

Predict Hydrophobicity and Hydrophilicity of a protein using H-Plot

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Abstract

Proteomics methodology has revolutionized by the arrival of computer programs which are used to study the structural and functional properties easily and feasibly. The H-Plot is the computer software which is used for the analysis of hydrophobicity or hydrophilicity of amino acids of a protein. It also give you information about the possible structure of a protein and can indicate potential transmembrane or surface regions in proteins. The application program that was considered suitable for the program is C#.

Keywords: Proteomics methodology, Predict Hydrophobicity etc.

Background

Proteomics methodology has revolutionized the way that proteins are studied and opened new channels to understanding both cell functions and the cellular changes involved in disease states.

A hydrophilicity plot is a quantitative analysis of the degree of hydrophobicity or hydrophilicity of amino acids of a protein. It is used to characterize or identify possible structure or domains of a protein.

The plot has amino acid sequence of a protein on its x-axis, and degree of hydrophobicity and hydrophilicity on its y-axis. There are a number of methods to measure the degree of interaction of polar solvents such as water with specific amino acids. For instance, the Kyte-Doolittle scale indicates hydrophobic amino acids, whereas the Hopp-Woods scale measures hydrophilic residues.[1]

Analyzing the shape of the plot gives information about partial structure of the protein. For instance, if a stretch of about 20 amino acids shows positive for hydrophobicity, these amino acids may be part of alpha-helix spanning across a lipid bilayer, which is composed of hydrophobic fatty acids. On the converse, amino acids with high hydrophilicity indicate that these residues are in contact with solvent, or water, and that they are therefore likely to reside on the outer surface of the protein.[2]

A computer program that evaluates the hydrophilicity and hydrophobicity of a protein has been devised. For this purpose, a H-Plot has been composed wherein the hydrophilic and hydrophobic properties of each of the 20 amino acid side-chains is taken into consideration.

Materials and methods

Availability and requirements Lists the following:

Project name: H-Plot

Project home page: Desktop Based

Operating system(s): Platform independent

Programming language: C#

Collection of Literature

All the relevant information stated in introduction and literature review of the thesis was gathered from authentic research papers and scientific journal.

Detailed Design

Algorithm of calculate hydrophobicity plot

```
for (int i = 0; i < textBox1.Text.Length; i++)
{
    int a = 0;
    a = a + i;
    textBox2.Text = Convert.ToString(a + 1);

    if (textBox1.Text[i] == 'A' || textBox1.Text[i] == 'a')
    {
        chart1.Series["H-Plot"].Points.AddXY(i, 1.9);
    }
    else if (textBox1.Text[i] == 'D' || textBox1.Text[i] == 'd')
    {
        chart1.Series["H-Plot"].Points.AddXY(i, 2.2);
    }
    else if (textBox1.Text[i] == 'T' || textBox1.Text[i] == 't')
    {
        chart1.Series["H-Plot"].Points.AddXY(i, -0.2);
    }
    else if (textBox1.Text[i] == 'Y' || textBox1.Text[i] == 'y')
```

```

{
chart1.Series["H-Plot"].Points.AddXY(i, -4.2);
}
else if (textBox1.Text[i] == 'N' || textBox1.Text[i] == 'n')
{
chart1.Series["H-Plot"].Points.AddXY(i, -3.3);
}
else if (textBox1.Text[i] == 'G' || textBox1.Text[i] == 'g')
{
chart1.Series["H-Plot"].Points.AddXY(i, -0.5);
}
else if (textBox1.Text[i] == 'Q' || textBox1.Text[i] == 'q')
{
chart1.Series["H-Plot"].Points.AddXY(i, 2.0);
}
else if (textBox1.Text[i] == 'K' || textBox1.Text[i] == 'k')
{
chart1.Series["H-Plot"].Points.AddXY(i, -4.0);
}
else if (textBox1.Text[i] == 'W' || textBox1.Text[i] == 'w')
{
chart1.Series["H-Plot"].Points.AddXY(i, 3.0);
}
else if (textBox1.Text[i] == 'I' || textBox1.Text[i] == 'i')
{
chart1.Series["H-Plot"].Points.AddXY(i, 4.3);
}
else if (textBox1.Text[i] == 'L' || textBox1.Text[i] == 'l')
{
chart1.Series["H-Plot"].Points.AddXY(i, 3.4);
}

else if (textBox1.Text[i] == 'M' || textBox1.Text[i] == 'm')
{
chart1.Series["H-Plot"].Points.AddXY(i, 2.0);
}

else if (textBox1.Text[i] == 'S' || textBox1.Text[i] == 's')
{
chart1.Series["H-Plot"].Points.AddXY(i, -1.0);
}

else if (textBox1.Text[i] == 'R' || textBox1.Text[i] == 'r')
{
chart1.Series["H-Plot"].Points.AddXY(i, -1.6);
}

else if (textBox1.Text[i] == 'C' || textBox1.Text[i] == 'c')
{
chart1.Series["H-Plot"].Points.AddXY(i, 2.7);
}

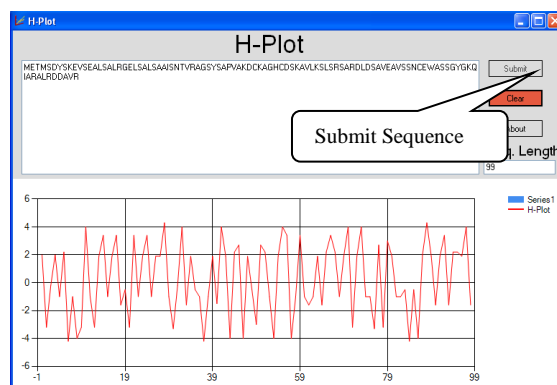
else if (textBox1.Text[i] == 'E' || textBox1.Text[i] == 'e')
{
chart1.Series["H-Plot"].Points.AddXY(i, -3.2);
}
else if (textBox1.Text[i] == 'H' || textBox1.Text[i] == 'h')

