V-BIND: Deep Geometric Transformers for SARS-CoV-2 Treatment Design

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This research presents a novel machine-learning approach for the identification of potential treatments against SARS-CoV-2, the causative pathogen of COVID-19. Despite the existence of effective vaccines, there is no widely accepted COVID-19 drug therapy. The proposed algorithm, called V-BIND, designs drug therapies in the form of artificial miniproteins that bind to the viral spike protein, thereby disabling SARS-CoV-2's attack method and preventing infection. A completely in-silico pipeline, V-BIND is the first fully AI-based method for the rapid development and prototyping of these COVID-19 miniprotein drugs. V-BIND consists of two parts: a novel deep neural network (named Geometric Transformer), inspired by advances from natural language processing, and an associated optimization module, used to design candidate miniproteins. Because it employs innovative techniques proposed herein (i.e., Manifold Attention), V-BIND designs potential COVID-19 drugs effectively and efficiently. Not only do V-BIND-created proteins bind potently to SARS-CoV-2, V-BIND designs them 10,000x faster than traditional approaches. This speedup allows for a significantly larger candidate drug pool, accelerating COVID-19 treatment development. V-BIND also operates de novo, meaning it is not constrained to proteins that already exist in nature. It therefore taps into the potential of trillions of unexplored proteins, some of which could contain the key to treating COVID-19. Crucially, V-BIND is universal: without any retraining, it is applicable to treatment design for any protein spike virus (e.g. HIV, influenza, and COVID-19 variants). V-BIND thus represents a powerful and versatile deep-learning tool in combating viral infection, potentially saving lives.

Awards Won:

Second Award of $2,000