

## Day 2:

Protein Name: Angiotensin Converting Enzyme 2

Protein ID: IPR001548

**Find the following Gene function details LOCATION**

Start: 19

End: 606

Family: Peptidyl dipeptidase / A

Clan: CL0126

Domain: Peptidase\_M2

Motif: HEXXH

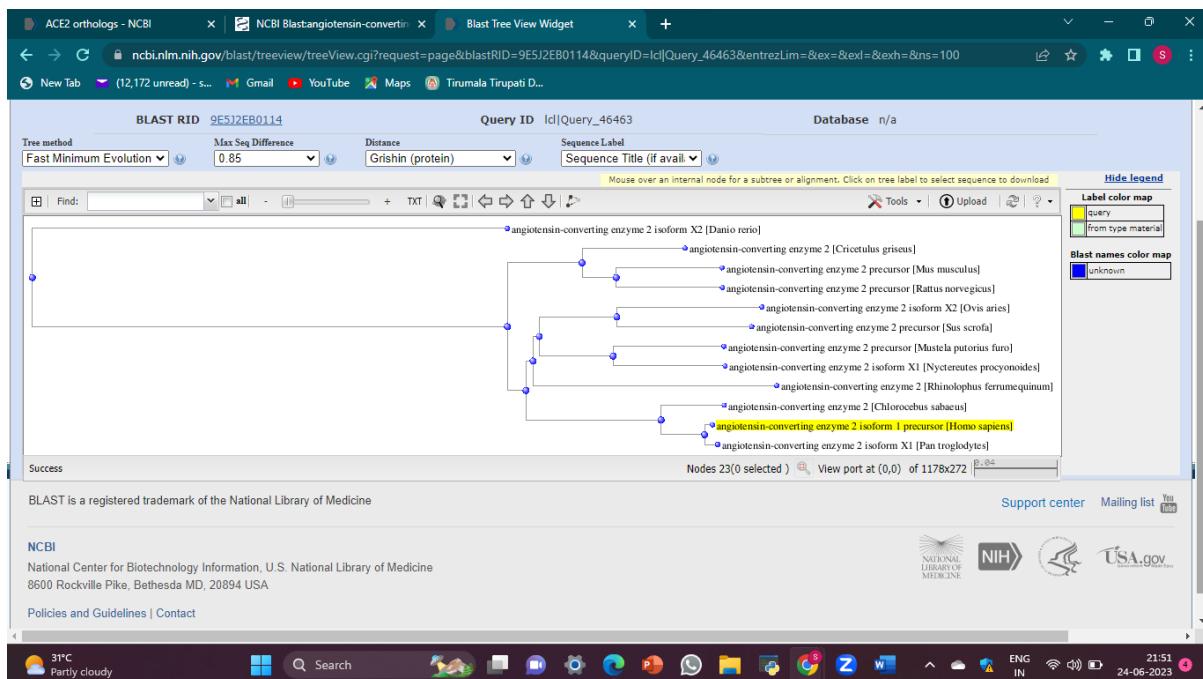
E value: 4.1e-245,4.2e-249

Description of function:

Peptidyl-dipeptidase A (angiotensin-converting enzyme or ACE) is a mammalian enzyme responsible for cleavage of dipeptides from the C-termini of proteins, notably converting decapeptide angiotensin I to the octapeptide angiotensin II. The enzyme exists in two differentially transcribed forms, the most common of which is from lung endothelium; this contains two homologous domains that have arisen by gene duplication. The testis-specific form contains only the C-terminal domain, arising from a duplicated promoter region present in intron 12 of the gene. Both enzymatic forms are membrane proteins that are anchored by means of a C-terminal transmembrane domain. Both domains of the endothelial enzyme are active, but have differing kinetic constants. ACE is well-known as a key part of the renin-angiotensin system that regulates blood pressure and ACE inhibitors are important for the treatment of hypertension.

