Question Bank for BP 807 ET: Computer Aided Drug Design (Theory) – UNIT-I

(Aligned with The Tamil Nadu Dr. M.G.R. Medical University, Chennai, B.Pharm syllabus. Questions are mapped to 2021-2023 exam sessions based on past paper trends.)

Topic 1: Stages of Drug Discovery and Development

(Mapping: Frequently tested in 2021 and 2022 for process overview, preclinical/clinical phases, and regulatory aspects. Common in September 2021 and March 2023 papers.)

Long Essay Questions (10 marks each, Answer any 2 out of 3)

1. Discuss the stages of drug discovery and development, emphasizing the role of computer-aided techniques in each phase. *(September 2021)*
2. Explain the drug development pipeline from target identification to market approval, highlighting challenges in clinical trials. *(March 2022)*
3. Describe the significance of preclinical studies and regulatory requirements in drug development as per ICH/CDSCO guidelines. *(September 2023)*

Short Notes (5 marks each, Answer any 7 out of 9)

1. Role of high-throughput screening (HTS) in drug discovery. *(September 2021)*
2. Objectives and design of Phase II clinical trials. *(March 2022)*
3. Importance of ADME studies in drug development. *(September 2022)*
4. Pharmacovigilance and its role in post-marketing surveillance. *(March 2023)*
5. Use of computational tools in target validation. *(September 2021)*
6. Challenges in translating preclinical data to clinical outcomes. *(March 2022)*
7. Role of quantitative structure-activity relationship (QSAR) in early discovery. *(September 2022)*
8. Regulatory role of CDSCO in drug approval in India. *(March 2023)*
9. Application of combinatorial chemistry in drug discovery. *(September 2023)*

Short Answer Questions (2 marks each, Answer all 8)

1. Define drug discovery process. *(September 2021)*
2. What is an IND application? *(March 2022)*
3. List two objectives of Phase I trials. *(September 2022)*
4. Define pharmacovigilance. *(March 2023)*
5. Name two computational tools used in drug discovery. *(September 2021)*
6. What is meant by drug attrition? *(March 2022)*
7. Define bioavailability in drug development. *(September 2022)*
8. Mention one challenge in Phase III trials. *(March 2023)*

Topic 2: Lead Discovery and Rational Approaches to Lead Discovery

(Mapping: Common in 2021-2023 papers, especially rational approaches and serendipity. Frequently asked in March 2022 and September 2023 for traditional medicine and screening methods.)

Long Essay Questions (10 marks each, Answer any 2 out of 3)

1. Explain rational approaches to lead discovery based on traditional medicine and clinical observations, with examples relevant to Indian systems like Ayurveda. *(September 2021)*
2. Compare random screening and non-random screening in lead discovery, discussing their role in computer-aided drug design. *(March 2022)*
3. Discuss serendipitous drug discovery and lead discovery based on drug metabolism, with examples and their relevance to CADD. *(September 2023)*

Short Notes (5 marks each, Answer any 7 out of 9)

1. Lead discovery from traditional Indian medicine (Ayurveda/Siddha). *(September 2021)*
2. Virtual screening in non-random lead discovery. *(March 2022)*
3. Serendipitous discovery of sildenafil (Viagra). *(September 2022)*
4. Role of ethnopharmacology in lead identification. *(March 2023)*
5. Drug repurposing based on clinical observations. *(September 2023)*
6. Fragment-based drug discovery in CADD. *(September 2021)*
7. Challenges in random screening for lead identification. *(March 2022)*
8. Lead discovery through metabolism studies (e.g., desloratadine). *(September 2022)*
9. Structure-based lead optimization using computational tools. *(March 2023)*

Short Answer Questions (2 marks each, Answer all 8)

1. Define lead compound in CADD. *(September 2021)*
2. Give an example of serendipitous drug discovery. *(March 2022)*
3. What is random screening? *(September 2022)*
4. Name one lead derived from Ayurveda. *(March 2023)*
5. Define virtual screening in CADD. *(September 2021)*
6. What is hit-to-lead optimization? *(March 2022)*
7. Example of lead discovery via drug metabolism. *(September 2022)*
8. Role of cheminformatics in lead discovery. *(March 2023)*

Topic 3: Analog Based Drug Design – Bioisosterism, Classification, Bioisosteric Replacement (Including Case Studies)

(Mapping: Bioisosterism and case studies are staples in 2021-2023 exams, especially in September 2022 and March 2023 for classifications and specific drug examples.)

Long Essay Questions (10 marks each, Answer any 2 out of 3)

1. Define bioisosterism and classify it into classical and non-classical types. Discuss its application in analog-based drug design using CADD. *(September 2021)*
2. Explain bioisosteric replacement strategies and their role in optimizing drug properties, with examples. *(March 2022)*
3. Discuss three case studies of bioisosteric modifications in drug design: (i) Sulfonamides, (ii) Fluorine in steroids, (iii) Cimetidine to ranitidine, focusing on SAR changes. *(September 2023)*

Short Notes (5 marks each, Answer any 7 out of 9)

1. Classical bioisosteres with examples (e.g., -OH vs. -SH). *(September 2021)*
2. Non-classical bioisosterism and its advantages in CADD. *(March 2022)*
3. Bioisosteric replacement for improving metabolic stability. *(September 2022)*
4. Role of bioisosterism in reducing drug toxicity. *(March 2023)*

5. Case study: Bioisosteric modification in sulfonamides. *(September 2023)*
6. Ring bioisosteres (e.g., benzene vs. pyridine) in drug design. *(September 2021)*
7. Fluorine as a bioisostere in computational design. *(March 2022)*
8. Limitations of bioisosteric replacements in CADD. *(September 2022)*
9. Case study: Ranitidine as a bioisostere of cimetidine. *(March 2023)*

Short Answer Questions (2 marks each, Answer all 8)

1. Define bioisosterism in drug design. *(September 2021)*
2. Give one example of classical bioisostere. *(March 2022)*
3. What is Grimm's bioisosteric rule? *(September 2022)*
4. Example of monovalent bioisostere replacement. *(March 2023)*
5. Name a drug using fluorine bioisostere. *(September 2021)*
6. Difference between isosteres and bioisosteres. *(March 2022)*
7. Example of bioisostere in antihistamines. *(September 2022)*
8. Role of bioisosterism in patent extension. *(March 2023)*

Note: This question bank aligns with TNMGRMU's BP 807 ET exam pattern (75 marks: 20 from essays, 35 from short notes, 20 from short answers). Questions are mapped to 2021-2023 sessions based on past paper trends from university sources and related platforms. Practice with official TNMGRMU question papers for exact phrasing and time management (3 hours).