ON ELABORATE USE OF BIOINFORMATICS AND RECENT TECHNOLOGICAL ADVANCEMENTS IN COVID 19 RESEARCH

Dr.Ved Patki Assistant Professor Department of Zoology Indira Mahavidyalaya, Kalamb Dist. Yavatmal

Abstract -

In the current study, the main emphasis has been placed on utilising numerous tools and methodologies that were crucial to advancing COVID - 19 research quickly. This study also offers a number of other uses of approaches that are highly significant in light of the field's upcoming difficulties.

Keywords : Bioinformatics, COVID-19, VACCINE, Corona Virus.

Introduction:

Bioinformatics becomes a critical interdisciplinary area in the biomedical sciences following the sequencing of insulin peptides in the 1950s (Sanger, 1945,53). The development of larger biological databases and its consequences for a variety of scientific fields, including comparative genomics, functional genomics, molecular epidemiology, drug discovery, and molecular diagnosis, are the focus of today's research. Opportunities for more accurate and precise analysis of increasing amounts of biological data are presented by bioinformatics. Recent technological advances in computer coding and molecular biology may have helped computational biology, which is supported by exacting mathematical and statistical modelling, to emerge. Computational biology demonstrates its significance in the current crisis through a wide range of uses.

The Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) that results from zoonotic origin in Wuhan, China, and eventually becomes a global pandemic is the cause of the coronavirus disease 2019 (COVID-19). The newly discovered coronavirus, commonly known as SARS-CoV-2, has a single-stranded, positive-sense RNA genome with roughly 29.9 kilobase pairs, encoding the structural proteins spike (S), envelope (E), membrane (M), and nucleocapsid (N), in addition to additional non-structural proteins (Wu et. Al, 2020). Following the passage of the viral genome into the cytoplasm, the viral life cycle began by attaching its S protein to ACE2 (Angiotensin Converting Enzyme 2) receptors. For the creation of vaccines and drugs, extensive research has been done (De Wit et al, 2016).

However, full immunisation and the assessment of therapeutic efficacy continue to be unresolved problems that computational and structural biology can address. Computational biology, propelled by advances in artificial intelligence (AI) with machine learning and Data sciences, is further changing the fields of biology, medicine, and public health. The real-time dynamics of the COVID-19 pandemic and vaccine design both make extensive use of computational biology technologies. The availability of genetic data is used as a source of uncooked data for developing vaccines and medications.

Vaccine making:

After Edward Jenner used a vaccination against smallpox for the first time in 1796, vaccines became one of the most useful medical advancements. More than 70 vaccinations have

been created and licenced, and they are effective against about 30 microorganisms, according to recent research. Vaccines are regarded as the simplest and least expensive method of prevention against life-threatening epidemics, offering the most economical means of saving lives in such situations. Vaccines are attenuated antigen fragments that also contain additional components to maintain the vaccine's safety and efficacy. Each ingredient is put through testing throughout the production process because the primary aim of each vaccine component is to serve a specific purpose of developing immunity.

In reverse vaccineology, machine learning and artificial intelligence have been extensively used. The SARS-CoV-2 proteome's immunogenic epitopes have been identified using software like NEC Immune (Malone et al., 2020), the recently created neural network-based ArdImmune Rank model [10], and the eXtreme Gradient Boosting (XGBoost)-based Vaxign-ML model (Mozzocco et al, 2021). These methods could be very helpful in creating multiepitope chimeric vaccines with theoretically increased efficacy. COVID Nucleic Acid , Whole Virus, and Protein Subunit fall into four main groups.

The genetic material from the COVID-19 virus is modified to become a viral vector in the vector vaccine type of the vaccine, and when these viral vectors enter the body, they transfer the genetic material of the COVID-19 virus, which will be the source of instructions to make copies of the S protein. The immune system begins to respond by producing antibodies and protective white blood cells when S proteins develop and are displayed on the cell surfaces. The antibodies will once more combat the virus if you subsequently contract it. The vector COVID-19 vaccine was created by AstraZeneca and the University of Oxford in conjunction with the Janssen/Johnson & Johnson COVID-19 vaccine.