## Day 3: Phylogenetics

**Construct a Phylogenetic tree for components of Corona virus.**



## Day 4:

**Genome name( the one of your interest): Severe acute respiratory syndrome-related coronavirus**

**From RAST results:**

Mention the desired nucleotide sequence that you choose to perform BLAST on and fill in the following:

1.Nucleotide sequence :

gtgctttttgaccttttgcatttcctgttttaataatgcttattatgtttgcttctgaaatccaggatctagaagaacctgtaccaaaagtctaaacgaacatgaa  
cttctcattgttttgactgtatttctctatgcagttgcatatgcactgtgtacagcgctgtgcattctaa

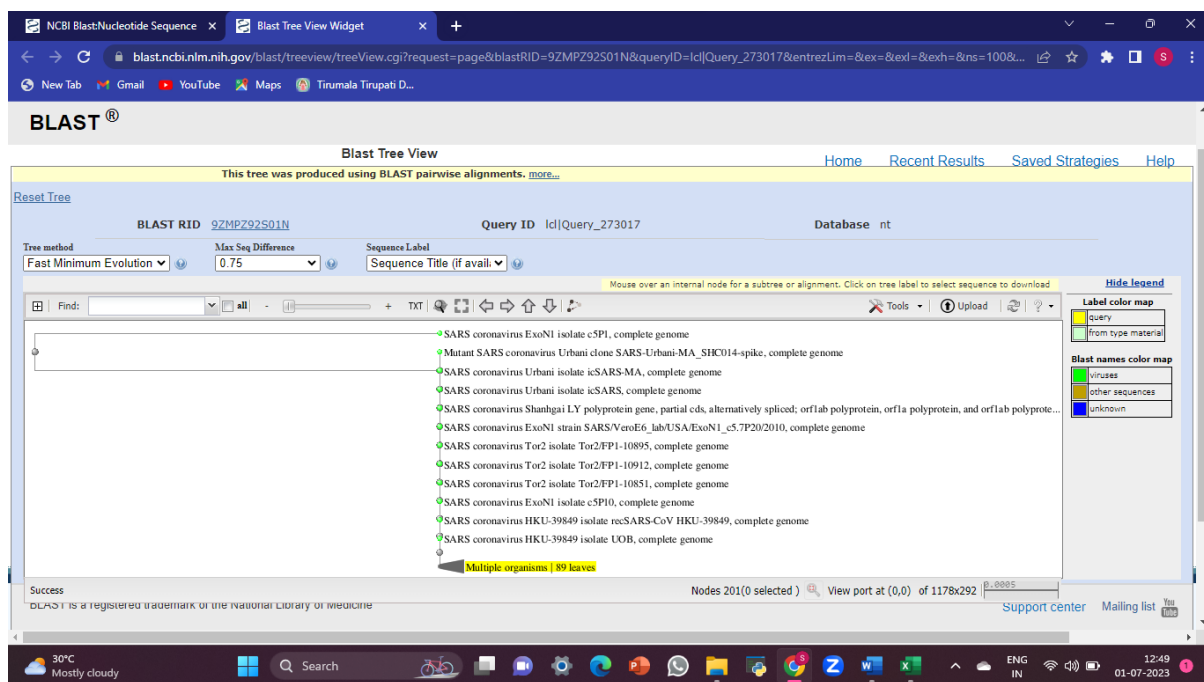
2.Location on the genome: AY274119.3\_27670\_27855

3.Start: 27670

4.End: 27855

5.Function : hypothetical protein.

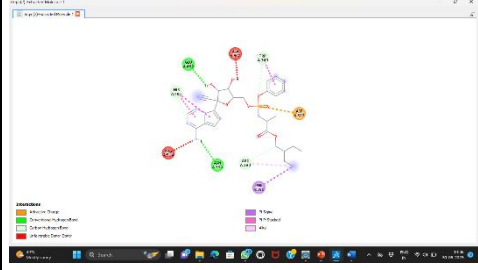
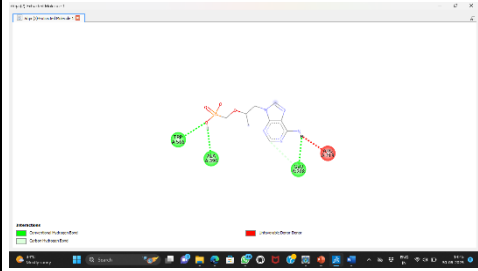
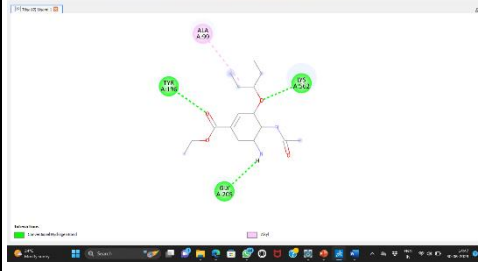
**Perform a BLAST on the nucleotide sequence and paste a screenshot of the obtained BLAST results:**



