

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATIONS-2022

M.Sc.-II Semester (BT)

COURSE CODE (CREDITS): 20MS1BT213 (2)

MAX. MARKS: 35

COURSE NAME: Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar, Dr. Tiratha Raj Singh

MAX. TIME: 2 Hours

Note: All questions are compulsory. Marks are indicated against each question in square brackets.

Q1. Realize the SOP method for MSA using a set of 5 sequences of length (7 characters or less) each. Use scoring system as follows: Match = 1, Mismatch = 0, Gap Penalty = -1. [4]

Q2. Differentiate between the following: [4*1.5=6]

- (a) Hamming vs Edit distance (b) Pairwise and Multiple sequence alignments
(c) Exact and Heuristic algorithms (d) BLAST and FASTA

Q3. Interpret various types of phylogenetic reconstruction methods. Describe UPGMA method for the sequences taken in Q1. [3]

Q4. Assess STAR alignment for the generation of MSA with an example data set. Use same scoring system as provided in Q1. [4]

Q5. Give brief account on the following questions in context to protein conformation:

- 1) Amino acids may exhibit different structural conformation in peptides. What will be the effect of a cis-conformation on energetics of a dipeptide containing arginine and phenylalanine residues? [2]
- 2) Proline is a special amino acid found in proteins. Briefly discuss its effects on the conformation of protein structure. [2]
- 3) Dihedral angle describes the rotation of the chain around the middle bond. Describe the properties and role of Omega (ω) dihedral in protein structure and how it's different from Ramachandran angles Phi (ϕ) and Psi (ψ). [3]

Q6. Considering an emergency situation such as COVID-19 for which no FDA approved drugs are available, how virtual screening approaches can prove to be useful for identifying potential drugs? [3]

Q7. Find out the score for alpha-helix for the given sequence using following 17x20 matrix. [3]
 Sequence: TAKVIEEVSDMFAFIARCL

Amino acid residue	Residue position† (centinats)																
	$j-8$	$j-6$	$j-4$	$j-2$	j	$j+2$	$j+4$	$j+6$	$j+8$	$j+10$	$j+12$	$j+14$	$j+16$	$j+18$	$j+20$	$j+22$	$j+24$
Gly	-5	-10	-15	-20	-30	-40	-50	-60	-80	-60	-50	-40	-30	-20	-15	-10	-5
Ala	5	10	15	20	30	40	50	60	65	60	50	40	30	20	15	10	5
Val	0	0	0	0	0	0	5	10	14	10	5	0	0	0	0	0	0
Leu	0	5	10	15	20	25	28	30	32	30	28	25	20	15	10	5	0
Ile	5	10	15	20	25	20	15	10	5	0	-10	-15	-20	-25	-20	-10	-5
Ser	0	-5	-10	-15	-20	-25	-30	-35	-39	-35	-30	-25	-20	-15	-10	-5	0
Thr	0	0	0	-5	-10	-15	-20	-25	-26	-25	-20	-15	-10	-5	0	0	0
Asp	0	-5	-10	-15	-20	-15	-10	0	5	10	15	20	20	20	15	10	5
Glu	0	0	0	0	10	20	30	40	50	60	70	78	78	78	78	70	60
Asn	0	0	0	0	-10	-20	-30	-40	-51	-40	-30	-20	-10	0	0	0	0
Gln	0	0	0	0	5	10	20	30	40	50	60	70	78	78	70	60	50
Lys	20	40	50	55	60	60	50	30	23	10	5	0	0	0	0	0	0
His	10	20	30	40	50	50	50	30	12	-20	-10	0	0	0	0	0	0
Arg	0	0	0	0	0	0	0	0	-9	-15	-20	-30	-40	-50	-50	-30	-10
Phe	0	0	0	0	0	5	10	15	18	15	10	5	0	0	0	0	0
Tyr	-5	-10	-15	-20	-25	-30	-35	-40	-45	-40	-35	-30	-25	-20	-15	-10	-5
Trp	-10	-20	-30	-40	-50	-60	-70	-80	-90	-100	-110	-120	-130	-140	-150	-160	-170
Cys	0	0	0	0	0	0	-5	-10	-13	-10	-5	0	0	0	0	0	0
Met	10	20	25	30	35	40	45	50	53	50	45	40	35	30	25	20	10
Pro	-10	-20	-30	-40	-50	-60	-70	-80	-90	-100	-110	-120	-130	-140	-150	-160	-170

Q8. Find out residues forming alpha-helix in the given sequence considering the below statistical propensities for alpha helices. [5]

Sequence:

NYSVSRLIFVRHMGGIL

TABLE 5.2 Chou-Fasman parameters

Residue	P_{α}	
Glu	H α 1.53	1.0
Ala	1.45	
Leu	1.34	
His	h α 1.24	
Met	1.20	
Gln	1.17	
Trp	1.14	
Val	1.14	0.5
Phe	1.12	
Lys	l α 1.07	
Ile	1.00	0
Asp	l α 0.98	
Thr	0.82	
Ser	0.79	
Arg	0.79	-1.0
Cys	0.77	
Asn	b α 0.73	
Tyr	0.61	
Pro	B α 0.59	
Gly	0.53	