CASE STUDY BASED PUZZLE

BP807 ET:COMPUER AIDED DRUG DESIGN

UNIT 3: MOLECULAR MODELING AND VIRTUAL SCREENING TECHNIQUES

Case Study Title

"Virtual Hunt for a New Antibacterial Drug"

Background

A pharmaceutical research team is working on discovering a new antibacterial drug to combat drug-resistant bacteria. Traditional lab screening is costly and time-consuming, so the team decides to use molecular modeling and virtual screening techniques to identify a promising lead compound.
You are part of the computational drug discovery team. Solve the following puzzles step by step to help the team select the best drug candidate.

PUZZLE 1: Identify the Technique (Concept Matching)

Match the research task with the correct molecular modeling technique.

Task	Technique Options
A. Predicting 3D structure of a target protein	1. Molecular Docking
B. Studying ligand–protein interaction	2. Virtual Screening
C. Screening 10,000 compounds quickly	3. Homology Modeling
D. Analyzing stability of protein–ligand complex over time	4. Molecular Dynamics

☞ Puzzle Question:
Match A–D with the correct technique numbers.

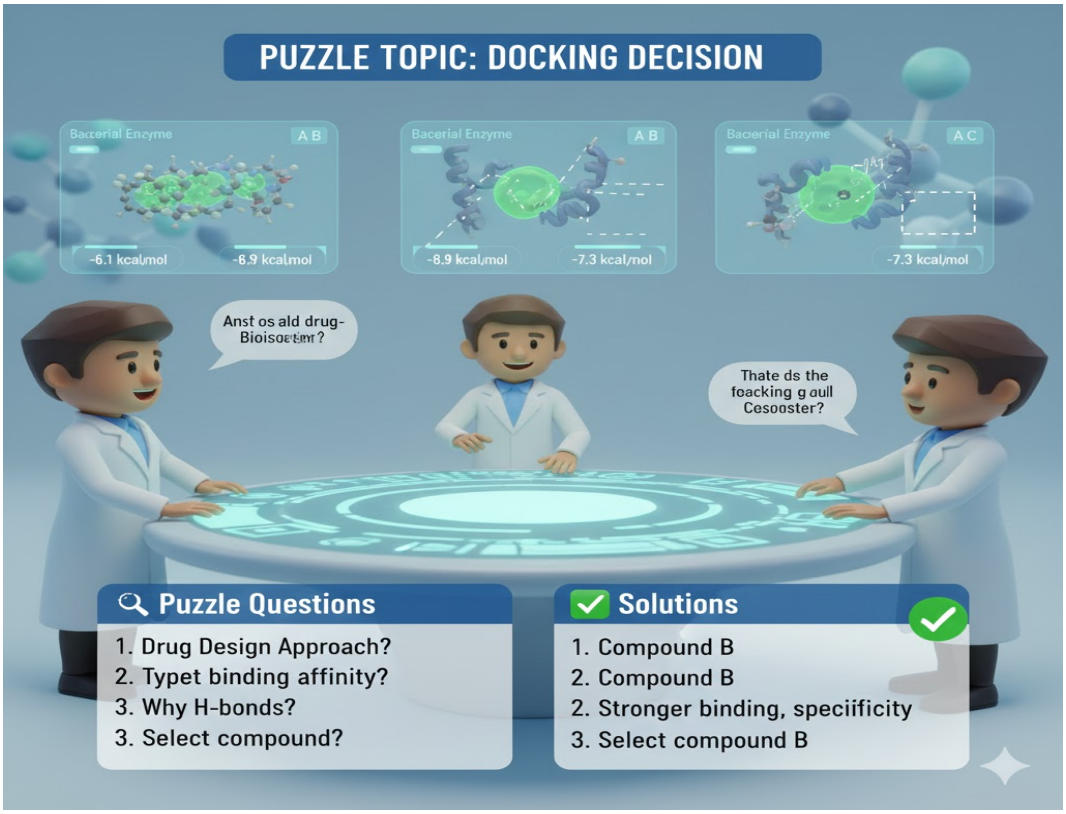
PUZZLE 2: Docking Decision Puzzle

The team docked three compounds (A, B, C) into the active site of a bacterial enzyme.