## Day 5 & 6: Molecular Docking

**Protein Name:** SARS-CoV2

**Protein ID:** 7DQA

Ligand Name	Ligand ID	Follows Lipinski Rule?	Energy value	Dock Image
Remdesivir	121304016	No	-8.5	
Tenofovir	464205	Yes	-6.6	
Oseltamivir	65028	Yes	-5.8	

## Day 7: Heatmap analysis

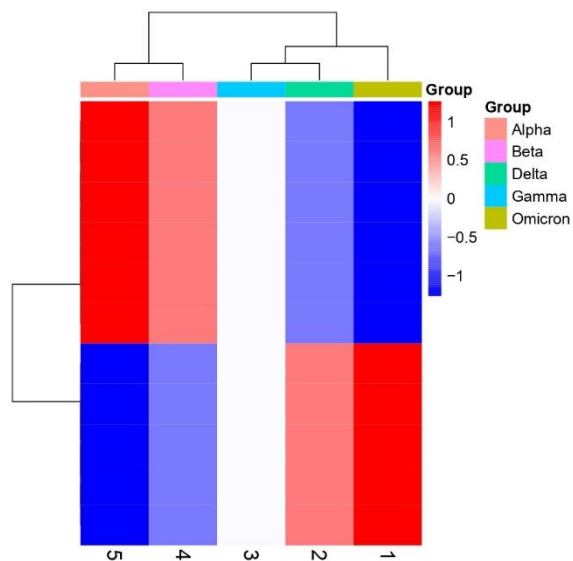
### Input details

1. Gene(s) Name: ACE2
2. Protein(s) Name: Angiotensin-converting enzyme 2

### Input data Table:

ORF	Alpha	Beta	Gamma	Delta	Omicron
ORF1a	5	4	3	2	1
ORF1b	4	3	2	1	0
ORF3a	3	2	1	0	-1
ORF6	2	1	0	-1	-2
ORF7a	1	0	-1	-2	-3
ORF7b	0	-1	-2	-3	-4
ORF8	-1	-2	-3	-4	-5
N	0	1	2	3	4
M	1	2	3	4	5
S	2	3	4	5	6
L	3	4	5	6	7
ORF10	4	5	6	7	8

Output:



## Day 8 & 9: Homology Modelling

**Disease:** Mycobacterium Tuberculosis

**Protein:** C-type lectin (CLR)

**Gene:** CLEC4D

**PDB:** Q8WXI8

**Target**

UniProt BLAST Align Peptide search ID mapping SPARCL UniProtKB

**Q8WXI8: CLC4D\_HUMAN**

**Names & Taxonomy**

Subcellular Location

**Disease & Variants**

**PTM/Processing**

**Expression**

**Interaction**

**Structure**

**Family & Domains**

**Sequence**

**Similar Proteins**

**Function**

Calcium-dependent lectin that acts as a pattern recognition receptor (PRR) of the innate immune system. It recognizes damage-associated molecular patterns (DAMPs) of pathogen associated molecular patterns (PAMPs) of bacteria and fungi (PubMed 23602766, PubMed 23191456). The PAMPs include alpha-mannans on A. Calicoccus hephaea and mycobacterial trehalose 6,6'-dimethylol (TDM) (PubMed 23602766, PubMed 23191456).

# Sequence

The screenshot displays the Swiss-Model web server interface. At the top, there is a navigation bar with links for 'Home', 'About', 'Contact', 'FAQ', 'Help', 'News', and 'Links'. Below this, the 'SWISS-MODEL' logo is prominent. The main content area shows a 'United Project' section with a 'Model Results' tab selected. The 'Model Results' section displays a 3D ribbon diagram of a protein structure, colored by domain (blue, green, red, orange, yellow, purple). The structure is shown in a side view, with a detailed view of the active site region highlighted in blue and red. The interface includes various controls for viewing the model, such as 'Zoom', 'Rotate', 'Translate', and 'Reset'. The bottom of the page features a footer with the text 'SWISS-MODEL: A Protein Structure Prediction Service' and a copyright notice for 2019.

<https://github.com/Shalini3008>