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,

"LGASGIAAFAFGSTAILIILFNMAAEVHFDPLQFFRQFFWLGLYPPKAQYGMGIPPL
HDGGWWLMAGLFMTLSLGSWWIRVYSRARALGLGTHIAWNFAAAIFFVLCIGCIHP
TLVGSWSEGVPFGIWPHIDWLTAFSIRYGNFYYCPWHGFSIGFAYGCGLLFAAHGA
TILAVARFGGDREIEQITDRGTAVERAALFW"

and for the secondary structure given,

"XHHHHHHHHHHHHHHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHXXHHHHHHHHHHHH
HHHHXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXHHHHHHHHHHH
HHHHHHHHHHHHHHXXXXXXXXXXXXXXXXXXXXXXXXXX"

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	Methionine = 3
Cysteine = 2	Asparagine = 2
Aspartic Acid = 0	Proline = 1
Glutamic Acid = 1	Glutamine = 0
Phenylalanine = 10	Arginine = 3
Glycine = 13	Serine = 6
Histidine = 3	Threonine = 3
Isoleucine = 10	Valine = 2
Lysine = 0	Tryptophan = 6
Leucine = 12	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	Methionine = 0.75
Cysteine = 0.5	Asparagine = 0.67
Aspartic Acid = 0	Proline = 0.11
Glutamic Acid = 0.2	Glutamine = 0
Phenylalanine = 0.5	Arginine = 0.33
Glycine = 0.52	Serine = 0.67
Histidine = 0.43	Threonine = 0.375
Isoleucine = 0.59	Valine = 0.28
Lysine = 0	Tryptophan = 0.54
Leucine = 0.6	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.