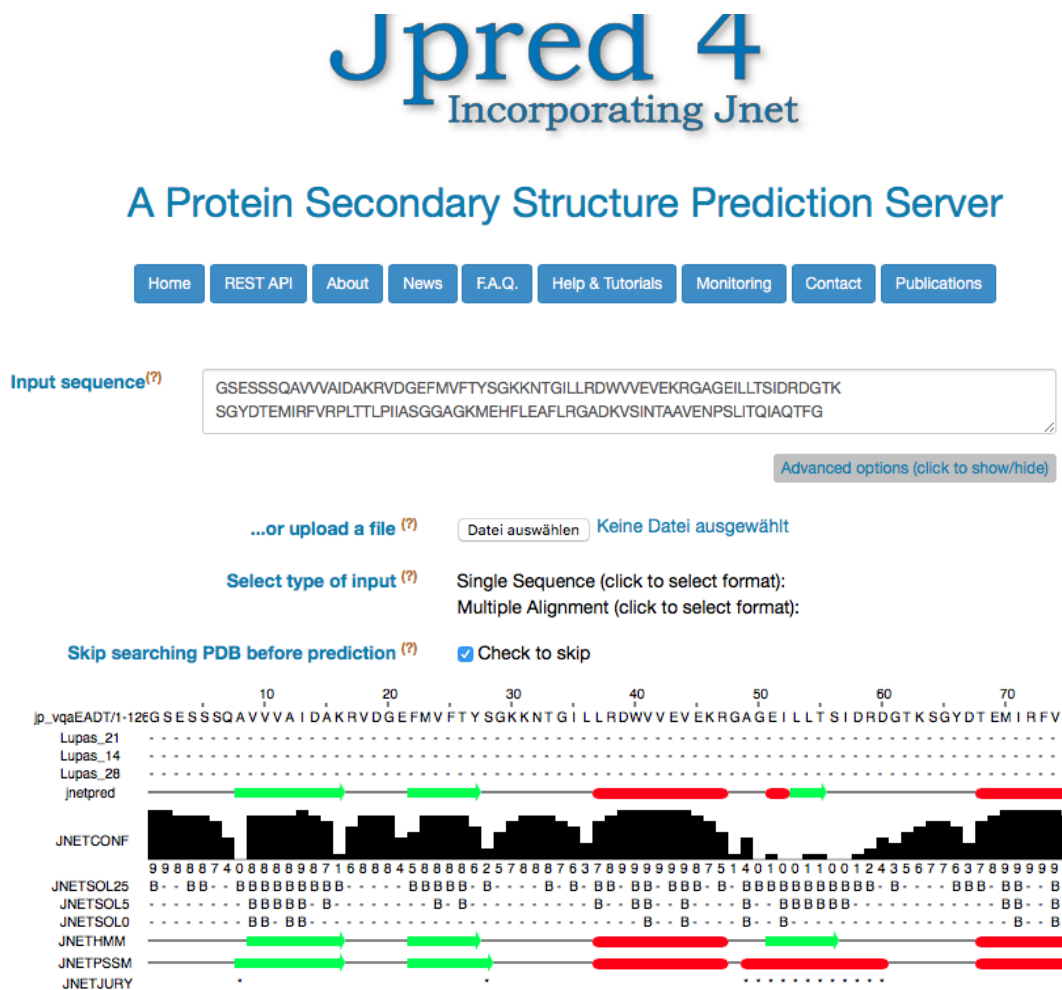# Assignment 9—Grundlagen der Bioinformatik

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1 Secondary structure using JPRED4

1. *Note: there is only first part of the result presented, because a window size is too small for the whole sequence.

The sequence for which the prediction was made is on the top of the picture.