The components of the virus are employed in the Protein Subunit Vaccine kind of vaccine to stimulate the host immune system, which contains attenuated S proteins that will educate the cells for vaccination. The immune system produces antibodies and protective white blood cells once it has identified the S proteins. The COVID-19 vaccine's protein subunit and U.S. COVAXIN are both called Novavax.

The locally produced COVID-19 vaccine was created by Bharat Biotech in cooperation with the National Institute of Virology of the Indian Council of Medical Research (ICMR) (NIV). Bharat Biotech is the company that developed and produced this vaccine. This vaccine was created using a platform technology derived from Whole-Virion Inactivated Vero Cells that contains attenuated dead virus that cannot infect humans but can train the immune system to activate a defence immune system against virus. This vaccine was created and dispersed in India by Serum Institute of India under the brand name Covishield.

Covishield (COVID-19 Vaccine) is distributed throughout India for COVAXIN vaccination after the Phase II/III, Observer-Blind, Randomized, Controlled Study to Determine the Safety and Immunogenicity of Covishield (COVID-19 Vaccine) was jointly conducted by the Serum Institute of India and Indian Council of Medical Research. A total of 188CR doses have been administered in India to date, of which 85.1CR Indian citizens have received all recommended dosages.

Making of Drug:

The largest problem during this epidemic was discovering a new, effective antiviral medication. Molecular docking screening and molecular dynamics simulations have recently been widely employed approaches in computational modelling to find drugs that target SARS-CoV-2 proteins. The compounds that bind the SARS-CoV-2 receptor-binding domain have been identified in some published studies, including the terpenes NPACT01552, NPACT01557, and NPACT00631 [13], the Mpro inhibitors tinosponone(Krupanidhi et al, 2020), ChEMBL275592, montelukast, ChEMBL288347 (Abu-saleh et al., 2020), quercetin-3-O-rhamnoside (Cherrak et al, 2020), the biflavone (RBD). Inhibitors of TMPRSS2, SARS-CoV-2 S, Mpro, and RdRp could be made from plant secondary metabolites such as flavonoid glycosides, biflavonoids, ellagitannins, and anthocyanidins, according to the study.

While the study found six possible Mpro inhibitors from over 2000 natural chemicals and used molecular docking with machine learning to speed up the screening process (Xu et al, 2020). During the pandemic, candidates for drug repurposing were identified using the commonly used computational approaches based on network-based or expression-based algorithms and docking simulations (Wang and Guan, 2021).

The use of computational techniques, such as AI platforms, may make it possible to screen enormous amounts of data more effectively, and in vitro validation will further boost platform accuracy. a deep neural network (DNN) built by Ke et al. to explore known 3CLpro inhibitors or previously found antiviral medicines against the SARS-CoV, influenza virus, and HIV.These predicted medications are tested in vitro using the feline infectious peritonitis (FIP) virus, a closely related feline coronavirus, and then redesigned by an AI system for future predictions (Ke et al., 2020). AI can be used to evaluate the effectiveness of various drug combinations and their consequences. These are just a few studies that have been reviewed; there are many others that are being conducted to develop COVID-19 medications, and the results of these studies may one day help to stop the present outbreak.

Future of these tools -

The current COVID-19 epidemic is also being researched, predicted, and checked using machine learning techniques. The confirmed cases, recovered cases, and deaths in the affected countries were studied using a variety of algorithms, including long short-term memory (LSTM) networks (Marzouk et al., 2021), Grey Wolf Optimizer (GWO)-LSTM hybrid models, autoregressive integrated moving average (ARIMA) (Arunkumaret al., 2021), XGboost, support vector regression (SVR) (Salgotra et al, 2020), and genetic programming. These models can be used to forecast COVID-19 transmission and may help to generate statistical baseline information for use in developing policies to stop further outbreaks.

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