CODE NO: 1223/PCI

FACULTY OF PHARMACY

M.Pharmacy (Pharmaceutical Chemistry) II-Semester (PCI) (Main)

Examination, August 2018

Subject: Computer Aided Drug Design

Time: 3 Hrs **Max. Marks: 75**

Note: Answer any Five questions. All questions carry equal marks

1. a) Discuss abt Substituent Hydrophobicity constant, Hammet constant and Taft steric constant
   b) Give a hypothetical Hansch equation for compnds with higher log p Values and explain each term (8+7)

2. a) Enumerate the steps involved in 3D QSAR studies to predict the biological activity
   b) Write the advantages of Free Wilson analysis (8+7)

3. a) Write a note on molecular mechanics
   b) Discuss abt the importance of energy minimization in molecul ar modeling (8+7)

4. a) Explain abt varis docking methods and write their advantages
   b) Discuss abt Knowledge based and Consensus scoring techniques in docking (8+7)

5. a) What is homology modeling and enumerate steps involved in homology modeling (9+6)
   b) Write a short note on de novo drug design

6. Write a short note on
   a) Drug likeness screening
   b) Pharmacophore based virtual screening (8+7)

7. a) Explain the techniques to predict the active site of a receptor in denovo drug design
   b) Explain, how new DHFR inhibitors are designed using molecular docking? (8+7)

8. Write a short note on
   a) Requirements to perform QSAR studies with suitable example
   b) Statistical methods used in QSAR (8+7)

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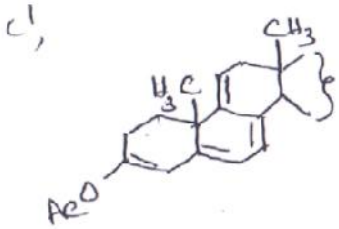
(i)



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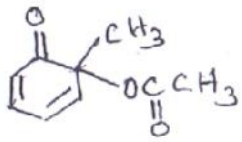

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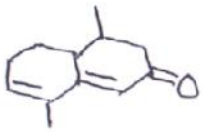

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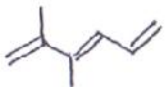
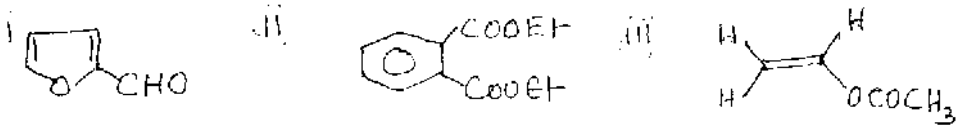


8. a) Draw a rgh HNMR Spectra for the following compnds with proton splitting



b) How do y interp ret the following functional grps in IR? (any six)

i) NO_2 ii) SO_2 iii) NH_2 iV) R - C(=O) - OR V) CONH

Vi) COOH Vii) CN Viii) CHO ix) - C(=O) - V) OH (9+6)

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