**B. Pharm Final Year (8 th SEMESTER)**

#### **COMPUTER AIDED DRUG DESIGN**

**LONG ESSAYS (10 Marks)**

1. Explain various stages involved in drug discovery.
2. Explain the electronic and stearic parameters in QSAR with their applications.
3. Explain the different types of Molecular docking studies.
4. Explain various physicochemical parameters of QSAR with examples.
5. Elaborate De Novo drug designing giving emphasis on various approaches involved.
6. Elaborate Analog based drug designing giving emphasis on objectives and categories of analog designing.
7. What is a lead molecule? Discuss the various stages involved in identification of a lead molecule.
8. What is QSAR? Explain the Hansch analysis and Free Wilson analysis.
9. Define and classify Molecular docking and discuss various steps involved in the flexible docking.
10. Discuss classical and non-classical bioisosteric replacement strategies in analog based design of drugs with examples.
11. What is QSAR? Explain the electronic and steric parameters to be considered in QSAR analysis.
12. Define pharmacophore and discuss concept of pharmacophore mapping and pharmacophore based Screening.
13. What is lead compound? How lead compounds are generated and optimized in drug discovery?
14. Define and classify Molecular docking and discuss various steps involved in the flexible docking.
15. Discuss Hammett’s Substituent constant and Taft’s steric constant and give their importance.
16. Discuss the various Stages of drug discovery and development.
17. Explain the Hansch analysis and Free Wilson analysis and relationship between them.
18. Define and classify Molecular docking and discuss various steps involved in the flexible docking.
19. Explain Hansch analysis and Free Wilson analysis along with its advantages and disadvantages.
20. Explain various rational approaches to lead discovery.
21. Describe the virtual screening techniques.
22. What is docking? Explain the different types of docking and their applications.
23. Explain in detail the lead discovery based on drug metabolism and clinical observation with examples and structures.
24. Explain the concept of Quantitative structure activity relationship (QSAR). Enlist the different QSAR parameters.
25. Classify bio-isosterism approach with examples. Discuss of bio-isosterism replacement strategy with one case study.
26. Describe the theoretical determination of partition coefficient and electronic parameters in QSAR.
27. Define the term pharmacophore. Explain about the pharmacophore mapping suitable example
28. Define lead? Explain the different stages of drug discovery.
29. Explain in detail the history and development of QSAR.
30. Explain the different types of virtual screening techniques with examples.

**SHORT ESSAYS (5 Marks)**

1. Explain Bioisosterism. Classify with examples.
2. Explain few methods of determination of Partition coefficient.
3. Define Bioinformatics. Mention applications of bioinformatics.
4. Explain various approaches for De Novo design.
5. Explain Pharmacophore mapping and its applications.
6. Write a note on chemoinformatics in the drug discovery process.
7. Discuss the role of molecular and quantum mechanics in drug discovery.
8. Write a note on various parameters of molecular mechanics.
9. Explain different methods in determination of energy minimization.
10. What properties a lead compound should possess to develop as an orally active compound.
11. Discuss Hammett’s substituent constant and Taft’s steric constant and its role in predicting biological activity.
12. Explain the role of Pharmacophore.
13. Discuss various databases used in drug design and discovery.
14. What is automated De Novo design? Explain various stages involved in De Novo drug design.
15. Write a short note on energy minimization.
16. Discuss global minima.
17. Write a note on the role of bioinformatics in the drug discovery process.
18. Explain various parameters of molecular mechanics.
19. What is analog Based Drug Design? Explain with suitable examples.
20. Discuss about similarity based methods used in virtual screening.
21. Discuss Comparative Molecular Field Analysis (CoMFA)
22. Discuss the important aspect of pharmacophore mapping.
23. Discuss the importance of prediction and analysis of ADME properties in drug design
24. Briefly explain the importance of various databases in drug design?
25. Write a note on various energy minimization techniques used in molecular modeling study.
26. Briefly explain quantum mechanical approach in drug design
27. Explain in brief about the molecular mechanics in drug design
28. Define Lead molecule? Discuss Lead discovery in drug design.
29. Discuss about similarity based methods used in virtual screening.
30. Explain Hansch analysis and give its application.
31. Distinguish between Rigid docking, Flexible docking.
32. Discuss the importance bioinformatics in drug design
33. Enlist the various databases applications in drug design?
34. Explain the concept of molecular mechanics in drug design.
35. Discuss the role of quantum mechanical approach in drug design
36. Explain global energy minimization.
37. What is analog Based Drug Design? Explain with suitable examples.
38. Discuss the role of quantum mechanical approach in drug design.
39. Write a note on pharmacophore mapping.
40. Give an account of brief history and development of QSAR.
41. Discuss the importance Chemoinformatics in drug design
42. Enlist the various databases applications in drug design?
43. Explain various energy minimization techniques used in molecular modeling.
44. Discuss the various steps involved in pharmacophore based virtual screening.
45. Explain the various parameters of molecular mechanics in drug design.
46. Discuss the various stages involved in identification of a lead molecule.
47. Explain the role of quantum mechanical approach in drug design.
48. Discuss about similarity based methods used in virtual screening.
49. Describe the concept of molecular mechanics in drug design.
50. Explain various energy minimization techniques used in molecular modeling.
51. Discuss the importance of prediction and analysis of ADME properties in drug design
52. Discuss the importance Chemoinformatics in drug design
53. Discuss the important aspect of pharmacophore modeling.
54. Write experimental method of determination of logP.
55. Explain Hammett’s and Taft’s constants of QSAR.
56. Explain de novo drug design.
57. Discuss concept of pharmacophore mapping.
58. Write note on ADME databases.
59. Discuss importance of quantum mechanics in drug design.
60. Define bio-isosterism? Classify bio-isosterism with examples.
61. Write a note on Conformational analysis.
62. Explain different methods in determination of energy minimization.
63. Define bioinformatics? Explain its application in drug discovery.
64. Write a note on Chemoinformatics.
65. Explain serendipitous drug discovery with examples.
66. Explain about the molecular mechanics principles.
67. Explain the approaches for de novo drug design.
68. Explain different methods in determination of energy minimization.
69. Explain Hansch analysis and give its applications.
70. Explain the pharmacophore based screening.
71. Write a note ADME databases.
72. Discuss in brief various parameters of quantum mechanics
73. Write a note on a) Random and non-random screening.
74. Differentiate molecular mechanics and Quantum mechanics.
75. Define the term virtual screening. Explain the concept.
76. Define Chemoinformatics? Explain steps involved in chemical data curation.
77. Write a note on different stages of drug discovery.
78. Discuss the parameters of Hansch and Free Wilson analysis.
79. Discuss various methods for determination of energy minimization.
80. Define molecular docking. Explain rigid docking
81. Write note on ADME databases.
82. Write a note on analog based drug design.
83. Enlist the differences between SAR and QSAR?
84. Explain the different approaches of de novo drug design.
85. What is bioinformatics? Explain the applications of bioinformatics.
86. Give a brief account of flexible docking.
87. Describe in detail about chemoinformatics.
88. Explain energy minimization methods.
89. Explain in detail molecular mechanics.
90. Explain the process of global conformational minima determination.

