EUYSRA Research Project Resources

# Project Vision:

These are a few ideas that we can build from, and the research topic does not necessarily have to be solely on SARS-CoV-2. It could also be on the drug, the ACE-2 receptor or any COVID-related research areas. To make this chemistry related, there should be plan for some lab-based practical work, complimentary to the computational part of the project.

## Computational part:

Building a computational model of the receptor-binding activities of SARS-CoV-2 to the ACE-2 receptor. Making an educational video for this procedure.

## Synthetic Part:

Synthesis of COVID-related drugs or their analogue and finding an optimised synthetic route?

# SARS-CoV-2 and Coronavirus Disease 2019: What We Know So Far:

* SARS-CoV-2 and Coronavirus Disease 2019: What We Know So Far

https://www.mdpi.com/2076-0817/9/3/231/htm?fbclid=IwAR23jVKF4Ss0rXAGDsvUHz5yJld54ljB1H0LS8O0fsNMitAhuHmowPEftMY

Diagram

Description automatically generated

# Possible research directions:

* All current COVID-19 Research Topics:

https://covid19-hpc-consortium.org

https://covid19-hpc-consortium.org/projects/5ed56e51a21132007ebf57bf

## Computational:

* Python: https://towardsdatascience.com/exploring-covid-19-research-publications-407f8c2aa842
* Computational structure-based drug design: Identifying antivirals from natural products targeting SARS-CoV-2:
* https://covid19-hpc-consortium.org/projects/5f57ef263a7a0a0084807f9e
* The Analysis of Binding SARS-CoV-2 to Various Substrates:
* https://covid19-hpc-consortium.org/projects/5f57ee873b6653007d01446e
* SARSCOV2/COVID19 protein interruption search with existing active compounds using quasi-quantum simulation:
* https://covid19-hpc-consortium.org/projects/5f60f47b165888007deb5b8a
* Coarse-grained Modeling of SARS-CoV-2 Spike Protein Intermediates on the Pathway to Membrane Fusion
* https://covid19-hpc-consortium.org/projects/5f60f4cc165888007deb5b8d
* The Competition of Antiviral Drugs with ATP to Inhibit the SARS-CoV-2 RNA-dependent RNA Polymerase: A Key to Enhanced Drug Screening:
* https://covid19-hpc-consortium.org/projects/5f08dfa109c9030080f3197d

## Synthetic:

* Reflections on treatment of COVID-19 with traditional **Chinese medicine**:

https://cmjournal.biomedcentral.com/articles/10.1186/s13020-020-00375-1?fbclid=IwAR0j80nnMq0-tRip3gVP3n5lod9nR4ytm9upoQYe\_wx3UhDO63xSn9q4THc