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

[LP 947] NOVEMBER 2019 **Sub. Code: 2947**

M.PHARM. DEGREE EXAMINATION
(PCI New regulations 2016)
SEMESTER-II
BRANCH–II – PHARMACEUTICAL CHEMISTRY – MPC
PAPER III – COMPUTER AIDED DRUG DESIGN

Q.P. Code : 262947

Time : Three hours **Maximum : 75 Marks**

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

1. Explain various physico chemical parameters involved in the study of Quantitative Structure Activity Relationship.

2. a) Write a note on various energy minimization techniques used in molecular modelling study.
   b) Explain briefly about the molecular modelling approaches in the discovery of DHFR inhibitors

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

1. Write a note on 3D-QSAR approach.
2. Brief out on ligand based drug design.
3. State the Lipinski's rule of five and explain the importance of the parameters in drug discovery.
4. Write a note on 3D structure alignment.
5. Explain De Novo drug design.
6. Brief out on PLS & CoMFA analysis.
7. Brief out on fragment based drug design.

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