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ASIA EDITION

Korea identifies repurposed drugs for COVID-19 treatment via virtual screening assays

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Identification of seven potential drugs out of the 38 drugs initially selected



A joint research group from Korea Advanced Institute of Science and Technology (KAIST) and Institut Pasteur Korea has identified repurposed drugs for COVID-19 treatment through virtual screening and cell-based assays.

The research team suggested the strategy for virtual screening with greatly reduced false positives by incorporating pre-docking filtering based on shape similarity and post-docking filtering based on interaction similarity.

This strategy will help develop therapeutic medications for COVID-19 and other antiviral diseases more rapidly. This study was reported at the Proceedings of the National Academy of Sciences of the United States of America (PNAS).

Researchers screened 6,218 drugs from a collection of FDA-approved drugs or those under clinical trial and identified 38 potential repurposed drugs for COVID-19 with this strategy.

Among them, seven compounds inhibited SARS-CoV-2 replication in Vero cells. Three of these drugs, emodin, omipalisib, and tipifarnib, showed anti-SARS-CoV-2 activity in human lung cells, Calu-3.

The experimental results showed that the virtual screening strategy reached a high hit rate of 18.4%, leading to the identification of seven potential drugs out of the 38 drugs initially selected.

“We plan to conduct further preclinical trials for optimizing drug concentrations as one of the three candidates didn’t resolve the toxicity issues in preclinical trials,” said Woo Dae Jang, one of the researchers from KAIST.