Seat No.: _____ Enrolment No._____

GUJARAT TECHNOLOGICAL UNIVERSITY

M. PHARM. - SEMESTER – II • EXAMINATION – WINTER 2012

Subject code: 2920201 Date: 12-01-2013

Subject Name: Drug Design and Discovery

Time: 10.30 am - 01.30 pm Total Marks: 80

Instructions:

1. **Attempt any five questions.**
2. **Make suitable assumptions wherever necessary.**
3. **Figures to the right indicate full marks.**

Q.1.a. Give detail account on importance of stereochemistry and hydrogen bonding in drug action. **(10)**

b. What is structure based drug design? How it is achieved ? What is the importance of target structure ? How is it derived? **(06)**

Q.2.a. What are the methods used to identify lead molecule ? **(05)**

b. Write a note on lead modification and lead optimization. **(06)**

c. Write a note on Importance of isosterism in drug design. **(05)**

Q.3.a. What are the different targets for drug in biological system ? Give mechanism of action each. **(10)**

b. What are the different approaches for new drug discovery? Discuss in brief about each. **(06)**

Q.4.a. QSAR is an important tool of drug design - How? Discuss basic principle of Hansch and Free Wilson model. **(10)**

b. How capacity factor (k') is determined experimentally. **(03)**

c. Calculate first order molecular connectivity of paracetamol.
(δ value –NH- = 4, =O =6; -O- = 6; -OH = 5) **(03)**

Q.5.a. Following is an equation and statistical parameters obtained from Hansch analysis of a series. **(05)**

$\log IC_{50} = 3.22(\pm 0.54)\log P + 1.16(\pm 0.21)\sigma^{*} + 0.53(\pm 0.16)MR - 7.38(\pm 0.62)$

$n=21$; $r=0.926$; $r^2=0.858$; $s=0.316$; $F_{3,18}=14.36$

Interpret this equation and give your suggestions for lead modification to obtain more potent molecules.

b. What are the recent advances in QSAR ? Discuss in brief about the different types of models used for it. **(08)**

c. write a note on docking. **(03)**

Q.6. Write a short note on following **(16)**

i. Designing a drug based on enzyme inhibition
ii. Molecular mechanics in drug design.
iii. Pharmacophore mapping
iv. *De novo* drug design

Q.7.a. "Optimised lead doesnot guarantee Drug molecule" Why? What are the factors guiding optimized molecule to drug ? Discuss in brief about each with suitable examples. **(08)**

b. What is mean by Prodrug ? How does it change the various properties of the drug? Discuss with suitable example. **(08)**

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