Towards development of new drug against Novel COVID-19.

Background and Motivation:

Novel coronavirus (nCoV) first emerged in population in December 2019 and has rapidly gained foothold across the world resulting in WHO declaring it as pandemic. Spreading primarily through human contact, even asymptomatic transfer has been found to occur. As there is currently no known cure, urgent studies are needed in order to push forward for development of new drugs. It is evident that nCoV initially binds to the ACE2 receptor of human cells. Therefore, the antagonists to ACE II receptors would be used as therapeutic measures for Novel COVID-19. Recently, about 77 drugs were identified against viral spike protein of Novel COVID-19. To that end, we propose to use state-of-the-art bioinformatics approaches to identify lead compounds or most promising drugs candidates, which can be used safely against nCoV. The most promising candidates will be screened based on docking study against several unique protein targets available for Novel COVID-19. After screening, few candidates will be tested for investigation of drug like properties and toxicity etc. Furthermore, validation of activity of these drugs will be tested against pseudo viral strain of nCoV.

Objectives

- Selection of an appropriate inhibitor based on in-silico drug binding affinity assay using computational tools for different proteins required for propagation of COVID-19
- To investigate the drug like properties and toxicity evaluation of selected inhibitors.
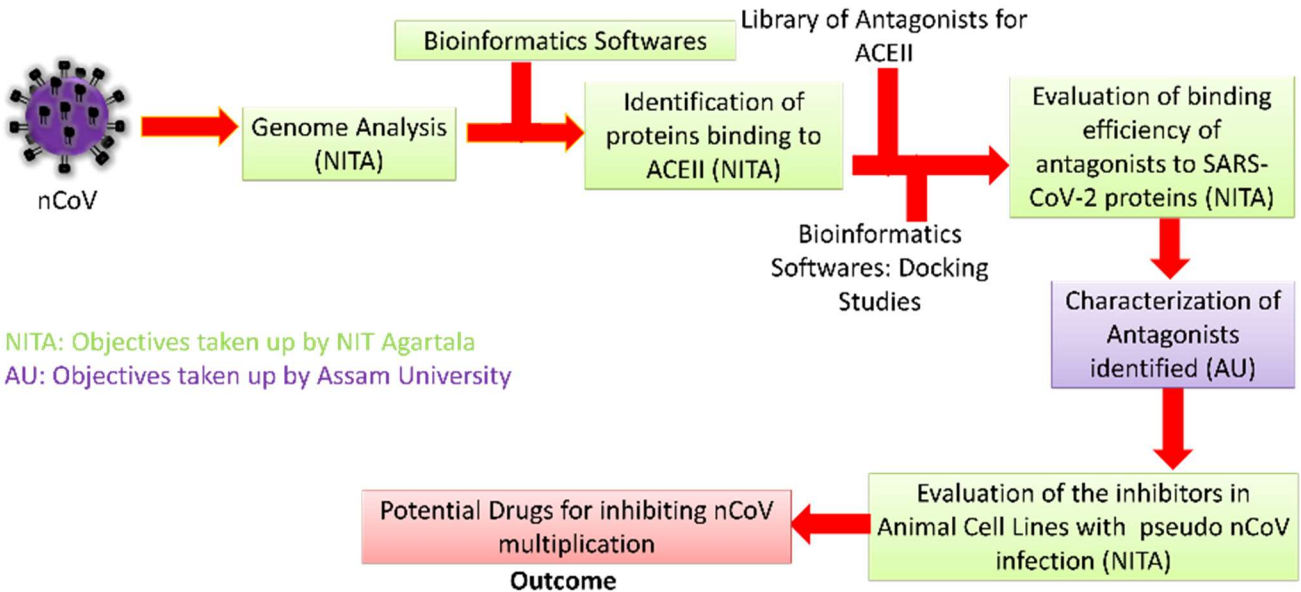- To study the activity of selected inhibitors against pseudo viral strain of nCoV.

Expected Outcome

A lot of research has been conducted and is still going on in various parts of the world on design of drug against **Novel COVID-19**. However in our country we are still in our initial stages in the field of drug development. We still lack an opportunity where the research on these aspects is being done with a holistic approach. We propose to develop **new drug molecules, which** would be the major outcome of this research work and would be much safe.

Expected Timeline: Work has been started and expected to be completed within 2 years

Remarks: Funding required Rs. 80.0 Lakh

Flow diagram

Genome Analysis (NITA) → Bioinformatics Softwares → Identification of proteins binding to ACEII (NITA) → Library of Antagonists for ACEII / Bioinformatics Softwares: Docking Studies → Evaluation of binding efficiency of antagonists to SARS-CoV-2 proteins (NITA) → Characterization of Antagonists identified (AU) → Evaluation of the inhibitors in Animal Cell Lines with pseudo nCoV infection (NITA) → Potential Drugs for inhibiting nCoV multiplication (Outcome)

NITA: Objectives taken up by NIT Agartala
AU: Objectives taken up by Assam University

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