Centre for High Performance Computing 2020 National Conference



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Novel Peptides as Potent Inhibitors of SARS-CoV-2 that work by Two distinct mechanisms: Molecular Docking and Dynamics Approach

Wednesday, 2 December 2020 12:15 (30 minutes)

The global outbreak of SARS-CoV-2 has caused high mortality rate and therefore requires an urgent identification of drugs and other interventions to overcome the disease. Scientist around the world are looking for new drugs or molecules to target the spike protein to prevent Covid-19 infection. We present molecular docking analysis of eight synthetic peptides against SARS-CoV-2 spike protein. Some interacted with the ACE2 while others interacted at the interface of the ACE2 and S protein. These peptides are potential molecules in preventing Covid-19 establishment and can be developed to new drugs.

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