**What are we doing?**

* We are taking a target biomolecule and predicting suitable inhibitor candidates through a structural-based manner. When enough data is given, ML can leverage the info to find patterns within the data to help us decide which compound is the most suitable.
* Virtual Screening: Computationally targeting a specific biomolecule within a cell to inhibit its growth and/or activation. Works well when we are given access to computationally and experimentally determined protein structures.
* Genome based vaccine design approach called “reverse vaccinology”.
* Usually we use rule-based filtering models.
  + But ML can create models that learn and generalize the patterns within the available data and make inferences from previously unseen data.
  + With DL, we can include automatic feature extraction from raw data itself. Moreover, DL’s feature extraction provides superior performance compared to general ML.
* GCNNs’ are a favorite

**What to target?**

* The neutralizing antibodies that block viral entry by targeting the viral spike protein.
* Targeting the enzymes that are essential for SARS – CoV – 2 replication.
  + RNA dependent RNA polymerase and protease

**Challenges**

**Resources**

* CoronaDB AI
* https://www.frontiersin.org/articles/10.3389/frai.2020.00065/full

**Antiviral Names**

* interferon alpha
* lopinavir/ritonavir
* chloroquine phosphate
* ribavirin
* arbidol

**Title: Comparing ML and DL algorithms for Drug Discovery for Covid-19**

**Comparing their results on a standardized set of compounds**

**Langya Hanipa (Covid-19 sub-variant) Virus**