

SUBJECT: COMPUTER AIDED DRUG DESIGN (BP807ET)

COURSE: FINAL YEAR B.PHARM

UNIT 2 : QUANTITATIVE STRUCTURAL ACTIVITY RELATIONSHIP(QSAR)

## SECTION – A : 2 MARK QUESTIONS

| Question Type | Question                                             | Mapping to TNMGRMU / GPAT / NIPER / Pharma Exams (Year) | Bloom's Taxonomy Level |
|---------------|------------------------------------------------------|---------------------------------------------------------|------------------------|
| 2 Marks       | Define QSAR.                                         | TNMGRMU (2019–2023)                                     | Remember               |
| 2 Marks       | Differentiate SAR and QSAR (any two points).         | TNMGRMU (2021), GPAT (2018)                             | Understand             |
| 2 Marks       | What is a physicochemical parameter?                 | TNMGRMU (2020)                                          | Remember               |
| 2 Marks       | Define partition coefficient (log P).                | GPAT (2019), Pharma Interviews                          | Remember               |
| 2 Marks       | What is Hammett's substituent constant ( $\sigma$ )? | TNMGRMU (2022)                                          | Remember               |
| 2 Marks       | Define Taft's steric constant.                       | GPAT (2020)                                             | Remember               |
| 2 Marks       | Mention any two applications of QSAR.                | Pharma Company Exams (2021)                             | Understand             |
| 2 Marks       | What is Hansch analysis?                             | TNMGRMU (2023), GPAT (2017)                             | Remember               |
| 2 Marks       | What is Free–Wilson analysis?                        | NIPER (2018)                                            | Remember               |
| 2 Marks       | Expand CoMFA and CoMSIA.                             | TNMGRMU (2022)                                          | Remember               |

## SECTION – B : 5 MARK QUESTIONS

| Question Type | Question                                                                 | Mapping to TNMGRMU / GPAT / NIPER / Pharma Exams (Year) | Bloom's Taxonomy Level |
|---------------|--------------------------------------------------------------------------|---------------------------------------------------------|------------------------|
| 5 Marks       | Compare SAR and QSAR with suitable examples.                             | TNMGRMU (2020, 2022)                                    | Understand             |
| 5 Marks       | Explain the history and development of QSAR.                             | TNMGRMU (2019)                                          | Understand             |
| 5 Marks       | Describe different types of physicochemical parameters used in QSAR.     | GPAT (2021)                                             | Understand             |
| 5 Marks       | Explain experimental methods for determination of partition coefficient. | TNMGRMU (2021)                                          | Apply                  |

|         |                                                                      |                           |            |
|---------|----------------------------------------------------------------------|---------------------------|------------|
| 5 Marks | Discuss Hammett's substituent constant and its significance in QSAR. | GPAT (2019)               | Analyze    |
| 5 Marks | Explain Taft's steric constant with examples.                        | TNMGRMU (2023)            | Understand |
| 5 Marks | Describe the basic principle of Hansch analysis.                     | GPAT (2018), NIPER (2017) | Analyze    |
| 5 Marks | Explain Free-Wilson analysis and its assumptions.                    | TNMGRMU (2022)            | Analyze    |
| 5 Marks | Write a short note on 3D-QSAR.                                       | TNMGRMU (2020)            | Understand |
| 5 Marks | Write differences between CoMFA and CoMSIA.                          | GPAT (2022)               | Analyze    |

## SECTION – C : 10 MARK QUESTIONS

| Question Type | Question                                                                             | Mapping to TNMGRMU / GPAT / NIPER / Pharma Exams (Year) | Bloom's Taxonomy Level |
|---------------|--------------------------------------------------------------------------------------|---------------------------------------------------------|------------------------|
| 10 Marks      | Explain the principles, advantages and limitations of QSAR in drug design.           | TNMGRMU (2019–2023)                                     | Analyze                |
| 10 Marks      | Discuss SAR versus QSAR in detail with suitable drug examples.                       | TNMGRMU (2021), Pharma Exams                            | Analyze                |
| 10 Marks      | Describe physicochemical parameters used in QSAR and methods of their determination. | GPAT (2020), NIPER (2019)                               | Apply                  |
| 10 Marks      | Explain Hansch analysis with equation, parameters and significance.                  | GPAT (2018, 2021)                                       | Analyze                |
| 10 Marks      | Describe Free-Wilson analysis, assumptions, advantages and limitations.              | TNMGRMU (2022)                                          | Analyze                |
| 10 Marks      | Explain 3D-QSAR approaches with emphasis on CoMFA.                                   | GPAT (2019), NIPER (2020)                               | Evaluate               |
| 10 Marks      | Discuss CoMSIA method in detail and compare it with CoMFA.                           | TNMGRMU (2023)                                          | Evaluate               |
| 10 Marks      | Write a detailed note on the role of QSAR in modern drug discovery.                  | Pharma Company Exams (2021–2023)                        | Evaluate               |