In silico Accelerated Drug Discovery and Development Utilizing Human Physiological Modeling and Simulation

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The research and development of new medicine are expensive and time-consuming: the entire process from discovery to distribution takes up to 12 years, costing as much as $2.5 billion USD. Human physiological modeling and simulations can be an alternative to accelerate the process and leverage high-performance computing, artificial intelligence, and petabytes of data collected over years of pharmaceutical research. This research developed a novel software application, PhySim, to aid pharmaceutical scientists in (1) analyzing pharmacokinetic and drug-likeness properties of new molecules; (2) performing visual simulations of certain heart performance indicators; (3) predicting the efficacy of new molecular entities based on comparisons to known molecules using Artificial Intelligence/Machine Learning/Deep Learning models; and (4) virtually screening the efficacy of thousands of molecules in batches. Due to the complexity of the human body, simulating even a single organ system requires significant time and resources. Therefore, this research project limits its scope to the human heart, as cardiovascular disease is the leading killer of men and women worldwide. PhySim allows researchers to extend and create full-scale physiological models and simulations to accelerate the discovery and development of new medications. PhySim can be deployed on the cloud, allowing global scholars to crowdsource and identify promising molecules from millions of known molecules. PhySim could allow the discovery of new pharmaceuticals that cost considerably less than existing treatments, along with cures for common diseases as well as rare diseases.

Awards Won:
Air Force Research Laboratory on behalf of the United States Air Force: Glass trophy and USAF medal for each recipient
Air Force Research Laboratory on behalf of the United States Air Force: First Award of $750 in each Regeneron ISEF Category, FOR 2023 ONLY: EBED WILL HAVE TWO
Patent and Trademark Office Society: Second Award of $500