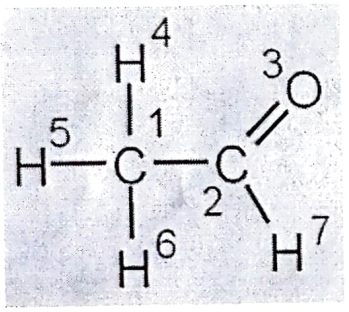
JAMIA HAMDARD
Department of Computer Science & Engineering
School of Engineering Sciences & Technology
New Delhi-110062

Paper Name:Chemoinformatics, chemogenomics and immunoinformatics
Paper Code: MCSB 204
Time: 2.5 Hours

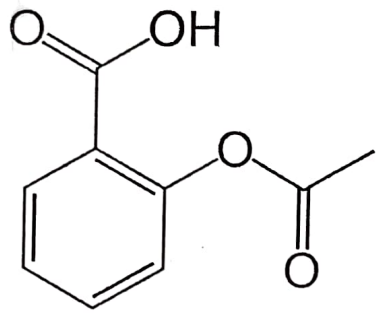
Maximum Marks: 60

Section A

Q.No.	Question	Marks	CO	BL
1.	What is an B cell and T cell epitopes? Name at least two-two tools for Bcell and Tcell epitope prediction.	4	CO1 CO3	BL1
2.	Write the adjacency matrix (with and without H- information) of the following compound. 	4	CO4 CO5	BL1 BL2 BL5
3.	What is drug metabolism? Name a few types of reactions involve in drug metabolism. What are the two phases of drug metabolism? How rate of drug metabolism effect different patients?	4	CO2	BL1 BL2 BL3
4.	Name at least 4 chemoinformatics databases and their uses and applications.	4	CO5	BL1 Bl3
5.	Explain the followings: • statistical mechanics • macroscopic and microscopic properties of a molecular system	4	CO4 CO5	BL1 BL2

Section B

Note: Attempt any four.

Q.No.	Question	Marks	CO	BL
1.	What is reverse vaccinology? How reverse vaccinology and machine learning is used for developing covid 19 vaccine?	10	CO1 CO2 CO3	BL1 BL3 BL5
2.	What do you understand by the term classical force field? What are bonded and non-bonded terms in a force field?	10	CO2	BL1 BL2 BL3
3.	What Is Morgan Algorithm? Explain the numbering scheme and iteration steps in Morgan Algorithm for the following compound. 	10	CO4 CO5	BL1 BL2 BL3 BL4
4.	Explain the following with examples in detail: • Molecular surface and algorithms to visualize molecular surfaces. • Molecular substructure searching algorithm	10	CO2 CO4 CO5	BL1 BL2 BL3
5.	What is CANGEN algorithm and its uses? What are the initial set of invariants for each atom in CANGEN Algorithm for numbering the atoms in a molecule? How do we calculate rank and new invariant at each iteration?	10	CO2 CO4 CO5	BL1 BL2 BL3 BL4
6.	Explain the following: • Parmacogenetics • Genetic drug response profile • different layers of InChI notation • SMILE, provide few examples.	10	CO2 CO3 CO4 CO5	BL1 BL2 BL3