

## CASE STUDY BASED PUZZLE

BP807 ET:COMPUER 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

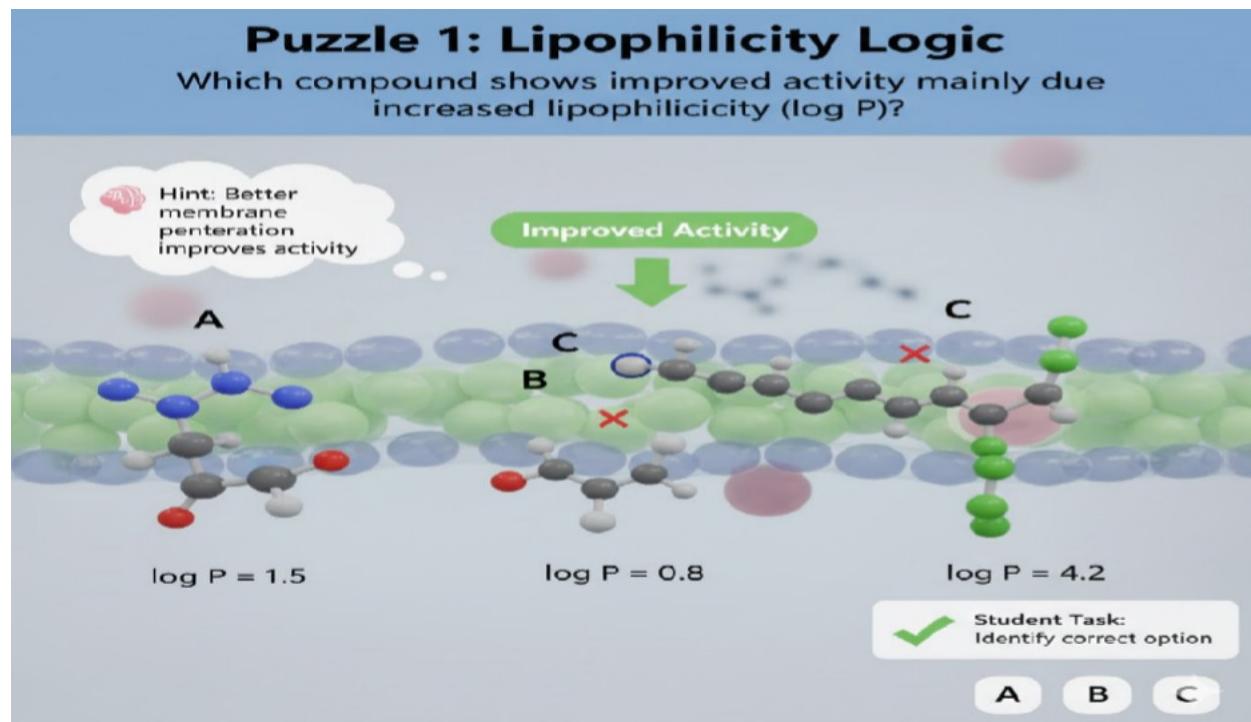
Which compound shows improved activity mainly due to increased lipophilicity ( $\log P$ )?

☞ Options: A / B / C

☞ Hint: Better membrane penetration improves activity.

**Puzzle 1: Lipophilicity Logic**

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



Hint: Better membrane penetration improves activity

Improved Activity

**Student Task:** Identify correct option

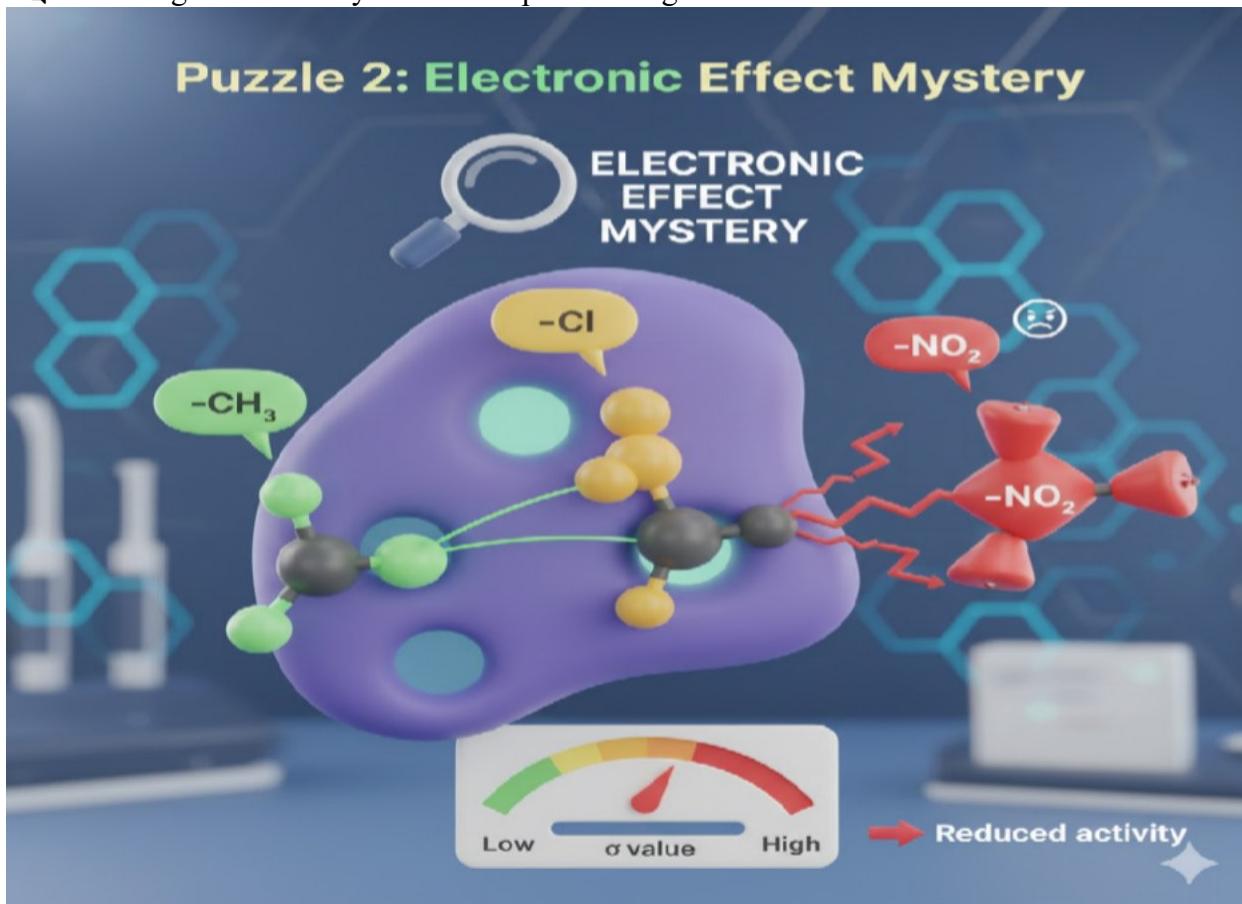
**A    B    C**

### 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  $\sigma$  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.

