CENTRAL UNIVERSITY OF SOUTH BIHAR

Department of Bioinformatics

End Term Open Book Examination   Session: **2020-22**   Semester -**2ⁿᵈ(Jan-June 2021)**

Programme: **M.Sc. (Bioinformatics)**   Date**:…………**
Course Code: **MSBIS2002C04**   Course Title: **Bio. Mol. Mod. & Simulation**
Duration: **2½ hours**   Course Credit: **04**
Max Marks: **50**

Note: Answer any 10 Questions each carry 5 marks.

Instructions:

1. *Preferably write your answers on A4 size plain paper (non-ruled) sheets.*
2. *Write your required details on the first page in the same order as specified below:*

Name:……………………… ……... Programme:………………. …...Semester: ……………..

Course Title:……………………………………………… Course Code:……………………

Total No. of pages Used:………… Date:…………… Signature:………………………….…

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3. *After completing the examination, write page number on the top right corner of each page in the format: 1/x, 2/x, …., x/x where 'x' is the total number of pages used. If you have used total 6 pages then your page numbers will be 1/6, 2/6,……….6/6.*

4. *The students have to write the answers on both side of the sheet (A4 size plain paper non ruled sheet).*

5. *The questions asked here are basically designed to assess the interpretation and application of knowledge, comprehension skills, and critical thinking skills rather than only recalling capacity.*

6. *Total twelve short answer questions of **five points each** are given covering the entire course content.*

7. *Answer **any ten** questions in total in maximum **two and half hours**.*

8. *The maximum limit to answer a question is 200 -300 words.*

9. *At the start of the examination all the questions will be released through e-mail and/or WhatsApp.*

10. *The total time limit to attempt the question paper is **two and half hours**. Along with the two and half hours, extra 30 minutes will be given for IT related activities such as downloading questions, scanning of answer sheets and uploading/emailing them.*

11. *After completing the examination within the stipulated time (two and half hours, scan your answer sheets or click pictures and submit it electronically in **one single file** (preferably PDF) to the course instructor through e-mail (**durgvijaysingh@cub.ac.in**) strictly within stipulated time limit for submission (Three hours). Before submitting, **rename your file and keep your name and enrolment number as file name.***

12. ***Please note** that do not use these extra 30 minutes for writing answers. Rather, finish writing as soon as possible within two and half hours and immediately submit your answers in the prescribed way given below. **Due to any reason, if a student is unable to submit the answer sheet file within the time limit, the university will not consider this examination and conduct another examination in the conventional mode whenever the conditions return to normal and circumstances permit or the university deems suitable. No other option or reason shall be entertained***.

13. *In case you feel difficulty in submitting the answer sheet file through e-mail, then you are required to submit it to the concerned course instructor through WhatsApp **within the stipulated time only** and email it later on (within 48 hours) along with the screen shots of WhatsApp submission.*

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Question Paper (Answer any 10 questions)

1. An oligopeptide of 13 amino acids (all amino acids are alanine) forms a typical helical conformation. Enumerate the number of hydrogen bonds in the helix? What will happen if the 7th amino acid is replaced with a proline amino acid?

2. What will happen if a native protein having four interchain disulphide bonds treated with the following.
    a. When it is treated with 8 M urea
    b. When protein is treated with 8M urea and β-mercaptoethanol
    c. Abrupt removal of both denaturing agents followed by the addition of trace amounts of β-mercaptoethanol.

3. Why biological samples were dried out and are damaged when electron beams hit the sample in a vacuum? How the problem was addressed? Which form of water allows the electron beams to reach up to the samples and why.

4. How many confirmations will be possible for the length of 100 amino acid proteins? Assume, each amino acid have only three conformational states. How much time will it require to sample all the conformations, if the fastest motion is assumed as 10^{-15} Sec? Do you think it is possible to sample all conformational states? If not, then how nature does the same?

5. A student wishes to model a protein that has shown a sequence identity of 20%. The amino acids secondary structure prediction shows that it belongs to the alpha-helix only protein family.
    a. Do you think the protein could be modelled? Explain with your reasoning?
    b. How much sequence identity is required to model a protein of length 25 amino acids and 250 amino acids?

6. What are the different parameters of protein structure validation? Discuss in terms of stereochemistry, folding and packing? Enlist the software suitable for each category.

7. What is the profile method of fold prediction (threading)? Discuss the importance of physicochemical descriptors used in the profile method of 3D structure prediction.

8. What was the drawback in the Verlet method and how velocity Verlet algorithm addresses the issue?

9. What artefacts may you see, if the simulation of a cytosolic protein is performed in a vacuum? What is the importance of periodic boundary conditions?

10. Why do we not prefer the ST2 water model for simulation? What is the benefit of considering water as rigid body geometry?

11. What is the optimum time step in MD simulation? What may happen if we consider very small and very large time steps? Explain with example.

12. How the simulation is performed at constant temperature and pressure? How the temperature and pressure are scaled?

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