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Research article

In-silico studies for design and development of inhibitor against Covid-19

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Abstract

Aim: The Covid-19 pandemic as declared by WHO, reported its first case in Wuhan, Hunei province, China. The infections have now been widespread and as of 30th March 2020, 6,93,224 infection cases and 33,106 deaths have been reported worldwide. This is an international concern related to public health. Several research studies are being carried on around the world to amid the crises. Various treatment and prevention hypothesis regarding vaccine development, repurposing of drugs along with development of new chemical entities are under investigation. Covid-19 is a virus from the coronavirus family of viruses of beta genus. It has similarity with the SARS-CoV which was reported earlier. We plan to propose a scaffold for designing peptide derived specific inhibitor against Covid-19.**Method:** Our strategy involves designing a peptide inhibitor that will interact with RBM of the SARS-CoV-2 and inhibit its entry inside the cell. We utilised online peptide designing platform called rosetta, Autodock Vena a computer aided drug designing software and Schrodinger's Drug Discovery Suite **Result:** We propose a peptide based on the sequence of human ACE2 which interacts strongly with RBM of the SARS-CoV-2. Interested readers can utilise the sequence for further modification of the peptide sequence to convert it into a peptidomimetic.**Conclusion:** Receptor binding motif of SARS-CoV-2 has stronger affinity towards the derived peptide so as to terminate the infection cascade. The proposed peptide can surely be used as scaffold for designing more active agents.