**SHORT Answers (2 Marks)**

1. Define Free Wilson Analysis with examples.
2. Write the applications of QSAR.
3. Enlist two ADME databases.
4. Mention two Biochemical databases.
5. Define Lead molecule with examples.
6. Explain Lipinski rule of 5.
7. Define Random screening for lead optimization.
8. Define COMFA and COMSIA.
9. Write applications of pharmaceutical databases.
10. Define Global minima.
11. Mention any two lead optimization techniques.
12. Define bioisosterism with examples.
13. Explain Hansch analysis.
14. Compare SAR and QSAR.
15. Define COMSIA with its two applications.
16. Explain Lipinski rule of 5.
17. Define cheminformatics and mention its two applications.
18. Enlist any two pharmaceutical databases.
19. How are ADME databases are obtained.
20. Define Local minima.
21. Enlist various stages of drug design..
22. Define Random screening and Non-random screening.
23. Define partition coefficient and log P.
24. Enlist electronic and steric descriptors of QSAR
25. Compare SAR versus QSAR.
26. Define pharmacophore and De novo drug design.
27. Define the terms Bioinformatics and chemoinformatics..
28. List out the various chemical databases.
29. Write a note on importance of biochemical databases.
30. What is Conformational Analysis and give its applications
31. What is serendipitous drug discovery?
32. List out the various chemical databases.
33. Expand and give importance of COMFA and COMSIA.
34. Enlist various stages of drug design.
35. Define chemoinformatics and give its applications.
36. Define and classify molecular docking.
37. Compare SAR versus QSAR
38. What is Conformational Analysis and give its applications
39. Give the importance of pharmaceutical databases.
40. What is Lipinski's Rule of five?
41. Define and Classify Bioisosterism.
42. Enlist 1D and 2D descriptors of QSAR.
43. Define partition coefficient and log P.
44. What is lead optimization?
45. Give the application of 3D QSAR.
46. What is drug likeliness? Explain.
47. List out biochemical database’s.
48. What is Conformational Analysis and give its applications.
49. Give the importance of pharmaceutical databases.
50. Give the importance of various ADME properties in drug design.
51. Define Random screening and Non-random screening.
52. What is Hammett substituent constant?
53. Explain Lipinski’s rule of 5.
54. Describe extra precision docking.
55. Define bioinformatics and give its applications.
56. What is Conformational Analysis and give its applications.
57. Define lead optimization.
58. Enlist 1D and 2D descriptors of QSAR.
59. Give the importance of pharmaceutical databases.
60. Enlist the various databases used in drug design?
61. Mention the electronic parameters used in QSAR studies
62. Mention the steric parameters used in QSAR.
63. Expand COMFA and COMSIA.
64. Random and non-random screening.
65. Define global and local minima.
66. Lipinski’s rule of five.
67. Define lead optimization.
68. Define Chemoinformatics.
69. Enlist biochemical database’s.
70. Application of chemical database’s.
71. Write the application of molecular modelling.
72. Expand COMFA and COMSIA.
73. Define Lipinski’s rule of 5 .
74. Enlist the various database’s used in drug design.
75. What is CADD? Enlist the applications.
76. Define global and local minima.
77. Importance of partition coefficient in the drug action.
78. Applications of Free Wilson analysis.
79. Give the importance of biochemical database.
80. What is lead optimization?
81. Define lead molecule.
82. Give two methods of lead optimization
83. Taft’s steric constant.
84. Expand COMFA and COMSIA.
85. Define global minima.
86. Enumerate the applications of QSAR
87. List out the various chemical database.
88. Lipinski’s rule of five.
89. What is bio-informatics?
90. Enlist any two biochemical database’
91. Define lead optimization?
92. What is drug design?
93. What is CoMFA and CoMSIA
94. Define QSAR.
95. In partition coefficient studies, why n-octanol is used?
96. Applications of chemical databases.
97. Name any two biochemical databases
98. Applications of ADME databases
99. Define molecular modeling?
100. What is Lipinski’s rule of five.