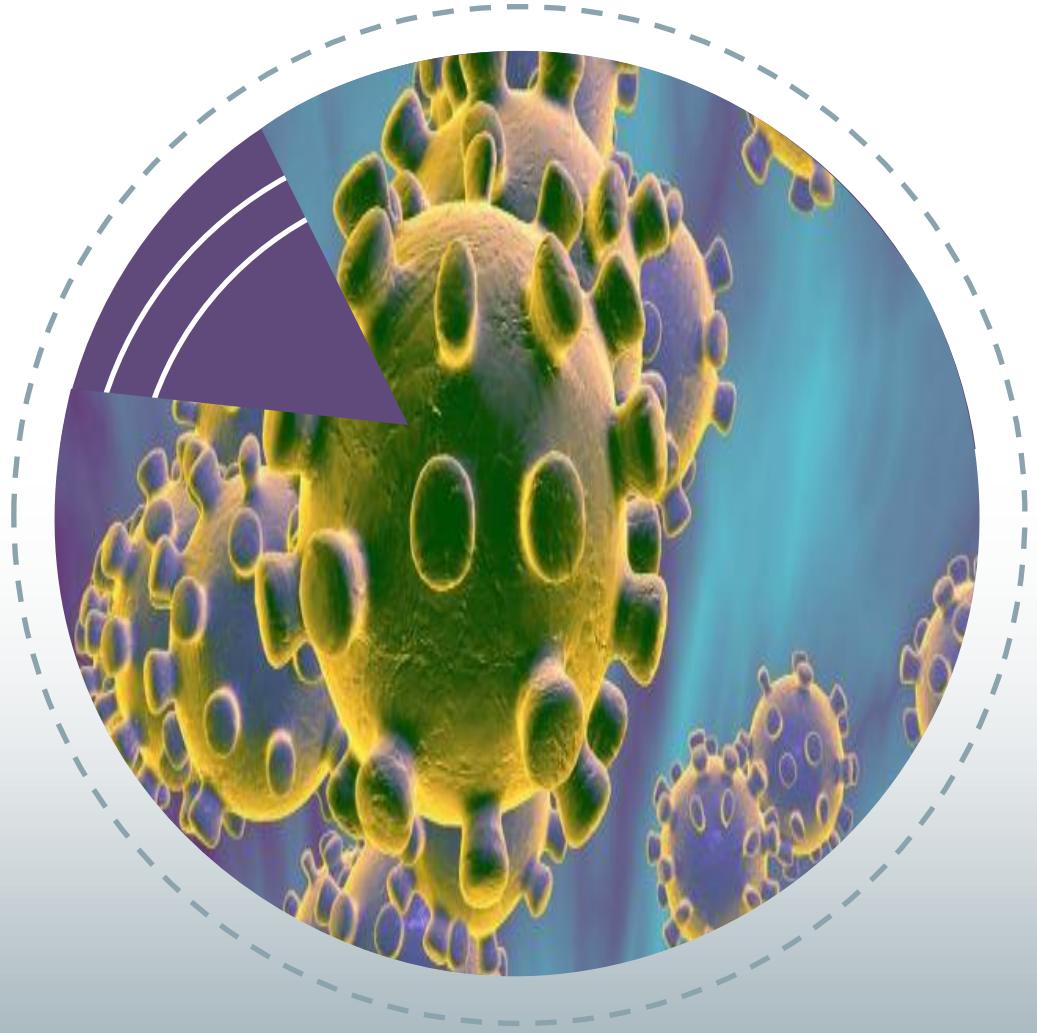
Ingenious e-Brain

Nurturing Innovations - Fostering Business



In-silico/Machine Learning/AI based prospects can Deal with Coronavirus Pandemic

Artificial Intelligence/Machine Learning Helps in Tackling COVID-19

OVERVIEW

- Advances and developments in algorithmic science, artificial intelligence, computing models and machine learning have made the process of drug discovery, development and commercialization easier and faster than conventional pharmaceutical processes.
- Before the introduction of these computational models, drug development process took about 10 years and a huge amount of money and still had a low success rate of approval from FDA. These tools could increase the success rate of drug discovery in the pharmaceutical industry, while considerably reducing costs.
- In pharmaceutical industry, these tools can help in extracting insights from huge experimental data, databases of structures, pursuing lead optimization, predicting binding of molecules to proteins and toxicity with unparalleled precision and accuracy

