

1. Estimate the pI of the peptide Asp-His-Glu-Lys-Arg-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 carboxy terminus. In terms of numbering peptides, 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 P1P53.m.

Solution:

Aspartic Acid (Asp) : 3.6 for N-terminus.

Threonine (Thr) : 2.09 for C-terminus.

Histidine (His) : 6 C+ charge

Carboxylic acid (Glu) : 4.25 C- charge

Lysine (Lys) : 10.53 C+ charge

Arginine (Arg) : 12.48 C+ charge.

$$[HX^+] = \frac{1}{1 + 10^{pH - pK_a}}$$

$$[X^-] = \frac{1}{1 + 10^{pK_a - pH}}$$

$$\frac{\text{charge}}{\text{Molecule}} = 0 = \sum [HX^+] - \sum [X^-]$$

$$f(pI) = \frac{1}{1 + 10^{pI - 3.6}} - \frac{1}{1 + 10^{2.09 - pI}} + \frac{1}{1 + 10^{pI - 6}} - \frac{1}{1 + 10^{4.25 - pI}} + \frac{1}{1 + 10^{pI - 10.53}} + \frac{1}{1 + 10^{pI - 12.48}} - \frac{1}{1 + 10^{2.09 - pI}}$$

Mathlab gives **PI = 7.98**

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Table of Contents Bioengineering Fundamentals Solutions

1. Understanding the eBook Bioengineering Fundamentals Solutions
 - The Rise of Digital Reading Bioengineering Fundamentals Solutions
 - Advantages of eBooks Over Traditional Books
2. Identifying Bioengineering Fundamentals Solutions
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Bioengineering Fundamentals Solutions
 - User-Friendly Interface
4. Exploring eBook Recommendations from Bioengineering Fundamentals Solutions
 - Personalized Recommendations

- Bioengineering Fundamentals Solutions User Reviews and Ratings
- Bioengineering Fundamentals Solutions and Bestseller Lists
- 5. Accessing Bioengineering Fundamentals Solutions Free and Paid eBooks
 - Bioengineering Fundamentals Solutions Public Domain eBooks
 - Bioengineering Fundamentals Solutions eBook Subscription Services
 - Bioengineering Fundamentals Solutions Budget-Friendly Options
- 6. Navigating Bioengineering Fundamentals Solutions eBook Formats
 - ePub, PDF, MOBI, and More
 - Bioengineering Fundamentals Solutions Compatibility with Devices
 - Bioengineering Fundamentals Solutions Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Bioengineering Fundamentals Solutions
 - Highlighting and Note-Taking Bioengineering Fundamentals Solutions
 - Interactive Elements Bioengineering Fundamentals Solutions
- 8. Staying Engaged with Bioengineering Fundamentals Solutions
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Bioengineering Fundamentals Solutions
- 9. Balancing eBooks and Physical Books Bioengineering Fundamentals Solutions
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Bioengineering Fundamentals Solutions
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Bioengineering Fundamentals Solutions
 - Setting Reading Goals Bioengineering Fundamentals Solutions
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Bioengineering Fundamentals Solutions
 - Fact-Checking eBook Content of Bioengineering Fundamentals Solutions

- Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
- 14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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