BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: B. TECH. **SEMESTER : V**
BRANCH: BIOTECH. **SESSION : MO/2022**

SUBJECT: BE328 MOLECULAR SIMULATION OF BIOMOLECULES

TIME: 3:00 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
***4*. Before attempting the question paper, be sure that you have got the correct question paper.**
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

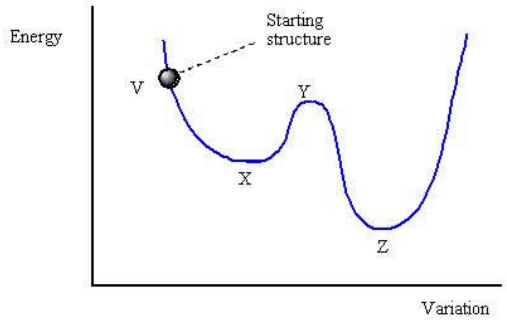
Q.1(a) Enlist and discuss all the criteria to rank the docked conformations [2]
Q.1(b) Explain all the components of the master equation of molecular docking. How different components contributes to the binding energy. [3]
Q.1(c) Explain one of the search algorithms in the context of molecular docking. [5]

Q.2(a) What are the main differences between molecular dynamics and molecular mechanics? [2]
Q.2(b) Enlist the major requirements of a good MD integrator in detail. [3]
Q.2(c) Discuss the different variants of the spherical cut-off scheme in detail with their limitations. [5]

Q.3(a) Explain the algorithm of monte Carlo simulations with its acceptance/rejection criteria. [2]
Q.3(b) What are the atom types in the force field? Why do we need them? [3]
Q.3(c) What is the forcefield? How are forcefields developed? Why can't we mix two force fields? Explain all in detail. [5]

Q.4(a) Why does cut-off not drastically reduce the computational time in MD? [2]
Q.4(b) In molecular mechanics force field contribution of the angle energy term of a water molecule is 18.16 kJ/mol for 120.6° angle. Calculate the equilibrium angle θ0 given that angle force constant k_θ is 55 kcal mol^{-1} $radian^{-2}$. Angle energy term is expressed as $E_\theta = ½\ k_\theta\ (\theta - \theta_0)^2$. [3]
Q.4(c) Discuss the necessity of a neighbor list in MD and explain one of the neighbor list algorithms in detail. [5]

Q.5(a) Plot mentioned below shows the stability of a molecule as its structure varied during the minimization process. What terms are used to describe points X and Z and why? [2]



Q.5(b) Considering the above graph, if energy minimization was carried out on a starting structure (point V), at which point would energy minimization stop and why? [3]
Q.5(c) Discuss one of the energy minimization algorithms in detail. [5]

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