APPLICATIONS

1. Improved Prediction
2. Drug discovery
3. Reducing time and streamline the process
4. Improve diagnostics

LinearFold

Recently release a tool that significantly mitigates COVID-19 prediction time from 55 minutes to 27 seconds

inferVISION

inferVISION, AI based software for quick diagnosis of disease. It can identify typical signs or partial signs of COVID-19 in suspected patients by looking out for signs of pneumonia

Baricitinib

Researchers based on Benevolent AI algorithm, were able to identify Baricitinib (used to treat Rheumatoid Arthritis) drug having high binding affinity to enzyme (AAK1) to reduce both the viral entry and the inflammation in patient population with 2019-nCoV acute respiratory disease

Alphafold System

Deepmind's new Alphafold system offers protein structure prediction associated with COVID-19. They hope to contribute to the scientific community's interrogation of how the virus functions, and serve as a hypothesis generation platform for future experimental work in developing therapeutics

Insilico Medicine

Insilico Medicine, based on its AI platform was able to filter out around hundreds of molecules for synthesis and tests. It's AI uses generative adversarial networks GANs to filter the molecule designs and prefers those that score highly for "drug-like" properties and for being chemically active1

Methodology & Approach

Technology Understanding

Assessment of different in silico/AI approaches being explored in the domain

Technology Details

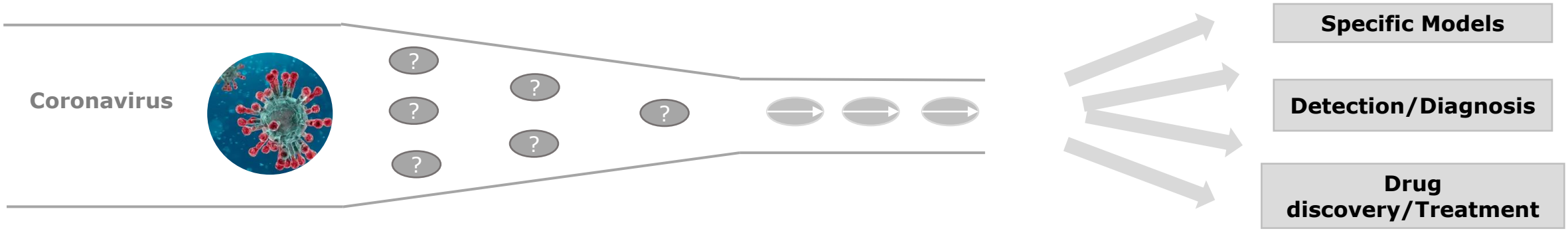
Understanding of the key features and application areas based on existing knowledge database

Insight Validation and Report Generation

Understanding the input parameters acting as a training data for various in-silico models in the domain

