CASE STUDY BASED PUZZLE

BP807 ET:COMPUER AIDED DRUG DESIGN

UNIT 3: MOLECULAR DOCKING

CASE STUDY PUZZLE

"Finding the Best Inhibitor for Enzyme X"

Background Scenario

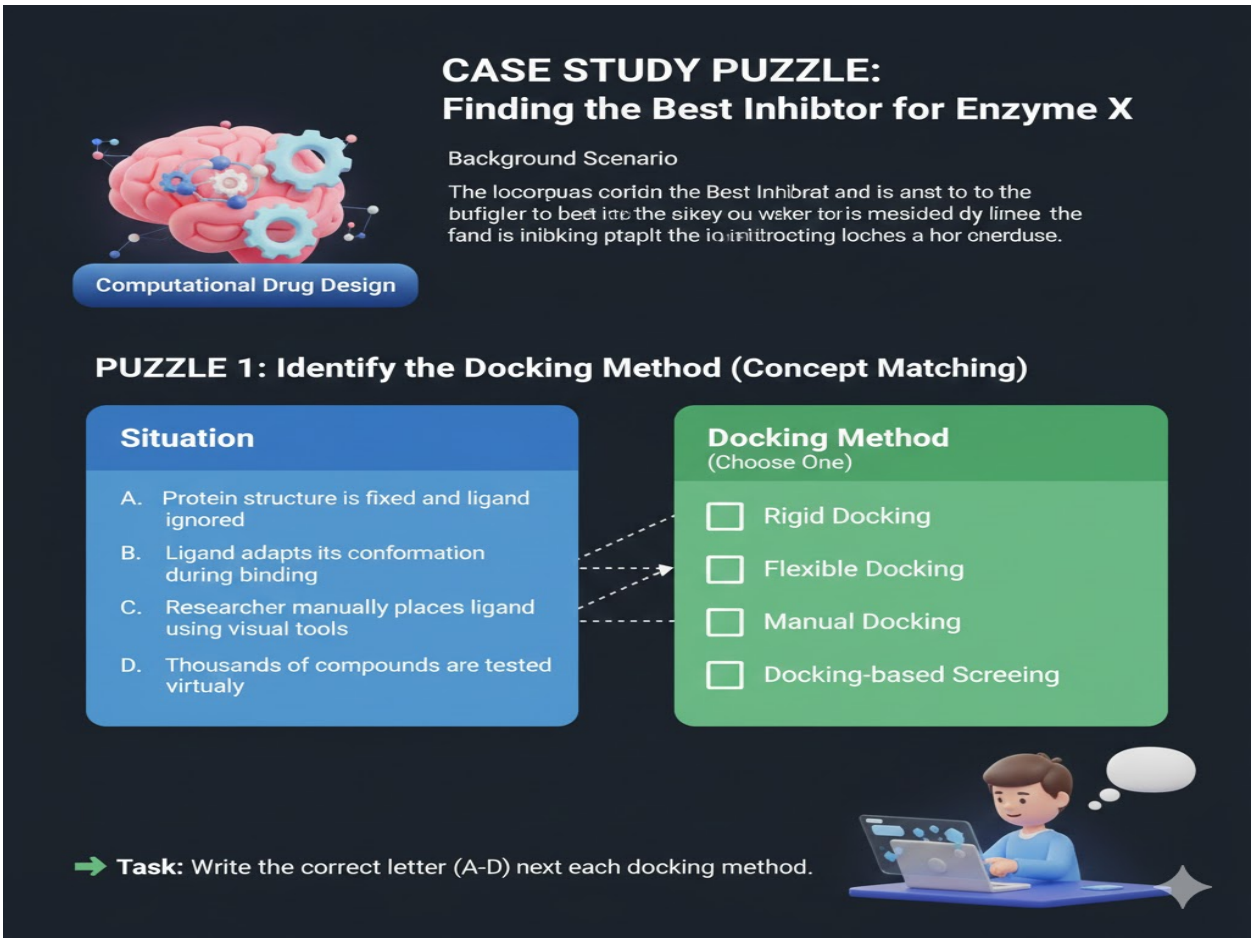
A pharmaceutical research team is working on Enzyme X, a key target involved in an infectious disease.
Three candidate ligands (L1, L2, and L3) have been identified from a compound library.
The team must choose the most suitable docking strategy and screen the best ligand efficiently.
You are part of the computational drug design team. Solve the following puzzles to help the team make correct decisions.

PUZZLE 1: Identify the Docking Method (Concept Matching)

Match the research situation with the appropriate docking type.

