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Developing a modified version of Generative Adversarial Network to predict the potential anti-viral drug of COVID-19

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Abstract

The advancements of computer science and its related fields are making our tasks easier in almost every scientific and non-scientific field. The use of machine learning in the field of drug discovery and development is accelerating so fast and helping us to discover anti-viral drugs for devastating viruses like coronavirus. The author will discuss using a deep reinforcement learning model 'ORGAN' which is a modified version of Generative Adversarial Network for predicting the potential anti-viral of coronavirus. The author used the deep reinforcement learning model (ORGAN) to generate potential candidates' drugs, with a of 0.2 and epochs of 240 and a sample set of 6400, 10 good sample SMILES were generated and the Solubility or LogP of these samples is 0.7098. Then using the coronavirus as a target, all the good samples of SMILES were bounded and the drug with the highest binding affinity (Most negative value) is C18H15ClN4O2 also known as Olutasidenib which can be the potential anti-viral drug of coronavirus.

Biography

Asif is a senior high school student at Notre Dame College, Dhaka who will graduate in November 2021. He is a machine learning enthusiast from an early age and attending MIT Beaver Summer Works in 2021 on Quantum Computing and machine learning. He is the youngest research work publisher in the field of computer science in Bangladesh in 2020. He is also the software engineer and editor of Young Scientists Journal which is the world's first peer-reviewed research journal for youths.

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