CHEM1200: Discovery in Biology

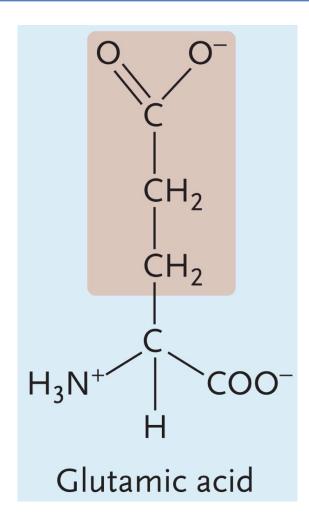
Week 8: Tutorial 2 (Chemistry of Life & Metabolism)

Yudai Matsuda

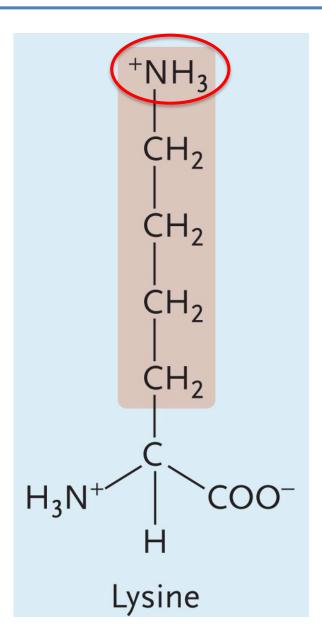
Assistant Professor, Department of Chemistry

(ymatsuda@cityu.edu.hk)

1. In the three-dimensional structure of a protein, if glutamic acid and lysine residues are adjacently located, what kind of chemical bond would they form? Also, draw chemical structures to explain how they form the chemical bond.



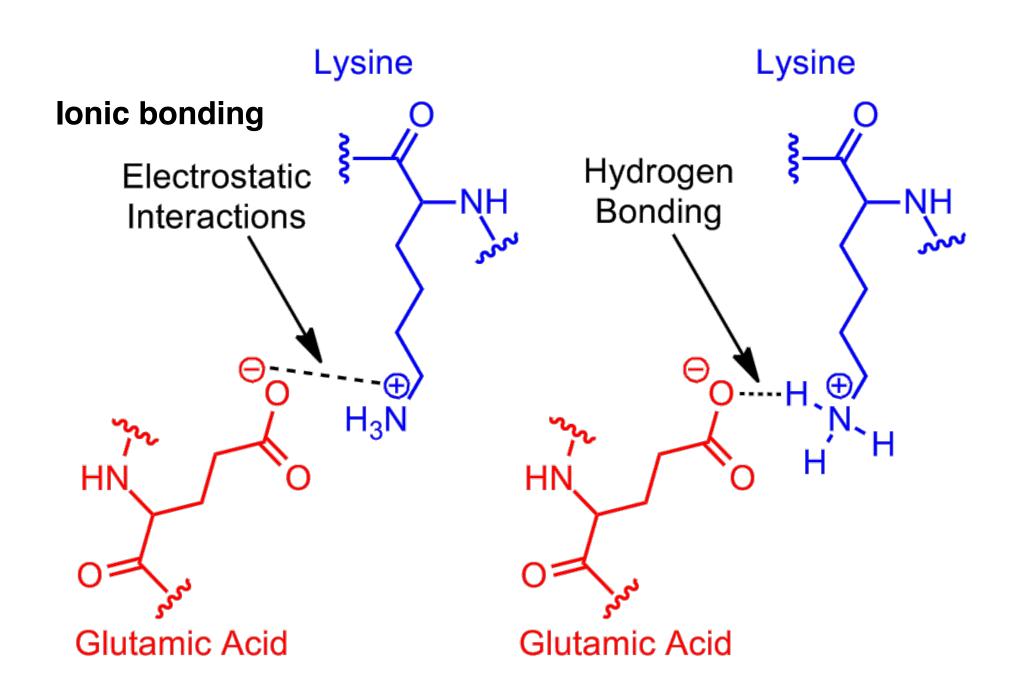
Negatively charged



Positively charged

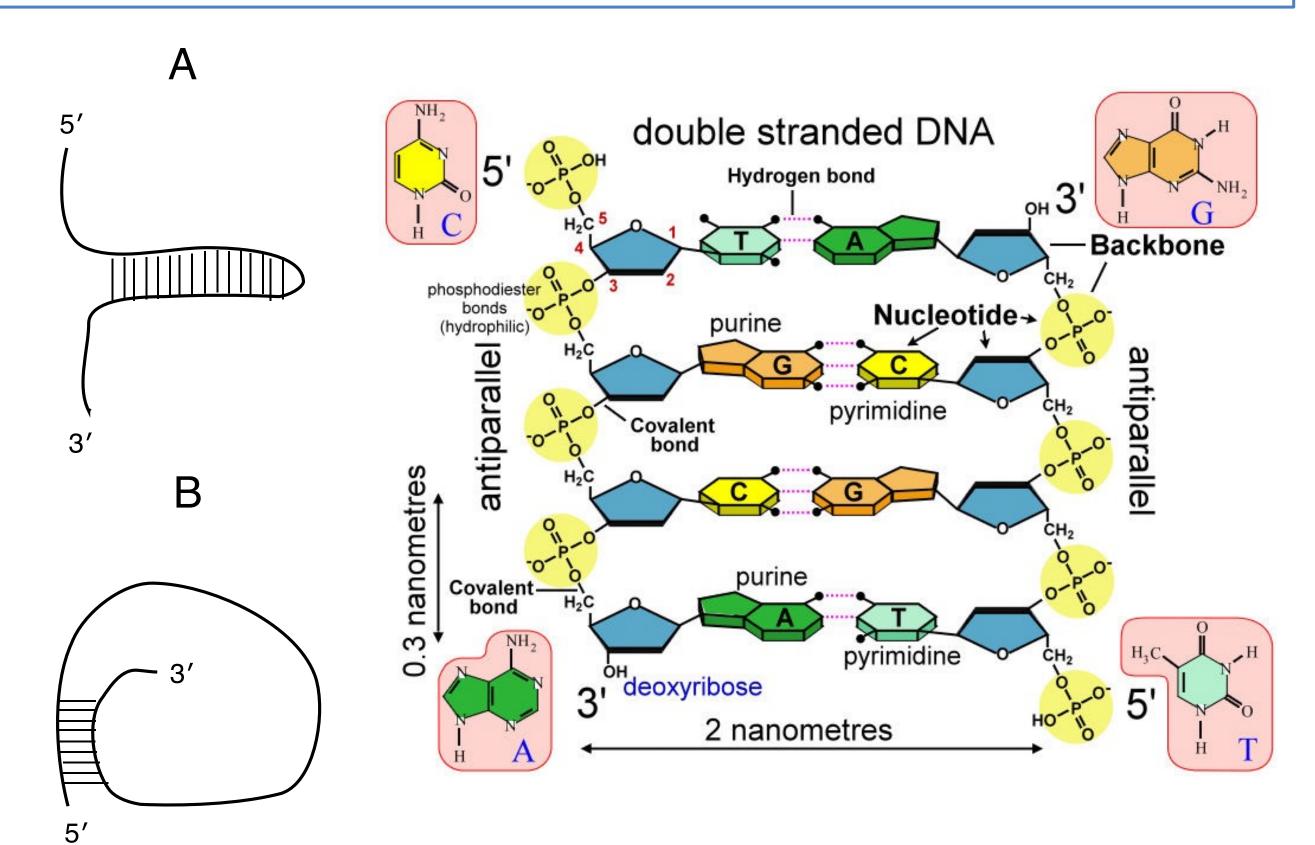
Hydrogen atoms bound to nitrogen (Hydrogen bond donor?)

1. In the three-dimensional structure of a protein, if glutamic acid and lysine residues are adjacently located, what kind of chemical bond would they form? Also, draw chemical structures to explain how they form the chemical bond.

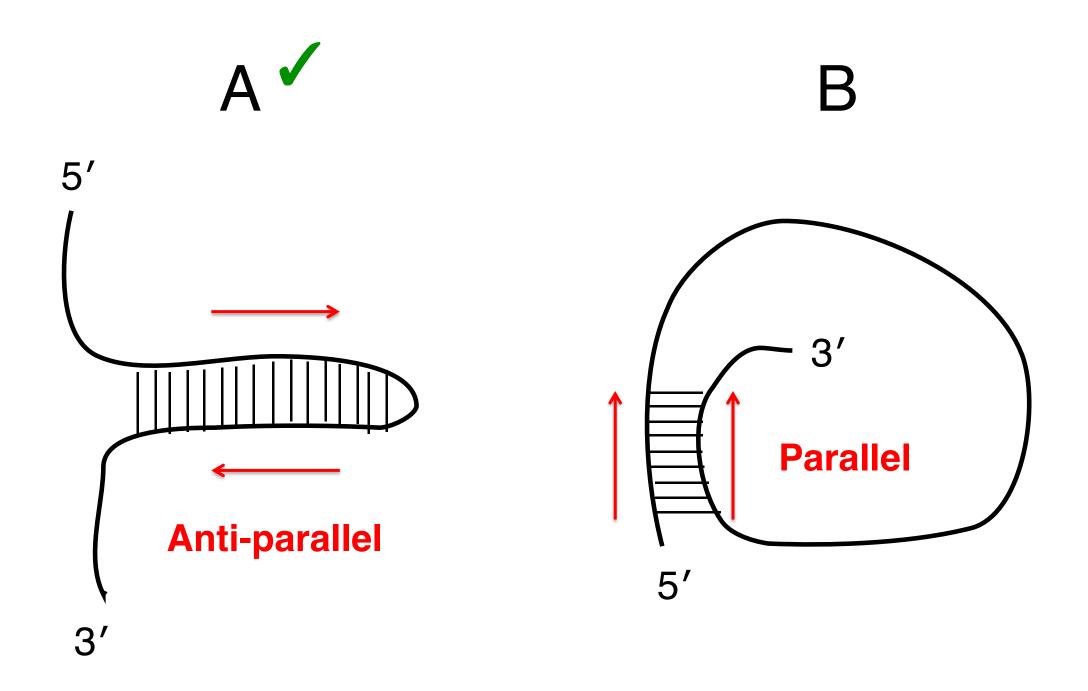


Salt bridge

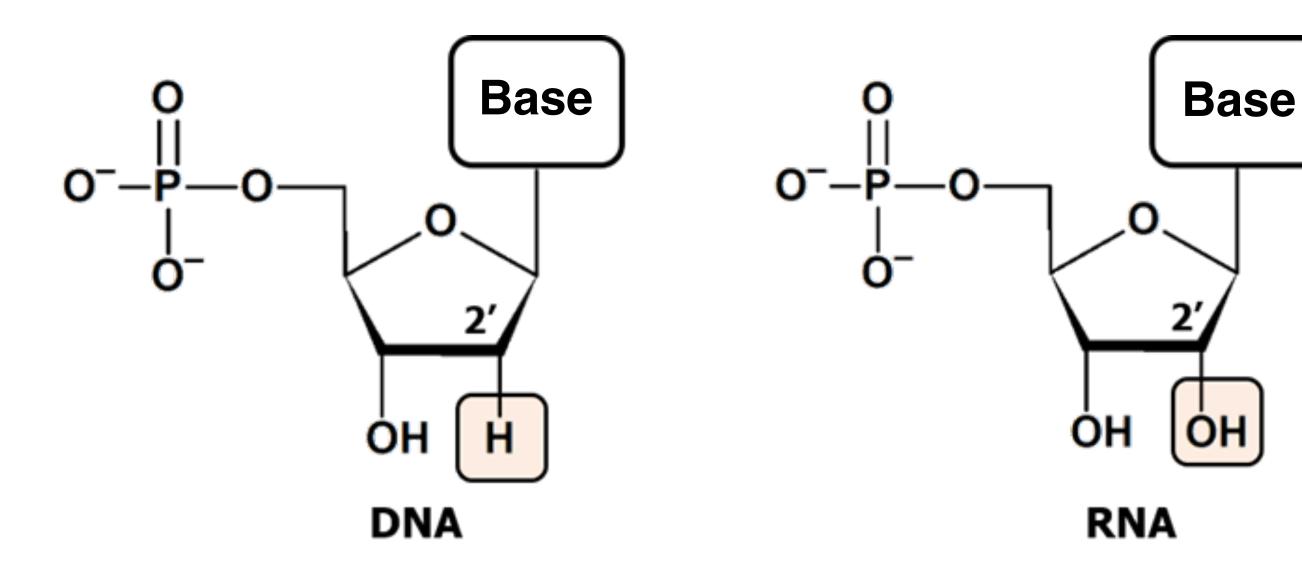
