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Grundlagen der Bioinformatik

Assignment 09

SoSe 2018

Submit electronically in Ilias by 2.7.2018, 10h

1 Secondary structure using JPRED4 (5 points)

Use the program `jpred4` hosted at `http://www.compbio.dundee.ac.uk/jpred/` to compute the secondary structure of the following sequence (but **not** using similarity to existing PDB entries):

```
GSESSSQAVVVAIDAKRVDGEFMVFTYSGKKNTGILLRDWVVEVEKRGAGEILLTSIDRDGTK
SGYDTEMIRFVRPLTTLPIIASGGAGKMEHFLEAFLRGADKVSINTAAVENPSLITQIAQTFG
```

What are the main secondary structure elements?

Note that the program reports following information:

- Jnet - Final secondary structure prediction for query

- jhmm - Jnet HMM profile prediction

- jpssm - Jnet PSIBLAST PSSM profile prediction

How do the results given for these items compare? For each pair, compute the percentage of amino-acids for which they make the same prediction.

Provide a sensible definition for when two different reports have identified essentially "the same" secondary structure feature. Then list, for each pair of reports, how many features either report contains and what percentage do they have in common?

2 Calculating hydrophobic moment (3 points)

Use the following sequence `LRDWVVEVEKR` to show in detail how the hydrophobic moment in the case of a possible α-helix is computed.

3 Maximizing hydrophobic moment (2 points)

Design a protein sequence of length 12 that has the maximum hydrophobic moment (for a α-helix).