

Optional Practice on Pain Medicine Binding

Explore how a hypothetical pain medicine binds to its target. Use a reversible-binding model to connect reaction rates, equilibrium, and receptor occupancy, then visualize the model with AI-assisted coding.

Optional and ungraded. No submission is required.

The model

A free drug molecule D binds to a free receptor R to form a drug–receptor complex C. The complex can also separate back into D and R.



[D], [R], and [C] are concentrations. In this simplified exercise, assume that greater receptor occupancy corresponds to a greater pain-relieving effect. This assumption does not describe every pain medicine.

Part 1 Understand the reaction

1. Write equations for $d[D]/dt$, $d[R]/dt$, and $d[C]/dt$, including both forward and reverse reactions.
2. Explain what $k_+[D][R]$ and $k_-[C]$ represent. Why does the forward rate depend on both free drug and free receptor concentrations?
3. At equilibrium, what must be true about the forward and reverse rates? Do the reactions stop?

Part 2 Calculate receptor occupancy

Assume the free drug concentration is held constant and the receptors have reached binding equilibrium. The fraction of receptors occupied by drug is:

$$\theta = [C] / R_{\text{total}} = [D] / (K_d + [D]) \quad \text{and} \quad K_d = k_- / k_+$$

Here $R_{\text{total}} = [R] + [C]$. Compare two hypothetical medicines: medicine A has $K_d = 1 \mu\text{M}$; medicine B has $K_d = 5 \mu\text{M}$.

1. Calculate θ for each medicine when $[D] = 1 \mu\text{M}$. Express the results as percentages.
2. Which medicine has greater occupancy at the same free drug concentration? How does this relate to K_d ?
3. If $[D]$ increases from 1 to 2 μM , does occupancy double? Calculate the new values and explain.

Part 3 Explore with AI assisted coding

Use an AI coding tool to create a simple script or browser demo. Read the generated code, identify the equation and parameters, and check the results before interpreting them.

Suggested coding prompt

Create a receptor-binding simulation using $\theta = D/(K_d + D)$. Plot receptor occupancy against free drug concentration from 0 to 20 μM for two hypothetical medicines with K_d values of 1 and 5 μM . Label both axes with units or percentages, include a legend, and make the K_d values easy to change. Show the calculated occupancy at $D = 1 \mu\text{M}$. Explain how the code implements the equation.

1. Run the code and compare its values at $[D] = 1 \mu\text{M}$ with your hand calculations.
2. Change one K_d value. Predict how the curve will change before running the code again.
3. Check that occupancy stays between 0 and 1, equals 0.5 when $[D] = K_d$, and approaches 1 as $[D]$ becomes much larger than K_d .
4. Explain what the curve tells you about receptor saturation and why increasing concentration has a smaller effect near saturation.

Part 4 Think about the physiology

1. Why might receptor occupancy alone be insufficient to predict how much pain relief a person experiences?
2. After a pill is taken, drug concentration changes as the drug is absorbed and eliminated. How does this differ from our assumption of constant free drug concentration?
3. What additional information would you need to extend this model to show how receptor occupancy changes over time?

All medicines and parameter values in this exercise are hypothetical and are not dosing guidance.