancer treatments. However, due to the vast number of potential drug monotherapies and combination therapies, in vitro testing is hindered by inefficiencies in time, cost, and scalability. Moreover, solutions using in silico modeling have focused on pure AI-based methods, lacking extensibility outside their training data. To address these challenges, I developed The Virtual Cell, an AI-driven simulation model that predicts cellular drug response by integrating genomics, proteomics, and rate law-based biochemical simulation. The model employs a novel elementary reaction prediction algorithm to create an internal reaction network from literature-backed protein signaling pathways, modeling the intracellular biochemical interactions. The Virtual Cell is initialized with functional genomic data and quantitative proteomic data to run simulated drug sensitivity experiments measuring in silico viability. In vitro kinetic drug monotherapy experiments were conducted for Capivasertib, Alpelisib, Tamoxifen, and Fulvestrant across the MCF-7, T-47D, MDA-MB-231, and MDA-MB-468 breast cancer cell lines. The model's reaction parameters were calibrated with machine learning to align in silico predictions with in vitro viability. Once calibrated, The Virtual Cell was used to predict novel combination therapies, which are then tested in vitro for validation. The Virtual Cell has shown remarkable accuracy in simulating combination therapy, allowing for increased efficiency of identifying new synergistic combinations. Overall, The Virtual Cell has the potential to transform oncology by reducing reliance on costly in vitro testing, advancing personalized and precision treatment strategies, and improving patient outcomes.

Awards Won: