Reg. No.										

Manipal Institute of Technology, Manipal

(A Constituent Institute of Manipal University)

VII SEMESTER B.TECH (BIOTECHNOLOGY)

END SEMESTER EXAMINATIONS, NOV/DEC 2015

SUBJECT: MOLECULAR MODELING AND DRUG DESIGN [BIO 401E]

REVISED CREDIT SYSTEM

Time: 3 Hours MAX. MARKS: 50

Instructions to Candidates:

- Answer **ANY FIVE FULL** questions.
- Missing data may be suitable assumed.

1A.	Describe about adrenergic, cholinergic and dopaminergic type of receptors. Illustrate the mechanism of ligand-gated ion channel receptors	**5**
1B.	Noradrenaline shows slight selectivity for the α-receptor, whereas isoprenaline shows selectivity for the β-adrenoceptor. Adrenaliene shows no selectivity and binds equally well to both α- and β-adrenoceptors. Suggest an explanation for these differences in selectivity.	**3**
1C.	Explain the role of carrier proteins. What would be the effect of a small molecule that blocks the re-uptake of seretonine?	**2**
2A.	How a drug can be smuggled into the cells? Explain with examples	**3**
2B.	Do natural products are successful as a drug? For what contribution the Nobel Prize in Physiology or Medicine was given this year? Explain the transformation of Avermectin to Ivermectin.	**5**
2C.	Do receptors are always membrane bound? Add few exceptions with examples	**2**
3A.	Differentiate the Lipinski's threshold for a drug, a herbicide and a pesticide	**3**
3B.	Design a competitive agonist for cAMP	**4**
3C.	How would you improvise the solubility and stability of the designed drug (**question 3B**)?	**3**

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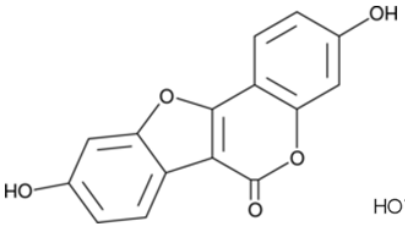
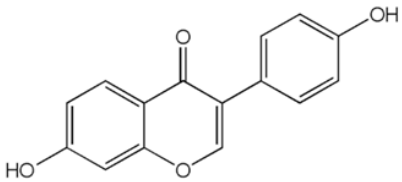
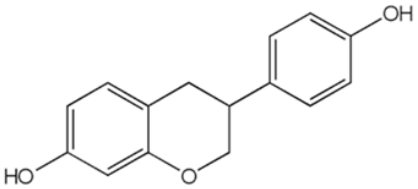
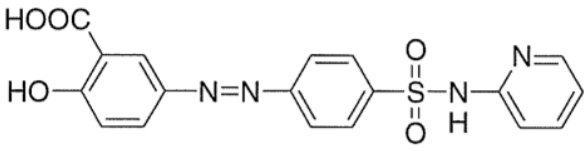
4A.	How good is to target nucleic acids? Explain the role of DNA intercalators, alkylating agents and chain cutters with an example each	**4**
4B.	Using the chemical graph theory compare the structural similarities of the following biologically active molecules (phytoestrogens)  **Coumestrol**  **Daidzein**  **Equol**	**4**
4C.	What are pharmacophores? Illustrate the pharmacophores for the structures showed in **question 4B**.	**2**
5A.	What is drug repurposing? Explain with some examples	**3**
5B.	Explain the metabolism of the 'Sulfasalazine'- a prodrug used against gut infections 	**3**
5C.	Penicillin methyl ester is an effective antibacterial agent in mice and rats, but it was found to be inactive in rabbit, dog and humans. Why does this happen? Also add your opinion on animal testing	**4**
6A.	Write a note on Quantitative Structure Activity Relationship (QSAR)	**3**
6B.	Johnson and Maggiora (1990) postulated that molecules having similar structures and properties should also exhibit similar activity – contemplate.	**3**
6C.	List out the challenges in drug design for the present and future.	**4**