2. Which of the following arrangements is/are possible in an RNA molecule? Please explain why. Note that the small lines represent hydrogen bonds.



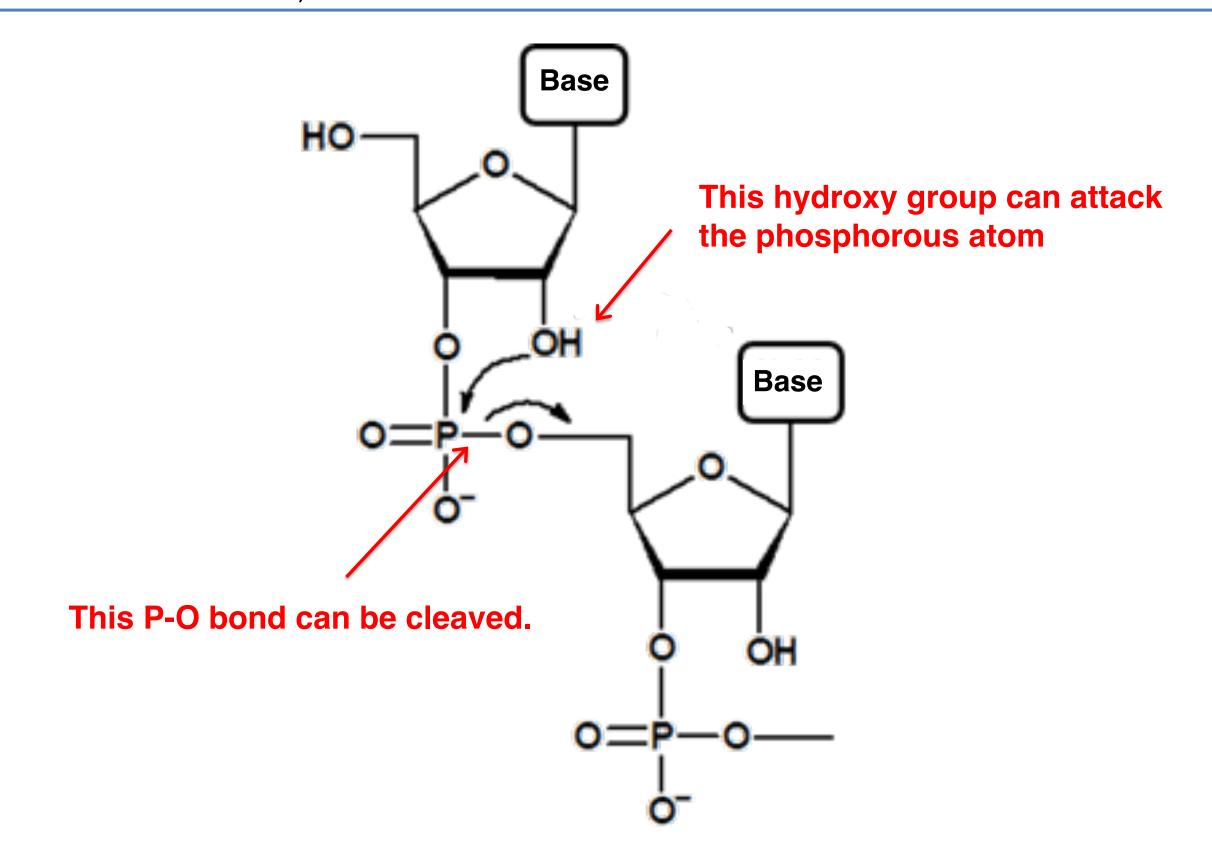
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3. RNA is less stable than DNA. Try to explain why (remember the structural difference between DNA and RNA).