```

```

{
chart1.Series["H-Plot"].Points.AddXY(i, -3.0);
}
else if (textBox1.Text[i] == 'F' || textBox1.Text[i] == 'f')
{
chart1.Series["H-Plot"].Points.AddXY(i, 3.0);
}
else if (textBox1.Text[i] == 'P' || textBox1.Text[i] == 'p')
{
chart1.Series["H-Plot"].Points.AddXY(i, -1.5);
}
else if (textBox1.Text[i] == 'V' || textBox1.Text[i] == 'v')
{
chart1.Series["H-Plot"].Points.AddXY(i, 4.0);
}
}

```



Algorithm of build hydrophobicity plot

```

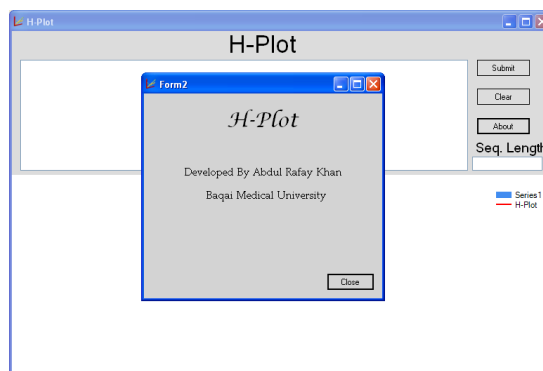
chart1.ChartAreas.Add("area");
chart1.ChartAreas["area"].AxisX.Minimum = 0;
chart1.ChartAreas["area"].AxisX.Interval = 10;
chart1.ChartAreas["area"].AxisY.Minimum = 0;
chart1.ChartAreas["area"].AxisY.Interval = 10;

//series is the the line on graph
chart1.Series.Add("H-Plot");

//type of chart
chart1.Series["H-Plot"].ChartType = SeriesChartType.Line;

//colour of lines
chart1.Series["H-Plot"].Color = Color.Red;

```



Results

H-Plot shows positive for hydrophobicity, these amino acids and negative for hydrophilicity in the form of line graph.

Conclusion

Using protein H-Plot, we can identify which kind of protein is being analyzed by examining the hydrophobic and hydrophilic regions of that protein. The structure of proteins defines their function. Using H-Plot, we can make predictions about the structure, which will enable us to make predictions about functions of proteins.

Download H-Plot from

https://www.dropbox.com/sh/x02r23eo9if23je/AAAqEIWVdpUe5_gjeaq6NWpMa?dl=0

References

- [1]. Kyte, J; Doolittle, R. F. (1982). "A simple method for displaying the hydropathic character of a protein". *Journal of Molecular Biology* 157 (1): 105–32. doi:10.1016/0022-2836(82)90515-0. PMID 7108955.
- [2]. Gasteiger E., Hoogland C., Gattiker A., Duvaud S., Wilkins M.R., Appel R.D., Bairoch A.; Protein Identification and Analysis Tools on the ExPASy Server; (In) John M. Walker (ed): *The Proteomics Protocols Handbook*, Humana Press (2005). pp. 571-607