Compound	Docking Score (kcal/mol)	Hydrogen Bonds
A	–6.1	1
B	–8.9	4
C	–7.3	2

☞ Puzzle Questions:

1. Which compound shows the best binding affinity?
2. Why are hydrogen bonds important in docking studies?
3. Which compound should be selected for further analysis?



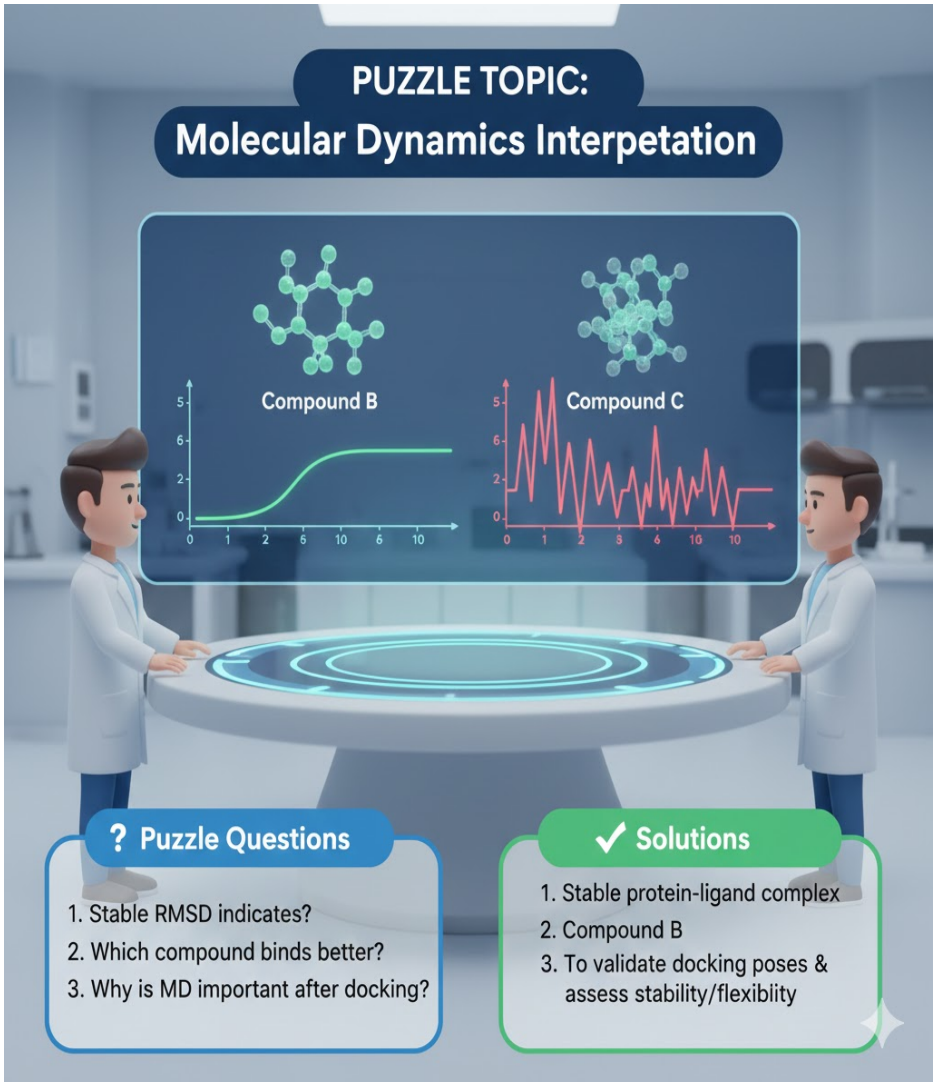
PUZZLE 3 : Molecular Dynamics Interpretation

During a 100 ns molecular dynamics simulation:

- Compound B shows stable RMSD
- Compound C shows large RMSD fluctuations

☞ Puzzle Questions:

1. What does stable RMSD indicate?
2. Which compound is more likely to remain bound in real biological conditions?
3. Why is molecular dynamics important after docking?


PUZZLE TOPIC:
Molecular Dynamics Interpetation
Compound B
Compound C
? Puzzle Questions
1. Stable RMSD indicates?
2. Which compound binds better?
3. Why is MD important after docking?
✓ Solutions
1. Stable protein-ligand complex
2. Compound B
3. To validate docking poses & assess stability/flexiblity