

CS482/682 W2022. Assignment 4

(Due date: April. 3, 2022)

This assignment requires you to use available public databases and software to study the RBD (receptor-binding domain) of the spike protein of SARS-Cov2 virus.

1. Find the RBD domain sequences for the following variants.
 - a. The earliest reported sequence: Wuhan-1
 - b. Alpha
 - c. Beta
 - d. Gamma
 - e. Delta
 - f. Omicron
2. Conduct a multiple sequence alignment of the protein sequences of the RBD domains. In the multiple alignment, highlight the amino acids that are different from the earliest reported sequence, Wuhan-1.
3. Predict the 3D structure of the RBD domains using the earliest sequence and the Omicron variant.
4. Superimpose the two predicted structures with any structure visualization software and label the positions of their different amino acids in the superimposed structures.

Detailed requirement:

Your submission is a pdf file that includes the following:

1. Your submission should include a list of sequences (one for each variant), together with a detailed description of the source where you get the sequence. Your sequence should only contain the RBD domains, but not the full sequence of the spike protein. Describe in enough detail so that another person can follow the steps to access the sequences as well. For each variant, there may be slightly different sequences available depending which source you get the sequence. You can use any sequence you found from any reputable sources. No need to be too obsessed by the precise boundaries of the RBD domain - being off by a few amino acids is fine.
2. You can use any existing multiple sequence alignment tool for this purpose. Your submission should include the multiple sequence alignment. It can be either a screenshot or in text format. The highlights of the different amino acids can be either produced by software or hand drawn. Describe what software you used.
3. Any 3D structure prediction software (standalone or online server) is fine. Describe what software you used.
4. Any visualization software that can do the job is fine. You'll need the software to have the ability to do the superimposition. Your submission will include two screenshots of the superimposed ribbon diagrams of the structures. The two screenshots are two observations from the opposite directions (180-degree flip) of the superimposed structures. You can either use the software to highlight the amino acids, or hand draw the positions of the different amino acids between the two sequences.