

R Programming: Acid Dissociation

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1 Introductory Reading

(Source: Dynamic Models in Biochemistry, Daniel E. Atkinson, et.al., Benjamin Cummings Publishing, 1987)

In chemistry, the dissociation of an acid, HA (where H is a hydrogen and A is a conjugate base) is a very important chemical process. We can show this with this equation:



From this, we can determine the acid dissociation constant, K_a , based on this equation:

$$K_a = \frac{[H^+][A^-]}{[HA]} \quad (2)$$

By taking the $-\log_{10}$ of both sides, we can derive the *Henderson-Hasselbalch* equation:

$$pH = pK_a + \log \frac{[A^-]}{[HA]} \quad (3)$$

From this, we can derive:

$$\frac{[A^-]}{[HA]} = 10^{pH - pK_a} \quad (4)$$

2 Computational Approach

3 Deliverable

You should submit your Netlogo model saved as "LastnameNLProject.nlogo". Make sure your code is well-documented, and that you have completed the **Information** section in the model interface.

Figure 1: Example Plot

