Teaching	with	Schrödinger	
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## Enzymes\_worksheet

## **Warm-Up Questions:**

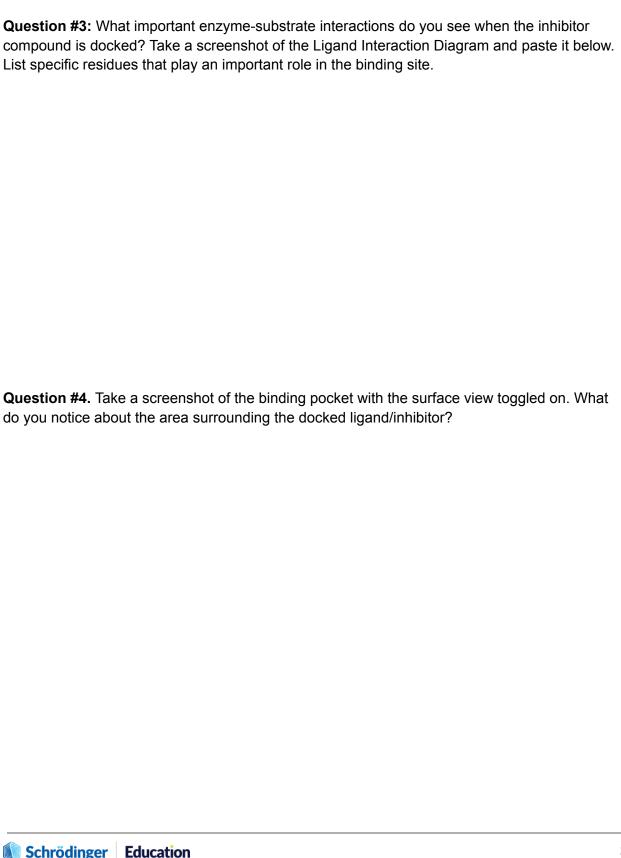
Read the Khan Academy article on **Enzymes** and answer the following questions:

- 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.



## **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.