

1. Estimate the pI of the peptide Asp-His-Glu-Lys-Thr. Asp is considered the first residue, since it has the amine group at the end, while Thr is considered the last residue as it has the carboxyl group at the end. In other words, Asp is at the N-terminus, or amino-terminus, while Thr is at the C-terminus, or carboxyl terminus. In terms of numbering, progresively, Asp is residue #1, while Thr is residue #6. For numerically solving for the pI , please use the bisection method. The written work should be part of the written work pdf while the .m file should be named P1P7Q3.m

Solution:

Aspartic Acid (CH_3COPO_4) : 9.6 for N-terminus.

Threonine (Thr) : 2.09 for C-terminus.

Histidine (His) : 6 (C δ) charge

Glutamic acid ($\text{C}_6\text{H}_5\text{O}_4$) : 6 (C δ) charge

Lysine (Lys) : 10.53 (C δ) charge

Alanine (Ala) : 6.09 (C δ) charge

$$[\text{Hx}^+] = \frac{1}{1 + 10^{pK_a - pI}} \quad [\text{X}^-] = \frac{1}{1 + 10^{pK_a - pI}}$$

$$\frac{\text{charge}}{\text{polaroid}} = 0 = \Sigma [\text{Hx}^+] - \Sigma [\text{X}^-]$$

$$\begin{aligned} f(\text{pI}) &= \frac{1}{1 + 10^{9.6 - \text{pI}}} - \frac{1}{1 + 10^{2.09 - \text{pI}}} \\ &+ \frac{1}{1 + 10^{6 - \text{pI}}} - \frac{1}{1 + 10^{6 - 2.09 - \text{pI}}} \\ &+ \frac{1}{1 + 10^{10.53 - \text{pI}}} + \frac{1}{1 + 10^{6 - 6.09 - \text{pI}}} - \frac{1}{1 + 10^{6 - 6.09 - \text{pI}}} \end{aligned}$$

mathlab gives $pI = 7.93$

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