Total No. of printed pages = 2

MPC 203T

Roll No. of candidate | | | | | | | | | | |

2023

M.Pharm. 2nd Semester End-Term Examination

COMPUTER AIDED DRUG DESIGN

Full Marks – 75

Time – Three hours

The figures in the margin indicate full marks for the questions.

1. Answer *all* questions : (10 × 2 = 20)

   (a) Differentiate between rigid docking and flexible docking.

   (b) What are the challenges stand up during De-novo design?

   (c) What is the meaning of serendipitious drug discovery:

   (d) Mention any two applications of Hansch analysis.

   (e) What do you mean by pharmacophore mapping?

   (f) What is the importance of log P during new drug discovery?

   (g) Mention any two software by which drug likeness can be determined.

   (h) Differentiate between global minimum conformation and bioactive conformation.

   (i) What is the main difference between structure based drug design and ligand based drug design?

   (j) Discuss in brief the importance of quantum mechanics in drug design.

2. Long answers (Answer *two* out of three) : (2 × 10 = 20)

   (a) What is Docking? Explain different types of docking and their applications.

   (b) Explain Hansch analysis and Free Wilson analysis with their advantages and disadvantages.

   (c) Elaborate De Novo Drug designing giving emphasis on various approaches involved.

[Turn over

3. Short answers (Answer *seven* out of nine) : $(7 \times 5 = 35)$

(a) Write a note on Homology modelling.

(b) Explain methods for determination of energy minimization.

(c) Discuss various databases used in drug discovery process.

(d) Discuss the importance of prediction and analysis of ADME properties in drug design.

(e) Discuss Lipinskis rule of five.

(f) Explain various parameters of molecular mechanics.

(g) Explain the role of pharmacophore.

(h) Discuss Hammett's substituent constant and Taft's steric constant.

(i) Discuss comparative molecular field analysis (CoMFA).