Situation	Docking Method (Choose One)
A. Protein structure is fixed and ligand flexibility is ignored	☐ Rigid Docking
B. Ligand adapts its conformation during binding	☐ Flexible Docking
C. Researcher manually places ligand using visual tools	☐ Manual Docking
D. Thousands of compounds are tested virtually	☐ Docking-based Screening

☞ Task: Write the correct letter (A–D) next to each docking method.



PUZZLE 2: Decision Puzzle – Choose the Best Docking Strategy

Research Conditions:

- Protein active site is known
- Ligand L2 has rotatable bonds
- Limited computational time
- Need accurate binding pose

Question:

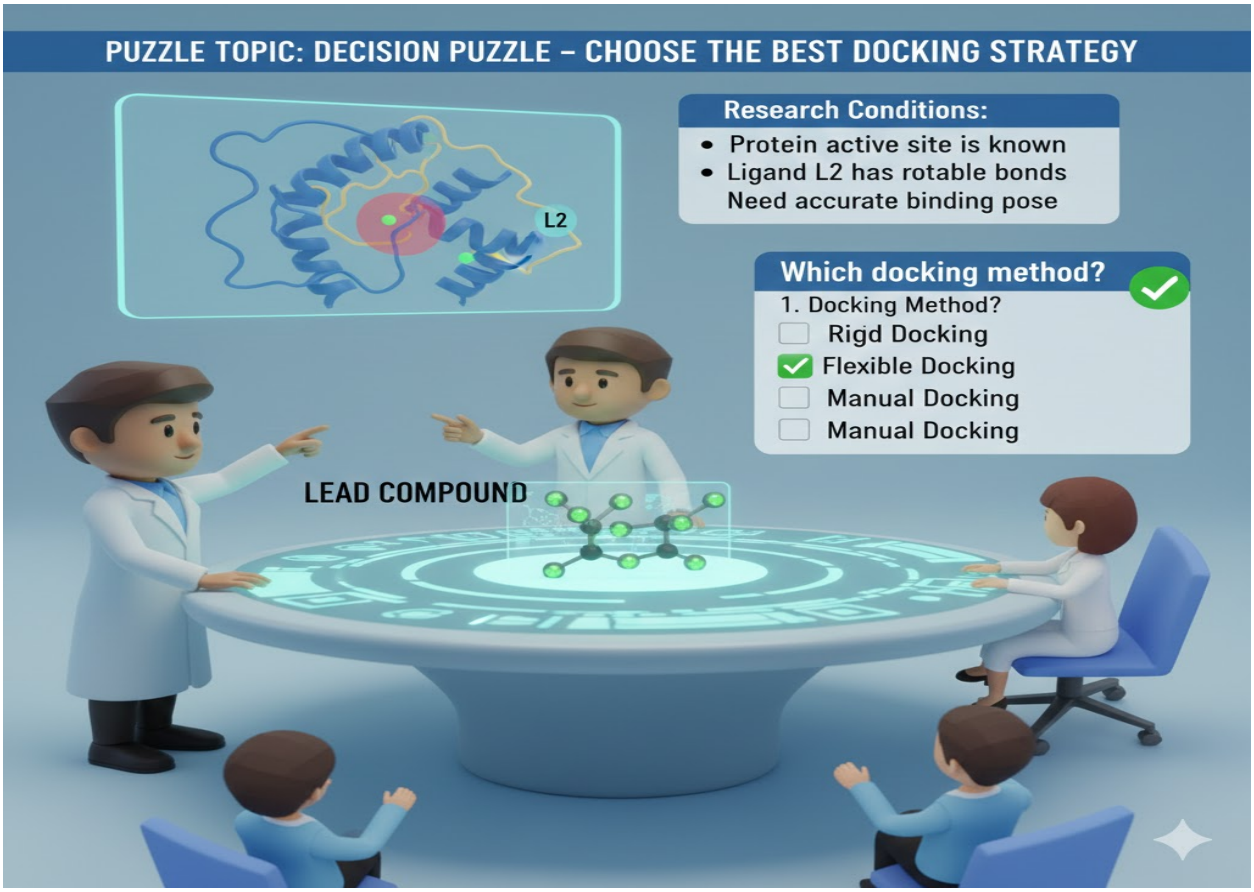
Which docking method should be selected?

☐ Rigid Docking

☐ Flexible Docking

☐ Manual Docking

☞ Hint: Think about ligand movement and accuracy.



