

Bioinformatics National Certification (BINC) Examination

Paper III

Total Time : 2 hrs

Max. Marks:100

Answer any one question.

Input files provided :

(GENE.txt, 1mbi.pdb, autocat.dat, codontab.txt)

1. Write a program in JAVA or PERL or PYTHON or in C the followings:

- a) Read the file provided (GENE.txt in FASTA format) and create complementary strand sequence.
- b) Find the ORFs on forward strand for the given nucleotide sequence using only start & end codon pattern.
- c) Convert each of the ORF into putative proteins using the standard codontab.txt (input provided).
- d) Read the 1mbi.pdb as provided from protein data bank. Extract all the coordinates of water Oxygen atoms. Calculate the distance between all the Oxygen and Identify which one pairs will form Hydrogen bonds between them (make a list by the residue number provided in PDB file starting form 160 to 278). (100 marks)

2. i) An autocatalytic reaction is described by the expression

$$x/P = [\exp(at) - 1] / [1 + b \exp(at)], \text{ with } a = (A + P)k \text{ and } b = P/A.$$

Write a program in C or JAVA or Perl or PYTHON to calculate x/P for three values of t ($t = 1, 2$ and 3) using a & b as given in the input file autocat.dat.

Report if the saturation is reached by printing a string, "The saturation is reached. The values are" and then print the value of (x/P , a , b and t) for the saturation point. Otherwise, print the message " The Saturation is not reached" . All your output, including these messages is to be saved in a file called autocat.out. (30 marks)

ii) Read the 1mbi.pdb as provided from protein data bank. Extract all the peptide bond containing atoms (only non-H) make a list as output. Calculate the omega torsion angle for each of the peptides. Calculate the probability of occurrence of $\omega = 180^\circ$ from the resulting data. Calculate the ratio of polar : non polar residues in the protein . (70 marks)