

CASE STUDY BASED PUZZLE

BP807 ET: COMPUTER AIDED DRUG DESIGN

UNIT 2: QUANTITATIVE STRUCTURE ACTIVITY

RELATIONSHIP (QSAR)

CASE STUDY PUZZLE

UNIT 2 – Quantitative Structure–Activity Relationship (QSAR)

Case Title: Improving the Potency of an Antibacterial Drug

A pharmaceutical research team is working on a new antibacterial drug (Compound X). Initial biological testing shows moderate antibacterial activity, but the team wants to improve its potency using QSAR principles instead of random trial-and-error synthesis.

The team synthesizes four analogues of Compound X by making small structural changes.

Puzzle 1: Lipophilicity Logic

Which compound shows improved activity mainly due to increased lipophilicity (log P)?

☞ Options: A / B / C

🧠 Hint: Better membrane penetration improves activity.

Puzzle 1: Lipophilicity Logic
Which compound shows improved activity mainly due to increased lipophilicity (log P)?

Hint: Better membrane penetration improves activity

Improved Activity

A

B

C

log P = 1.5

log P = 0.8

log P = 4.2

Student Task: Identify correct option

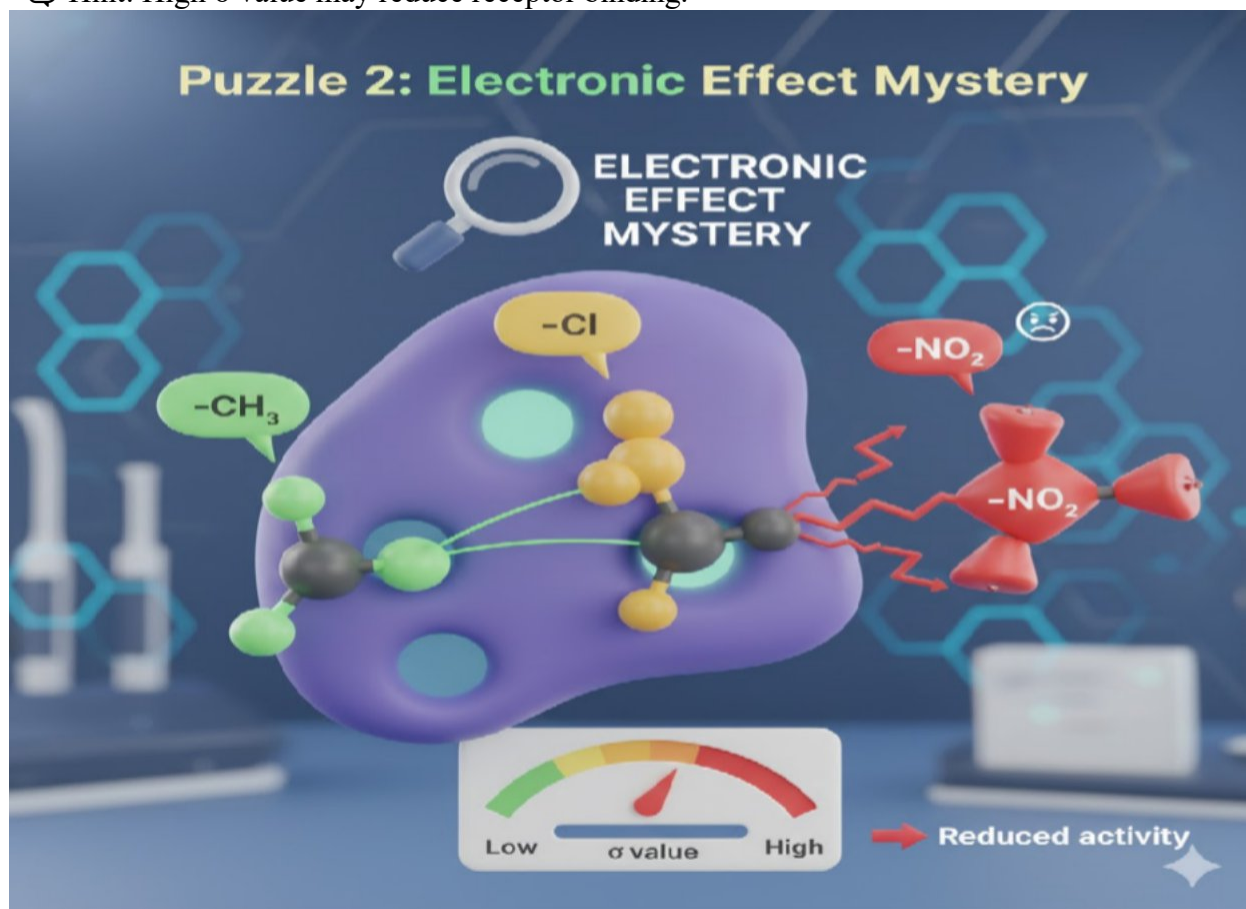
A B C

Puzzle 2: Electronic Effect Mystery

Which substituent reduced antibacterial activity due to strong electron-withdrawing nature?

☞ Options: $-\text{CH}_3$ / $-\text{Cl}$ / $-\text{NO}_2$

🧠 Hint: High σ value may reduce receptor binding.



Puzzle 3: Best Lead Compound

Based on QSAR parameters, which compound should be selected as the best lead molecule for further development?

☞ Options: A / B / C

🧠 Hint: Balance between lipophilicity, electronic effect, and steric bulk.