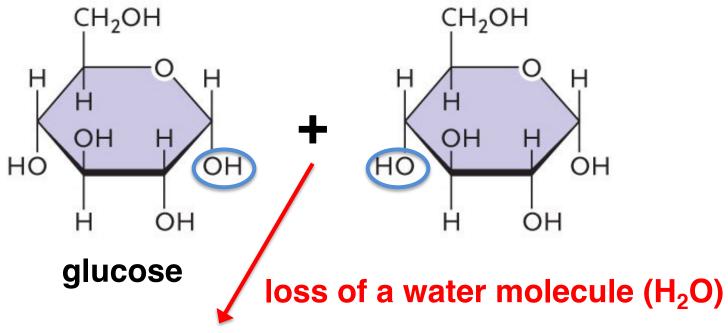


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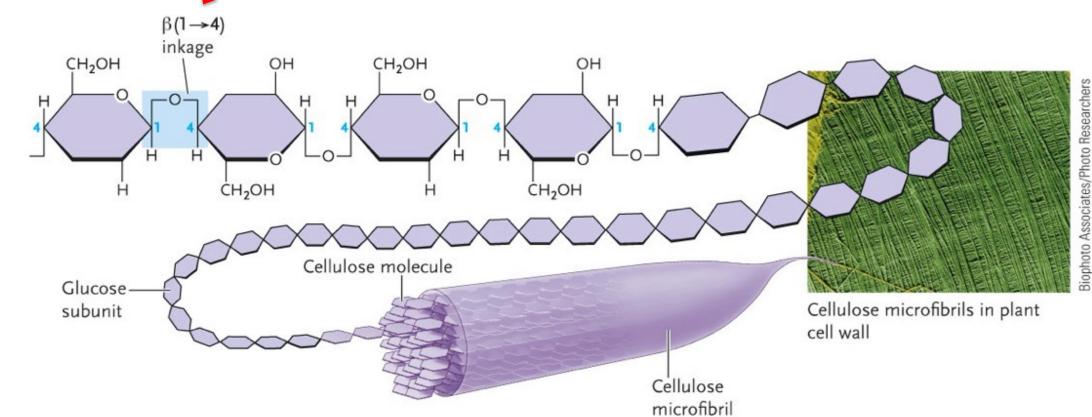
4. Suppose a cellulose molecule consists of 3000 glucose monomers. How many carbon, hydrogen, and oxygen atoms would it have?

Cellulose: Polymer of glucose (C₆H₁₂O₆)



c. Cellulose, the primary fiber in plant cell walls

Cellulose, formed from glucose units joined end to end by $\beta(1\rightarrow 4)$ linkages. Hundreds to thousands of cellulose chains line up side by side, in an arrangement reinforced by hydrogen bonds between the chains, to form cellulose microfibrils in plant cells.



4. Suppose a cellulose molecule consists of 3000 glucose monomers. How many carbon, hydrogen, and oxygen atoms would it have?

