INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

END SEMESTER EXAMINATION – BT 305: Computational Biology

April 29, 2024. Maximum Marks: 70 Time: 3 hours

Section A: 5 marks for each question

1. The SMILES representation of four molecules are as follows. Attempt to draw an approximate 2D structure of these molecules.

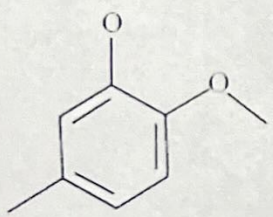
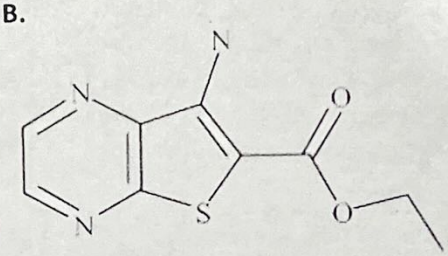
CCO

CC(=O)O

C1CCCCC1

c1cnccc1

2. Write the 1D string representation (SMILES) for the following molecules.

A.	B.
	

3. According to Hansch equation, how is the activity of a drug related to its hydrophobicity. How is the biological activity of a molecule related to its electronic characteristics and hydrophobicity?

4. Explain briefly the following concepts.
   A) Simulated Annealing B) Energy minimization C) RMSD based clustering D) Solvent accessible surface area.

5. A) Attempt to write an additive equation for free energy of binding in a molecular docking experiment.

   B) Free energy of binding can also be expressed based on simple molecular mechanics-based scoring functions. What are the most likely variables (or components) in such free energy estimations.

6. Explain briefly the following concepts.
   A) Pharmacophore B) Receptor C) Lipinski rule of five D) Molecular descriptor.

Section B: 20 marks for each question

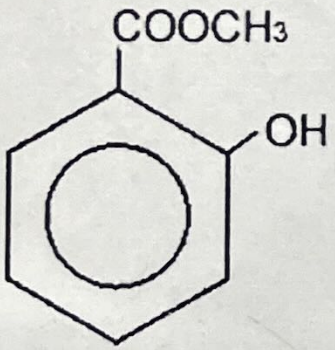
7. A) Bit strings for query and test molecules in a typical fingerprinting exercise is given below.

Mol 1	0	1	1	0	0	1	1	1	0
Mol 2	1	1	0	1	1	0	0	0	0
Mol 3	1	1	0	1	1	1	0	1	1
Mol 4	1	0	1	1	0	1	1	0	0

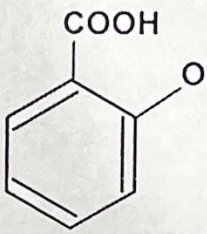
Calculate Tanimato coefficients for structure comparison and attempt the following question:

If receptors of the four candidate structures Mol 1 Mol 2 Mol 3 and Mol 4 are respectively Rec 1, Rec 2, Rec 3 and Rec 4. Which molecule is more likely to bind with maximum number of Receptors? Rationalize your answer?

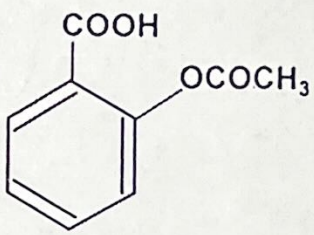
B) Suppose we are performing an experiment of structure based molecular profiling for methyl salicylate (below structure) in a structure pool of four members on the right hand side, how do we determine the closest structure by calculating Tanimato coefficient?



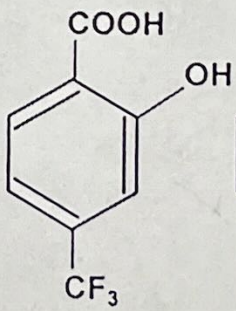
Salicylic acid



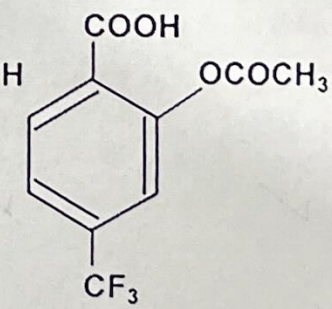
Aspirin



HTB



Triflusal



8. Using all three genetic operators (Selection, Crossover and Mutation), maximize the function $f(x) = x^3$, with 'x' lies in the interval 0 to 30. Generate initial population as 6, 9, 17 and 23.

End of Questions