MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

(A constituent unit of MAHE, Manipal)

VII SEMESTER B.TECH. END SEMESTER EXAMINATIONS

NOVEMBER 2019

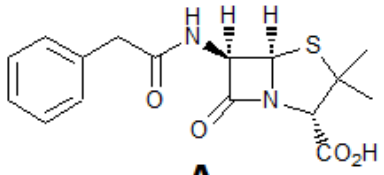
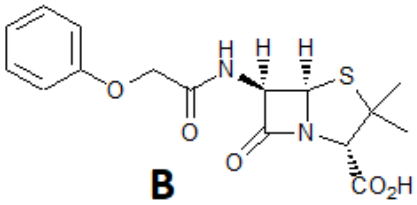
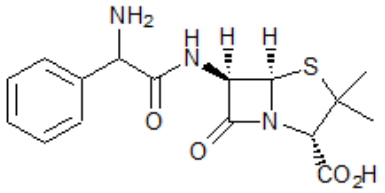
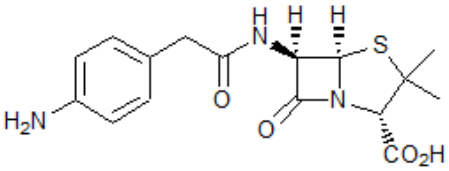
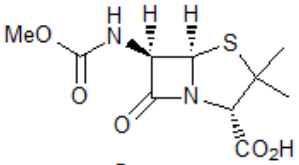
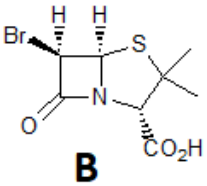
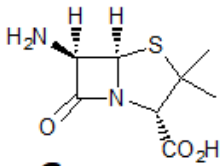
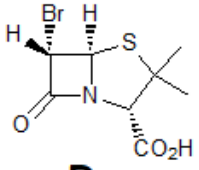
SUBJECT: [BIO 4012] Molecular Modeling and Drug Design [PE6]

Date of Exam: **28/11/2019** Time of Exam: 2-5 pm Max. Marks: **50**

Instructions to Candidates:

- Answer ALL the questions & missing data may be suitable assumed

1A.	Differentiate potency, affinity and efficacy of drugs with reference to the functional groups	**3**
1B.	Do any of the molecular descriptors relate to their potency, efficacy or affinity? Describe them	**4**
1C	Explain about receptor dimerization with an example	**3**
2A.	Membrane proteins account for up to two thirds of known drug targets, demonstrating they are "druggable". Among the membrane proteins integrated in the cell membrane. Which one would you choose druggable for treating cancer? Give explanation	**5**
2B.	Illustrate and describe the signal transduction pathway for G-protein coupled receptors	**5**
3A.	How would you assess whether natural compounds are lead-like or drug-like?	**4**
3B.	What are the advantages and disadvantages of natural products and lead compounds?	**3**
3C.	Differentiate prodrugs from leads	**3**
4A.	Describe about the set of methods used in ligand-based drug design	**4**
4B.	Write about the drug design strategies to increase solubility and stability of the drug?	**3**
4C.	Comment on network pharmacology and its applications in drug repurposing	**3**

5A.	Briefly discuss about the fundamentals of QSAR. Add a note on QSAR parameters related to chemical structure and biological activity	**5**
5B.	To produce a drug in large scale, fermentation is usually done to increase the yield of the desired product. Among the penicillin structures (given below), which one of the following penicillin cannot be produced by fermentation? Why?  **A**  **B**  **C**  **D**	**3**
5C.	Which of the following structures is crucial to the preparation of semi-synthetic penicillins? Why?  **A**  **B**  **C**  **D**	**2**