1. How many C, H, and O atoms are there in 3000 molecules of glucose?

Carbon: $6 \times 3000 = 18000$

Hydrogen: $12 \times 3000 = 36000$

Oxygen: $6 \times 3000 = 18000$

2. How many H and O atoms are lost as water molecule?

NOTE: 2999 (not 3000) molecules of water are lost

Lost hydrogen: $2 \times 2999 = 5998$

Lost oxygen: $1 \times 2999 = 2999$

3. So the answer is...

Carbon: 18000

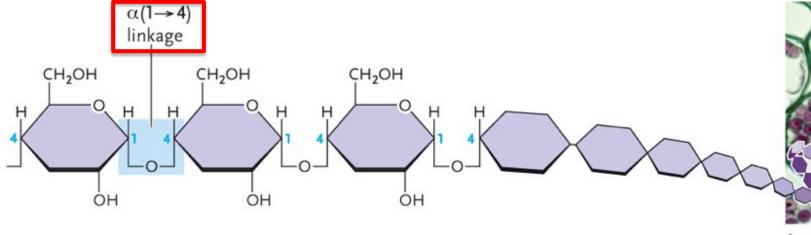
Hydrogen: 36000 - 5998 = 30002

Oxygen: 18000 - 2999 = 15001

5. We humans can digest starch but not cellulose. Why?

A. Amylose, a plant starch

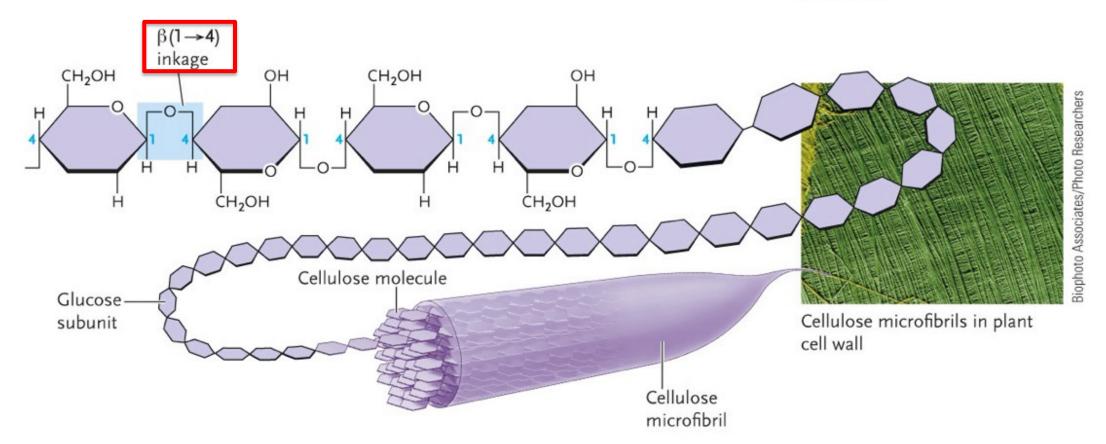
Amylose, formed from α -glucose units joined end to end in $\alpha(1\rightarrow 4)$ linkages. The coiled structures are induced by the bond angles in the α -linkages.



Amylose grains (purple) in plant root tissue

c. Cellulose, the primary fiber in plant cell walls

Cellulose, formed from glucose units joined end to end by $\beta(1\rightarrow 4)$ linkages. Hundreds to thousands of cellulose chains line up side by side, in an arrangement reinforced by hydrogen bonds between the chains, to form cellulose microfibrils in plant cells.



Humans have enzymes that can hydrolyze the α linkages but not β linkages.

6. Consider an enzyme that utilizes glutamic acid as a catalytic residue. This glutamate residue serves as a general acid to initiate the enzymatic reaction. When the glutamate was substituted with aspartate, the enzyme was still active. However, when substituted with glutamine, the enzyme completely lost its activity. Provide a plausive explanation for this observation.

