

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

[LQ 0121]

JANUARY 2021

Sub. Code: 2947

(APRIL 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. Discuss in detail the molecular and quantum mechanics in drug design.
2. a) Discuss in detail 3D-QSAR approaches and contour map analysis.
b) Explain homology modeling and the method adopted for the generation of the 3D structure of a protein.

II. Write notes on:

(7 x 5 = 35)

1. Briefly explain the Hammett equation parameters.
2. Discuss the statistical methods used in QSAR analysis.
3. Write a short note on global energy minimization.
4. Explain the physico chemical parameters that affect biological activity.
5. Write short note on De Nova drug design.
6. Short notes on pharmacophore mapping.
7. Explain insilico virtual screening protocols.
