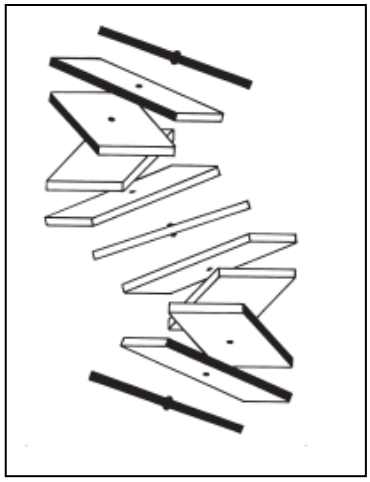
BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI (RAJ.)
FIRST SEMESTER 2023-2024
BIO F417, BIOMOLECULAR MODELING
COMPREHENSIVE EXAMINATION
TOTAL WEITAGE 35% Date: 20.12.2023 DURATION: 3Hrs. (Part A & Part B)
Total Marks (23+47) =70

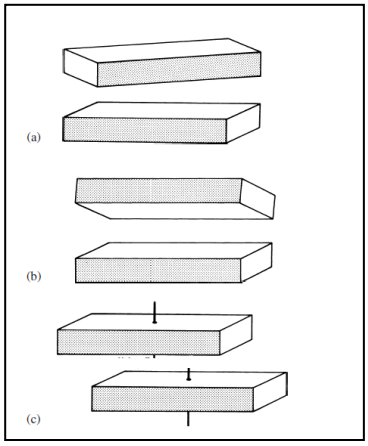
- **Answer Part A and Part B in separate answer sheets.**
- **Irrelevant answer may attract penalty.**

PART – A (CLOSED BOOK) (Max. duration: 1 Hr., Max. Marks 23)

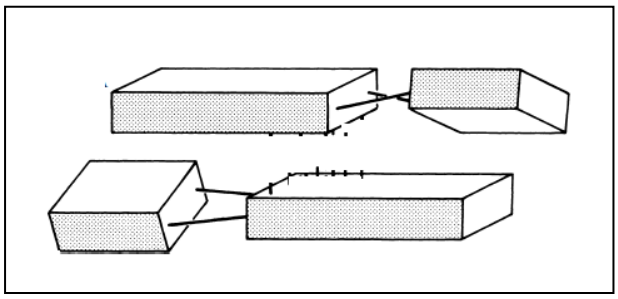
1. a) Mention all non-zero basepair and step parameters (which ever applicable) with appropriate sense (positive or negative) of each of the following set of figures. **[3X1.5=4.5]**

i) ii)





iii)



Ans: **Basepair** **Step**

i) **- Slide, +rise, +Twist,**
ii) **+Slide, +roll, +Twist**
iii) +Propeller Twist **+Rise**

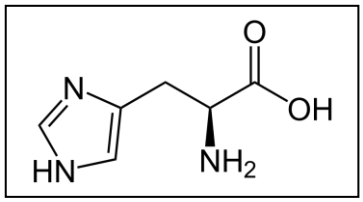
b) Explain with at least one example how does small motion of the basepair affects the overall structure of DNA. **[1.5]**

2.a) What would be the utility of Ramachandran Plot? **[1]**

b) What will be the importance of understanding secondary structural information of protein? **[1]**

c) Explain the hydrophobic collapse model of protein folding. **[2]**

3.a) Draw SMILE representation of the following molecule. **[2]**



Ans: O=C([C@H](CC1=CNC=N1)N)O

b) Why is model validation an important step in modeling technique? **[1]**

3. Write a short note on the following Term. [**2X5=10**]

i) CASP **ii**) Ab initio technique of protein modeling **iii**) Energy Minimization **iv)** DNA structural parameters **v)** Side chain rotamers.

****************************Good Luck**

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PART – B (OPEN BOOK) (Max. duration: 2 Hrs., Max. Marks 47)

1. The attached article is part of a research article in the area of molecular dynamics and protein folding. Read the article and answer the following questions.

i) What is the principle of MELD (modeling employing limited data), an enhanced sample technique? **[3]**

ii) What are the differences between the classical MD technique and ML x MELD x MD technique? **[3]**
iii) What are the advantages of using ML x MELD x MD technique? **[3]**
b) Write the abstract of this article. **[6]**
c) What is the objective/s of this study? **[3]**
d) Summarize the conclusion of this study. **[3]**
e) Suggest an appropriate title for this article. **[2]**
f) What would be the major challenge of studying protein folding through classical molecular dynamics techniques? **[4]**
g) What are the limitations of the techniques employed in this study? **[3]**

2. a) Predict the possible secondary structure of the following piece of polypeptide sequence using the Chou-Fasman method. **[6]**
Phe-Glu-Ala-Ala-Met-Cys-Lys-Trp-Glu-Ala-Gln
b) Draw Phe-Glu-Ala-Ala tetra-peptide with LDLD configuration on Cα atoms and with following torsion angles specification. **[5]**

ψ1(°)	ω1(°)	ϕ2(°)	ψ2(°)	ω2(°)	ϕ3(°)	ψ3(°)	ω3(°)	ϕ4(°)
180	180	0	180	0	180	0	180	0

c) Draw (Newman projection) each of the backbone torsion angles of a typical B-DNA structure. **[6]**

**********Good Luck**********