A reaction example

Can perform the protonation

Cannot perform the protonation

7. Related to question 6, you are now working on another enzyme with a glutamate residue that serves as a general acid to initiate the reaction. In this case, the substitution of glutamate with aspartate has led to the complete abolishment of the enzymatic activity. Provide a plausive explanation for this observation.

$$\sum_{i=1}^{N} C = C + H$$
Glu

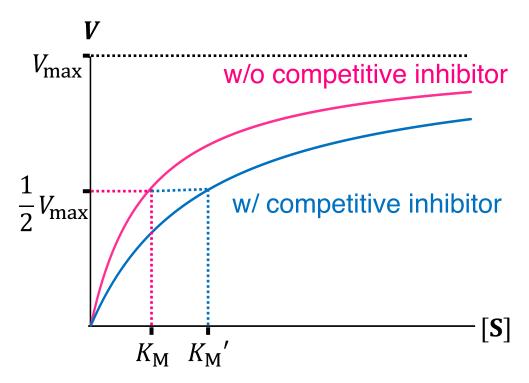
$$\sum_{i=1}^{N} C = C + H$$
Asp

The side chain of Asp is shorter than that of Glu.

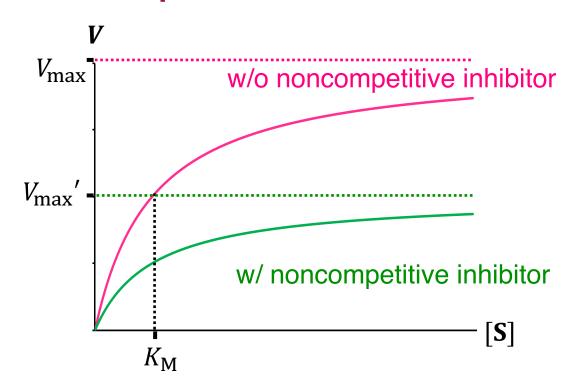
⇒ The distance between the Asp residue and the substrate might be too long for the Asp residue to perform the reaction.

8. You are now investigating the function of an enzyme and found that the enzymatic reaction is inhibited in the presence of a small molecule **A**. What experiment would you design to tell whether **A** serves as a competitive or a noncompetitive inhibitor?

Competitive inhibition



Non-competitive inhibition



A possible answer

Perform the enzymatic reaction under several different substrate concentrations in the presence of a fixed concentration of the inhibitor. Also perform the reactions in the absence of the inhibitor (control experiment).

If the inhibitor works in a competitive manner, the reaction rate will saturate at the same point as the reaction without the inhibitor at higher substrate concentration. In case of the non-competitive inhibition, the maximum reaction rate will be lower than that of the reaction without the inhibitor even at a high substrate concentration.

9. Use the Michaelis-Menten equation to complete the enzyme kinetic data set, when $K_{\rm M}$ is known to have a value of 1.00 mM (= mmol/L).

V (μM/min)
50.0
-
-
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-

Michaelis-Menten equation

$$V = \frac{V_{\text{max}}[S]}{K_{\text{M}} + [S]}$$

1. Determine V_{max}

$$50.0 \, [\mu\text{M/min}] = \frac{V_{\text{max}} \times 500 \, [\mu\text{M}]}{1000 \, [\mu\text{M}] + 500 \, [\mu\text{M}]}$$

$$V_{\text{max}} = 150 \, [\mu \text{M/min}]$$

2. Determine V at each [S]

[S] = 1.00 [mM]
$$\Rightarrow$$
 V = 75.0 [μ M/min]

[S] = 2.00 [mM]
$$\Rightarrow$$
 $V = 100 [\mu M/min]$

[S] = 3.00 [mM]
$$\Rightarrow$$
 $V = 113 [\mu M/min]$

[S] = 10.0 [mM]
$$\Rightarrow$$
 $V = 136 [\mu M/min]$