

# Enzymes\_worksheet

## Warm-Up Questions:

Read the Khan Academy article on [Enzymes](#) and answer the following questions:

- 1) What is a catalyst? How do they work?
  
- 2) Give an example of catalysis in your daily life. Identify the catalyst in your example.

## Computational Exercise #1: Simulating enzyme-substrate binding

**Question #1:** List one error that you identified to be a problem prior to running the Protein Preparation Workflow. Was it resolved after getting prepared?

**Question #2:** What amino acid residues do you notice in the binding site of TBK1 and what classification of amino acid does it fall under (i.e. (1) non-polar and neutral, (2) polar and neutral, (3) acidic and polar, or (4) basic and polar)? List them and take a screenshot of the binding site and paste it below.

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**Question #3:** What important enzyme-substrate interactions do you see when the inhibitor compound is docked? Take a screenshot of the Ligand Interaction Diagram and paste it below. List specific residues that play an important role in the binding site.

**Question #4.** Take a screenshot of the binding pocket with the surface view toggled on. What do you notice about the area surrounding the docked ligand/inhibitor?

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## Individual Exercises:

### Part A: Enzymes at play in COVID-19

- 1) Based on the description of SARS-CoV-2 above, identify the enzymes involved in the COVID-19 disease.
- 2) According to IUBMB nomenclature, what classification group(s) do the enzymes from Question (1) fall under?
- 3) What classification do the enzymes from Question (1) fall under?
- 4) Who/What does “host cell” refer to?
- 5) Based on what you have learned in this lesson so far, list one possible mechanism by which we can stop the activation of S proteins to prevent virus entry.

### Part B: Visualizing interactions in a SARS-CoV-2 enzyme-inhibitor complex

**Question #1:** Paste a screenshot of the binding pocket of TMPRSS2 below. What interactions do you see in the binding site of TMPRSS2? *Hint:* use the Ligand Interaction panel to visualize the 2D interactions.