An Intelligent Drug Discovery Engine for Personalized Medicine with Communication Dynamics

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Statement of the Problem: Recent advances in the biomedical sciences have resulted in innovative drug treatments. Yet making these treatments available to consumers remains a challenge. On average, it takes ten to fifteen years and 1.3 billion dollars to develop one new drug. The process involves a complex system of testing in which even qualified candidates have a failure rate of 80%. The main reason for this is that biological systems are complex. It is proposed that this complexity can be reduced by means of an intelligent engine designed for the drug discovery process. A quickened ability to provide new drug treatments to patients would have local and global impact. An intelligent drug discovery engine would be generalizable internationally.

A framework can be developed to study biological systems and improve the drug discovery process by using the novel theory of "communication dynamics". Current computational methodologies are based on physics-based modeling methods. This has great practical value for investigating particle structures and mechanisms in specific size scales, but has tradeoffs in theoretical perfection, physical accuracy, multi-scale integration, and computational scalability.

Communication dynamics proposes a "vector-frequency scheme" that combines space and frequency as one mathematical object. This model employs a uniformly applicable mathematical formula to describe physical realities at different scales. It provides modeling advantages in solving problems in heterogeneous biological systems with the possibility of whole system simulations.

Communication dynamics makes use of the least-action principle of information theory, which can aid in identifying the minimum necessary experimental and computational steps needed, and in defining the optimal routes for achieving better outcomes for drug-candidate screening. All resources relevant to drug discovery in the UAB system can be integrated into a dynamic research production system.

Desired Outcome: Make drug development practical by radically shortening development and testing time. The proposed platform has the potential to screen 20 million drug candidates in a few hours.

Plan of Work: The first step will be to create comprehensive knowledge maps of biological networks relevant to drug-biomarker interactions by integrating machine learning approaches and big data technology. The primary focus of modern biomedical science is to understand molecular level mechanisms and their pathological implications. However, the volume of data produced outstrips current analytical tools. Artificial intelligence approaches are increasingly recognized for their ability to accomplish this task. Our research approach will be to construct comprehensive pathway knowledge maps based on public databases, using the entities (nodes) in databases as keys to perform data mining from research journals and patents. Next, we will develop a fully automated AI system to continually expand and update the maps. Once the map system is generated, probabilistic models can be developed and applied to build predictive models for drug discovery. With this computational resource, it will be easier to understand disease models and predict potential drug candidates for potential drug targets.

The second step will be to develop a cloud-based virtual screening platform for drug candidate screening using conventional computational physics and deep learning models. Machine learning techniques will be used within the framework of computational molecular design to increase accuracy. It can also be used independently as black-box models, trained by experimental

data, to increase accuracy and decrease computational cost. Figure 2 displays a deep learning-based model of potential predictive power that has been created with training sets from Quantum Mechanics, Physical Chemistry, Biophysics, and Physiology. We propose to develop similar models to more accurately and efficiently predict desired molecular properties and to design novel functional drug molecules.

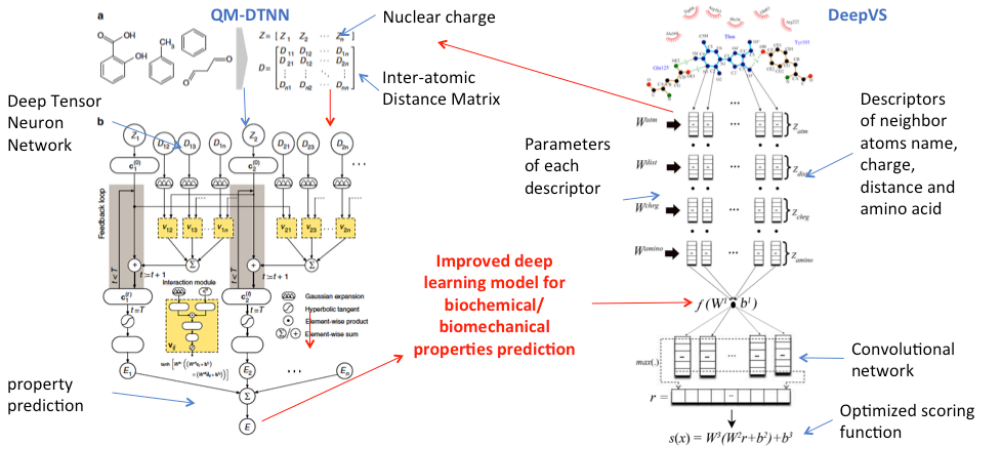

Figure 2. Deep learning algorithm in molecular property and binding prediction

The structure of the proposed platform is presented below in figure 3.

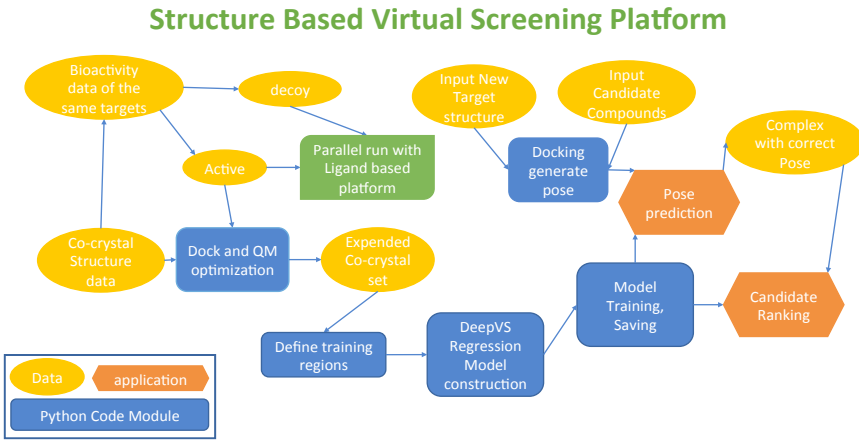

Figure 3. Structure based virtual screening platform for drug discovery

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