JNetPRED

The consensus prediction - helices are marked as red tubes, and sheets as dark green arrows.
Total query length 126
According to prediction:
# of ß-sheet amino acids: $9 + 6 + 3 + 4 = 22$
of α-strand amino acids 53:
As we can see the main structure according that prediction is α-strand.

jhmm - Jnet HMM profile prediction

of ß-sheet amino acids:23
of α-strand amino acids: 50
As we can see the main structure according that prediction is α-strand.

jpssm - Jnet PSIBLAST PSSM profile prediction

of ß-sheet amino acids:20
of α-strand amino acids:64
As we can see the main structure according that prediction is α-strand.

jpssm/jhmm

$\frac{matches}{Query.length} = \frac{67}{126} = 53,17\%$

jpssm/JNetPRED

$\frac{matches}{Query.length} = \frac{72}{126} = 57,14\%$

JNetPRED/jhmm

$\frac{matches}{Query.length} = \frac{69}{126} = 54,76\%$

Two different reports have identified essentially "the same" secondary structure feature, when the sum of amino acids, involved in either α-strand, β-sheet or neither of both structures, by every report makes the greatest part of all predictions we have observed in the report.

All reports contain 3 features : predicted α-strand, predicted β-sheet or not defined.

Predicted α-strand for each pair of reports $= \frac{\#matches}{maxNumberOfAlphaAA}$:

jpssm/jhmm:$\frac{50}{64} = 78,12\%$
jpssm/JNetPRED:$\frac{53}{64} = 82,81\%$
JNetPRED/jhmm:$\frac{57}{60} = 95\%$

Predicted β-sheet for each pair of reports $= \frac{\#matches}{maxNumberOfAlphaAA}$:

jpssm/jhmm:$\frac{17}{23} = 73,91\%$
jpssm/JNetPRED:$\frac{19}{23} = 82,61\%$
JNetPRED/jhmm:$\frac{20}{26} = 76,9\%$

2 Calculating hydrophobic moment

The amino acid sequence is LRDWVVEVEKR. The given formular to calculate the hydrophobic moment is:

$$\mathcal{M}^{\omega}(p,q) = [(\sum_{i=p}^{q} h(a_i)cos(i\omega))^2 + \sum_{i=p}^{q} h(a_i)sin(i\omega))^2]^{\frac{1}{2}}$$

According to the amino acid hydrophobic table(Kyte and Doolittle 1982):

$$h_L = 4 \quad h_R = -4.5 \quad h_D = -3.5 \quad h_W = -1 \quad h_V = -1.2 \quad h_E = -3.5 \quad h_R = -4.5$$

Besides, this should be an α-helix, which means $\omega = 100°$
Then just put this values into the formula and get the final outcome. The final outcome is 11.93.

3 Maximizing hydrophobic moment

$\omega = 100°, sin\omega > 0, cos\omega < 0, |sin\omega| > |cos\omega|$ Pick "I" with the largest positive h.
$\omega = 200°, sin\omega < 0, cos\omega < 0,$ Pick "R" with the smallest negative h.
$\omega = 300°, sin\omega < 0, cos\omega > 0, |sin\omega| > |cos\omega|$ Pick "R" with the smallest negative h.
$\omega = 400°, sin\omega > 0, cos\omega > 0,$ Pick "I" with the largest positive h.
$\omega = 500°, sin\omega > 0, cos\omega < 0, |cos\omega| > |sin\omega|$ Pick "R" with the smallest negative h.
$\omega = 600°, sin\omega < 0, cos\omega < 0$ Pick "R" with the smallest negative h.

$\omega = 700°, sin\omega < 0, cos\omega > 0, |cos\omega| > |sin\omega|$ Pick "I" with the largest positive h.

$\omega = 800°, sin\omega > 0, cos\omega > 0,$ Pick "I" with the largest positive h.

$\omega = 900°, sin\omega = 0, cos\omega = -1$ Pick "R" with the smallest negative h.

$\omega = 1000°, sin\omega < 0, cos\omega > 0, |sin\omega| > |cos\omega|$ Pick "R" with the smallest negative h.

$\omega = 1100°, sin\omega > 0, cos\omega > 0,$ Pick "I" with the largest positive h.

$\omega = 1200°, sin\omega > 0, cos\omega < 0, |sin\omega| > |cos\omega|$ Pick "I" with the largest positive h.

Therefore, the final determined sequence is "IRRIRRIIRRII"