THE TAMIL NADU DR. M.G.R. MEDICAL UNIVERSITY

[MPHARM 0921] SEPTEMBER 2021 Sub. Code: 2947
(OCTOBER 2020 EXAM SESSION)

M.PHARMACY DEGREE EXAMINATION
SEMESTER-II (PCI New regulations 2016)
PHARMACEUTICAL CHEMISTRY - MPC
PAPER III – COMPUTER AIDED DRUG DESIGN
Q.P. Code : 262947

Time : Three hours **Answer ALL Questions** **Maximum : 75 Marks**

I. Elaborate on: **(2 x 20 = 40)**

1. a) Explain briefly on various strategies utilized in homology modeling.
   b) Discuss briefly on various QSAR analysis methods in relation to biological activity.

2. a) Elaborate briefly on the strategic approaches on structure based and ligand based *In-silico* virtual screening protocols.
   b) Explain about the techniques utilized in De Novo drug design.

II. Write notes on: **(7 x 5 = 35)**

1. Write a brief note on the types of docking.
2. Brief on the development of HMG–CoA reductase inhibitors using molecular modeling strategies.
3. Give an account on CoMFA and CoMSIA methods in 3D QSAR studies.
4. Write a note on molar refractivity.
5. Brief a note on pharmacophore mapping techniques.
6. Derive Hammet substituent constant and explain the changes in its value related to electronic parameters.
7. Compare and contrast between global minimum conformation and bioactive conformation.

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