***Practicals – 11***

*-BS19B032*

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1) I wrote a code to calculate the propensity of the helix for all the 20 residues for the given sequence. I attached the code in submission.

For the given sequence,

"LGASGIAAFAFGSTAILIILFNMAAEVHFDPLQFFRQFFWLGLYPPKAQYGMGIPPLHDGGWWLMAGLFMTLSLGSWWIRVYSRARALGLGTHIAWNFAAAIFFVLCIGCIHPTLVGSWSEGVPFGIWPHIDWLTAFSIRYGNFYYCPWHGFSIGFAYGCGLLFAAHGATILAVARFGGDREIEQITDRGTAVERAALFW"

and for the secondary structure given,

"XHHHHHHHHHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHXXHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXHHHHHHHHHHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXXXX"

The propensity of the alpha helix for residues is:

Alanine: 1.55

Cysteine: 1.02

Aspartic acid: 0.0

Glutamic acid: 0.41

Phenylalanine: 1.02

Glycine: 1.06

Histidine: 0.87

Isoleucine: 1.2

Lysine: 0.0

Leucine: 1.22

Methionine: 1.53

Asparagine: 1.36

Proline: 0.23

Glutamine: 0.0

Arginine: 0.68

Serine: 1.36

Threonine: 0.77

Valine: 0.58

Tryptophan: 1.11

Tyrosine: 0.58

2) From, the given sequence, first we have to find the frequencies of amino acid residues. Then we have to find the frequencies of amino acid residues where helix is present.

**Frequency of amino acids:**

Alanine = 25

Cysteine = 4

Aspartic Acid = 5

Glutamic Acid = 5

Phenylalanine = 20

Glycine = 25

Histidine = 7

Isoleucine = 17

Lysine = 1

Leucine = 20

Methionine = 4

Asparagine = 3

Proline = 9

Glutamine = 4

Arginine = 9

Serine = 9

Threonine = 8

Valine = 7

Tryptophan = 11

Tyrosine = 7

**Frequency of amino acid with alpha helices:**

Alanine = 19

Cysteine = 2

Aspartic Acid = 0

Glutamic Acid = 1

Phenylalanine = 10

Glycine = 13

Histidine = 3

Isoleucine = 10

Lysine = 0

Leucine = 12

Methionine = 3

Asparagine = 2

Proline = 1

Glutamine = 0

Arginine = 3

Serine = 6

Threonine = 3

Valine = 2

Tryptophan = 6

Tyrosine = 2

Now, we have to calculate the ratio of frequency of helices formed in amino acid to frequency of amino acid.

Alanine = 0.76

Cysteine = 0.5

Aspartic Acid = 0

Glutamic Acid = 0.2

Phenylalanine = 0.5

Glycine = 0.52

Histidine = 0.43

Isoleucine = 0.59

Lysine = 0

Leucine = 0.6

Methionine = 0.75

Asparagine = 0.67

Proline = 0.11

Glutamine = 0

Arginine = 0.33

Serine = 0.67

Threonine = 0.375

Valine = 0.28

Tryptophan = 0.54

Tyrosine = 0.28

Now, ratio of helices formed in total sequence is,

= total alpha helix residues/total residues

= 98/200 = 0.49

Now, to find the propensity of alpha helix residues, we have divide the first found ratio for each amino acid residue by the ratio for complete sequences.

Therefore, the propensity values are:

Alanine = 1.55

Cysteine = 1.02

Aspartic acid = 0.0

Glutamic acid = 0.41

Phenylalanine = 1.02

Glycine = 1.06

Histidine = 0.87

Isoleucine = 1.2

Lysine = 0.0

Leucine = 1.22

Methionine = 1.53

Asparagine = 1.36

Proline = 0.23

Glutamine = 0.0

Arginine = 0.68

Serine = 1.36

Threonine = 0.77

Valine = 0.58

Tryptophan = 1.11

Tyrosine = 0.58

3) As per the given set of rules, I wrote a code to find helical and strand segments in given sequence. I attached the code in submission.

The results were:

**The Alpha Helix sequences are:**

RCELAAAMKRH

WVCAAKFESNF

MNAWVA

TDVQAW

**The Beta Strand Sequences are:**

LAAAM

WVCAA

YGILQI

AWVAWR

TDVQAWIR

For some segments, there was some ambiguity, so for them I found the propensity of helix and strand, and took the maximum value as its segment, as given in the rules.

* As helix propensity of ***LAAAM*** is greater than strand, it is a helical segment
* As strand propensity of ***WVCAA*** is greater than helix, it is a strand segment
* As strand propensity of ***TDVQA*** is greater than helix, it is a strand segment
* As helix propensity of ***DVQAW*** is greater than strand, it is a helical segment

Therefore, the final segments are:

**Helix:**

* RCELAAAMKRH
* KFESNF
* MNAWVA
* TDVQAW

**Strand:**

* WVCAA
* YGILQI
* AWVAWR
* TDVQAWIR

4) Verifying the helical and strand segments, using given rules.

Helix: MNAWVA

= 1 – 1 + 1 + 1 + 1 + 1

= 4

Since, the value is greater than or equal to 4, it is a helical segment.

Strand: YGILQI

= 1 + 0 + 1 + 1 + 1 + 1

= 5

Since, the value is greater than 3, it is a strand segment.

Hence, verified.