PUZZLE 3: Docking Score Mystery

After docking, the following binding scores were obtained:

Ligand Docking Score (kcal/mol)

L1 −6.2

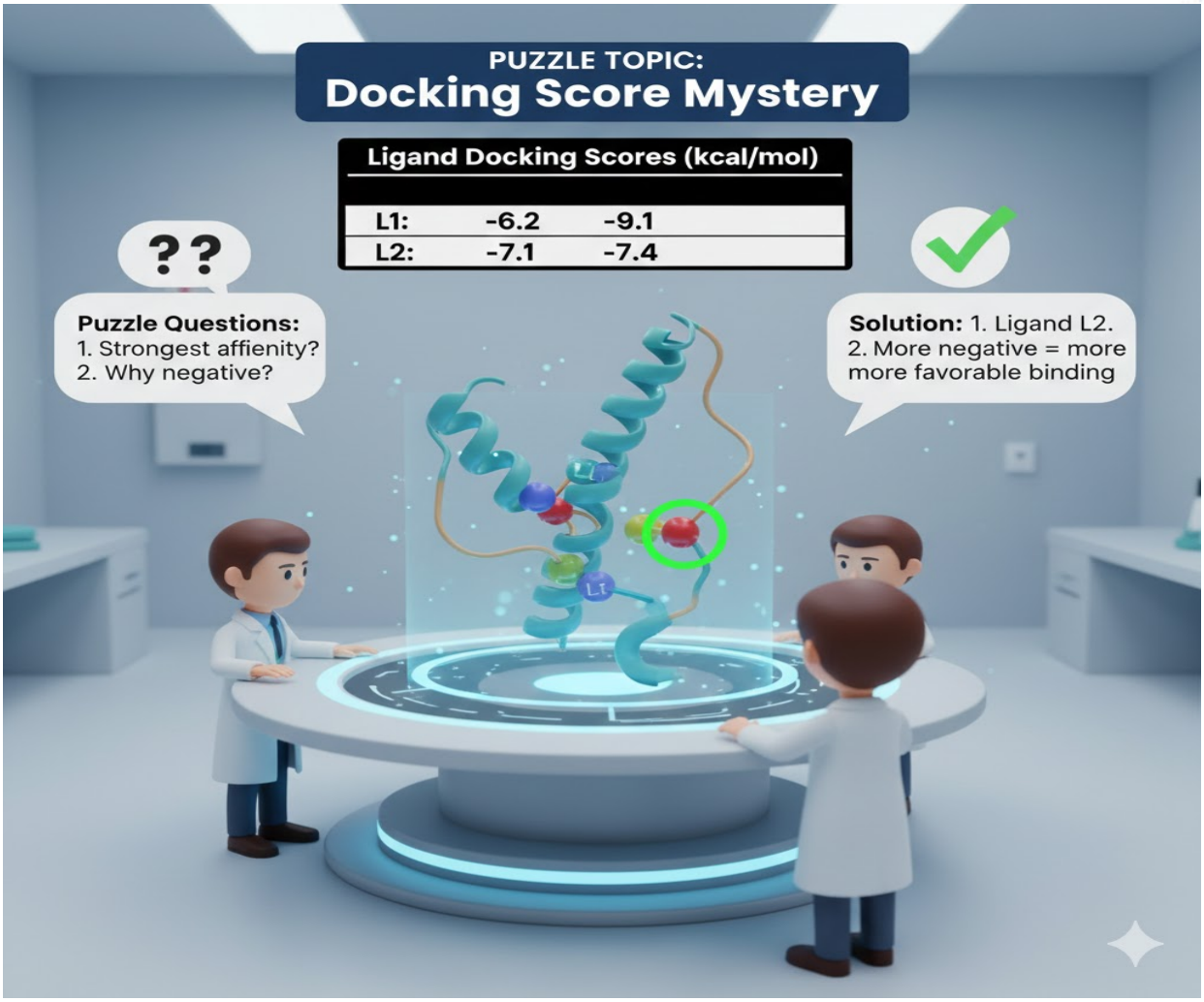
L2 −9.1

L3 −7.4

Questions:

1. Which ligand shows strongest binding affinity?
2. Why is a more negative docking score preferred?

☞ Answer format: Ligand name + 1 line justification.


PUZZLE TOPIC:
Docking Score Mystery
Ligand Docking Scores (kcal/mol)
L1: -6.2 -9.1
L2: -7.1 -7.4
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Puzzle Questions:
1. Strongest affienity?
2. Why negative?
Solution: 1. Ligand L2.
2. More negative = more
more favorable binding