GEBZE TECHNICAL UNIVERSITY, FACULTY OF ENGINEERING, DEPARTMENT OF BIOENGINEERING 2024-2025 FALL SEMESTER

BENG451: Introduction to Bioinformatics BSB511: Bioinformatics Fundamentals

HOMEWORK I

Please submit a single Jupyter notebook including your answers/solutions.

Pairwise protein sequence alignment

- Get familiar with dihydrofolate reductase by reading its PDB molecule of the month description at https://pdb101.rcsb.org/motm/34
- Retrieve the amino acid sequences of the enzyme dihydrofolate reducate from human and three additional organisms in FASTA format using Biopython.
- Perform pairwise alignments for each possible pair of these four sequences. Experiment with different scoring matrices (e.g., BLOSUM and PAM families) and tweak gap insertion/extension penalties. Again, you should use Biopythons align2 module to perform this.
- Report alignment results to highlight matches, mismatches, and gaps, as clearly as possible.
- You code should generate a FASTA file that includes your alignment results.
- Compare and discuss the alignment results, including identity and similarity scores. Which of the alignments was the most successful one? Why? (Hint: you may also include a short discussion of the structure of the protein based on what you know about protein sequence-structure-function relationship of the protein).

Please try to submit a comprehensive discussion. Your responses will be evaluated with great emphasis on your discussion as well.

