Reg. No.										

MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

A Constituent Institution of Manipal University

VII SEMESTER B.TECH. (BIOTECHNOLOGY)

END SEMESTER EXAMINATIONS, NOV/DEC 2017

SUBJECT: PE 6-MOLECULAR MODELING AND DRUG DESIGN [BIO 4012]

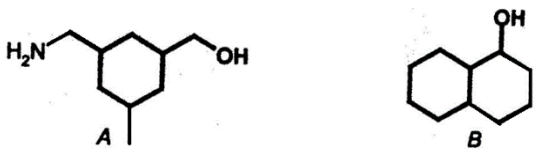
REVISED CREDIT SYSTEM

Time: 3 Hours MAX. MARKS: 50

Instructions to Candidates:

- Answer **ALL** the questions.
- Missing data may be suitably assumed.

1A.	Describe and illustrate the signal transduction mechanism of G-protein coupled receptors with stimulatory G protein (Gs)	**4**
1B.	Differentiate Agonists from Antagonists with an example each	**2**
1C.	'Structural proteins are not usually drug targets'. Describe an exception to this with examples	**4**
2A.	Describe about adrenergic, cholinergic and dopaminergic type of receptors	**3**
2B.	"Similar algorithms – diverse applications". Discuss its applicability on cheminformatics research with examples.	**4**
2C.	State the Lipinski's rule of 5 with explanation. Also mention the add-ons to this rule	**3**
3A.	What are chemical descriptors? Explain with examples	**3**

3B.	Define pharmacophore and emphasize on 3-Point Pharmacophore	**4**
3C.	What is comparative molecular field analysis? What are the recommendations to perform such CoMFA studies?	**3**
4A.	Whether enantiomers are agonists or antagonists? Explain with an illustration	**3**
4B.	How would you improvise the solubility and stability of the designed drug for a specific disease target?	**4**
4C.	A 32-year-old woman received cyclosporine as anti-rejection therapy followed by kidney transplant. She was also administered ketoconazole for treating fungal infection. A week later she developed worsening kidney failure and seizures? what happened?	**3**
5A.	Johnson and Maggiora (1990) postulated that molecules having similar structures and properties should also exhibit similar activity – contemplate.	**3**
5B.	Compute the similarity of the compounds 'A' and 'B' using Tanimoto coefficient 	**4**
5C.	Elaborate about the design considerations for a pesticide.	**3**