REINFORCEMENT LEARNING WITH REAL-TIME DOCKING OF 3D STRUCTURES FOR SARS-COV-2

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PATENT STATUS

Country	Type	Number	Dated	Case
Patent Cooperation Treaty	Published Application	WO2023/077124	05/04/2023	2022-030

BRIEF DESCRIPTION

The inventors propose a novel framework generating new molecules that potentially inhibit the Mpro protein, the main protease of SARS-COV-2. The technology combines deep reinforcement learning (RL) with real-time molecular docking on the 3d structure of Mpro using AutoDock Vina, an open-source program for doing molecular docking. A second second docking software, Glide, was used to validate the generated molecules. The AutoDock and Glide docking softwares showed consensus on 41 molecules as potential potent Mpro inhibitors that were sufficiently easy to synthesize.

The inventors show that this method samples the drug chemical space efficiently, covering a much broader space than molecules submitted to the COVID moonshot project, and the molecules have the correct shape and non-bonded interactions to fit into the binding pocket. Moreover, this approach only relies on the structure of the target protein, which means it can be easily adapted for future development of other inhibitors.

SUGGESTED USES

This technology can be utilized for pharmaceuticals.

ADVANTAGES

COVID-19, caused by SARS-COV-2, continues to be a global crisis. The development of an antivirus drug targeting the main protease of SARS-COV-2 (Mpro) is an important practice in fighting the disease.

In order to find the inhibitor with existing high-throughput approaches, researchers must search a massive chemical space for potent drug molecules that might interact strongly with the target protein. This makes it extremely difficult to identify promising search directions.

The inventors have presented a method enlisting deep learning methods that make exploring chemical spaces with specific biological relevance possible. Moreover, this technology designs molecules that more specifically inhibit a protein by taking advantage of the rapid acquisition of 3d protein structures related to SARS-COV-2.

RELATED MATERIALS

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