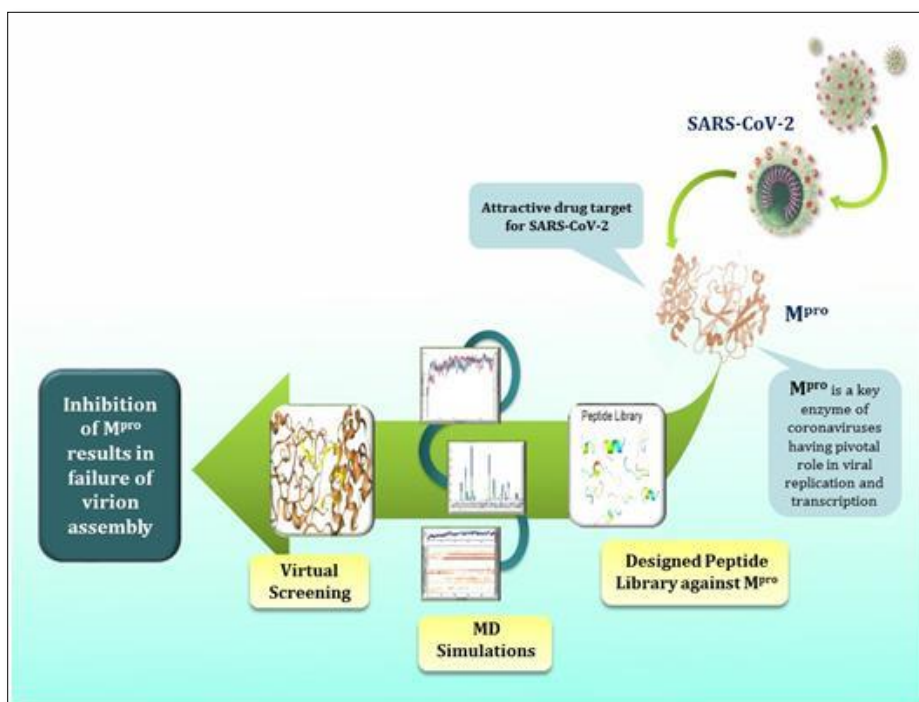


## Machine learning helps identify molecules with therapeutic potential against COVID

Dr. Shailza Singh's team at the Department of Biotechnology's National Centre for Cell Science (DBT-NCCS), Pune, have been involved in research aimed at identifying targets that could be used to design therapeutic peptides against many variants of the virus. For this purpose, they used machine learning algorithms to select specific viral sequences from among the diverse sequences reported from different parts of the world. They used a novel technique of combinatorial machine learning algorithm with an optimization algorithm, to design a novel set of peptides, from among which they identified peptides that showed a strong binding affinity towards  $M^{\text{pro}}$  using computational studies.



Machine learning helps identify potential therapeutic molecules that target the M<sup>pro</sup> protein of the COVID-causing virus

The molecule under examination as a target is " $M^{\text{pro}}$ ", the main protease enzyme of the COVID-causing virus. It is an attractive drug target since it is a key enzyme that plays a pivotal role in mediating viral multiplication. Moreover, humans do not have any molecule similar to this protein, which means that any therapeutic agent that blocks this protein would ideally not affect humans adversely.

These peptides could potentially serve to block the functionality of M<sup>pro</sup>, which could result in regulating the replication of the viral RNA, and may thus help in controlling the virus. Further experimental validation could help develop effective therapeutics in the future. These peptides show promise for safeguarding against viral variants that might arise in future as well, since the machine learning strategy used here was based on studying all the mutants available till date, which therefore takes into consideration the evolvability of the virus. These promising research outcomes have been accepted for publication in the international journal, *BBA Molecular Basis of Disease*.

The urgent need to tackle the current COVID-19 pandemic has fueled a surge in research aimed at rapid development of vaccines and therapeutics against this novel disease. Rising to this unprecedented challenge, the scientific community is using various tools and approaches to address this issue. In addition to the conventional approaches, modern tools in the researchers' arsenal that have been popular in the current war on COVID include computational biology, artificial intelligence and machine learning. These tools are being used to help identify viral components that could serve as targets for the development of vaccines and therapeutics.

**Link:** <https://www.sciencedirect.com/science/article/pii/S0925443920303264>

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