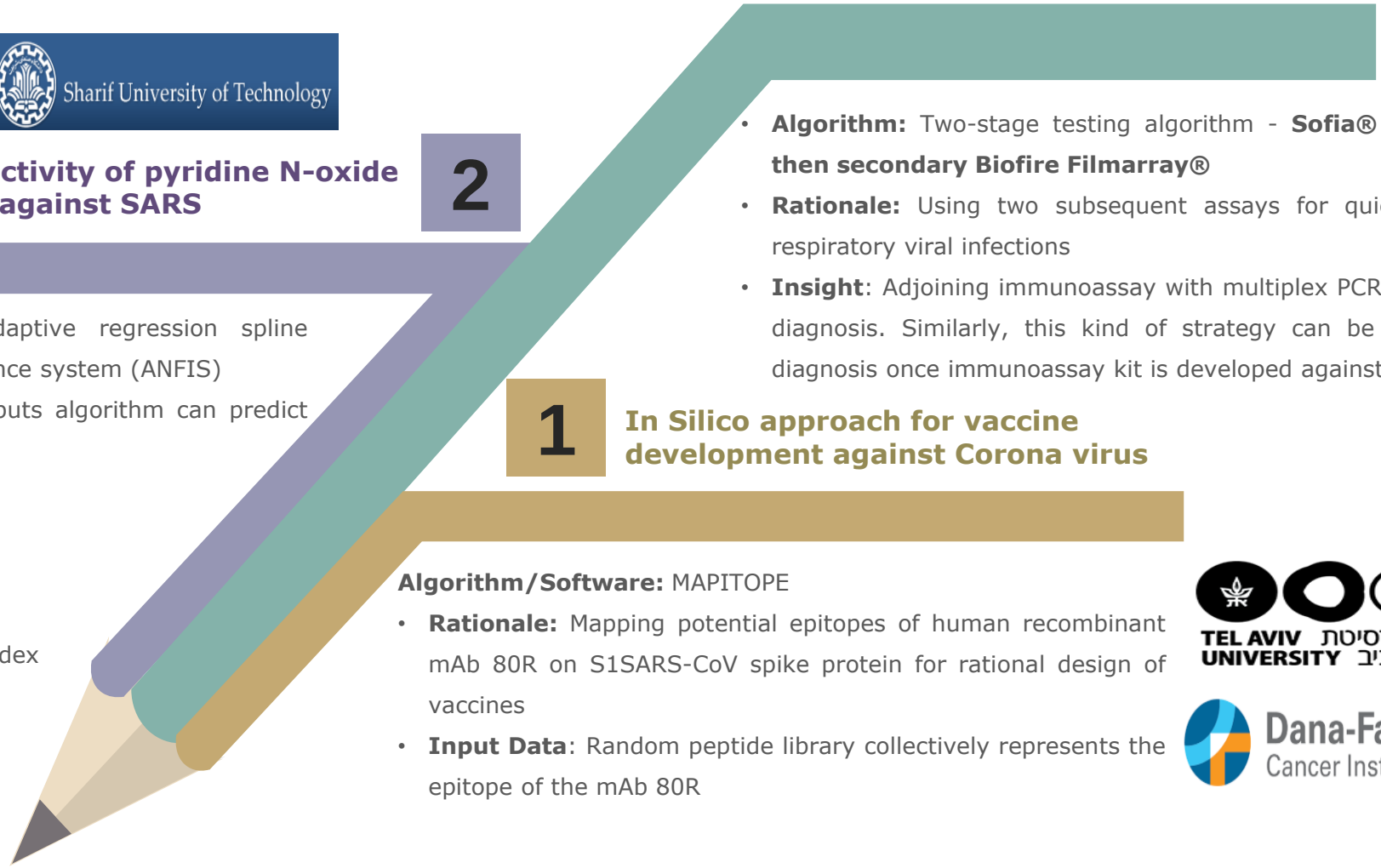
Identification of key parameters/indicators

Understanding the requirement → **Technology identification** → **Selection** → **Assessment** → **Focused areas**



IEBS having access to more than 40,000 literature covering various aspects related to work on detection/diagnosis, relationship between key parameters and working of viruses responsible for respiratory diseases, therapeutics/drug discovery and so on. Such existing database can help in deriving relationships between genes, diseases, d and biological pathways to identify the gaps and fulfill current requirement of researchers across the domain

Exemplary approaches employed by academic players



3 Diagnosis of respiratory viral infections

Tufts Medical Center

- **Algorithm:** Two-stage testing algorithm - **Sofia® immunoassay then secondary Biofire Filmarray®**
- **Rationale:** Using two subsequent assays for quick diagnosis of respiratory viral infections
- **Insight**: Adjoining immunoassay with multiplex PCR assists in quick diagnosis. Similarly, this kind of strategy can be used for quick diagnosis once immunoassay kit is developed against SARS-CoV

2 Inhibitory activity of pyridine N-oxide derivatives against SARS

Sharif University of Technology

- **Algorithm/Software**: Multivariate adaptive regression spline (MARS) and Adaptive neuro-fuzzy inference system (ANFIS)
- **Rationale:** By assessing the critical inputs algorithm can predict the activity of drug
- **Input Data:**
  - ❑ Solvation connectivity index
  - ❑ Length to breadth ratio
  - ❑ Relative negative charge
  - ❑ Harmonic oscillator of aromatic index
  - ❑ Average molecular weight
  - ❑ Total path count

1 In Silico approach for vaccine development against Corona virus

Algorithm/Software: MAPITOPE

- **Rationale:** Mapping potential epitopes of human recombinant mAb 80R on S1SARS-CoV spike protein for rational design of vaccines
- **Input Data**: Random peptide library collectively represents the epitope of the mAb 80R

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