B

List of Common Rate Laws

Abbreviations are given at the end of this appendix.

Mass-Action Rate Laws

2. Irreversible Mass-action (1.8)

$$v = k \prod_i S_i^{n_i}$$

3. Reversible Mass-action (1.10)

$$v = k_1 \prod_i S_i^{n_i} - k_2 \prod_i P_i^{m_i}$$

4. Modified Reversible Mass-action (1.19)

$$v = k_1 \prod S_i^{n_i} \left(1 - \frac{\Gamma}{K_{eq}}\right)$$

Non-Mechanistic Approximations

5. **Single Substrate Linear Model 8.1**

$$v = v_o + \frac{\partial v}{\partial S_o}(S - S_o)$$

6. **Linear Model Using Elasticities (8.5)**

$$v = v_o \left(1 + \sum_i \varepsilon^v_{S^o_i} \frac{\delta S_i}{S^o_i}\right)$$

7. **Power Law (8.6)**

$$v = k \prod_j S_j^{\varepsilon^i_j}$$

8. **Lin-Log Model (8.7)**

$$v = v_o \left[\frac{e}{e_o}\right]\left(1 + \sum_i \varepsilon^v_{S_i} \ln\left(\frac{S_i}{S^o_i}\right)\right)$$

Single Substrate Michaelis-Menten

10. **Briggs-Haldane (3.5)**

$$v = \frac{V_f\, \alpha}{1 + \alpha}$$

11. **Reversible Michaelis-Menten (3.19)**

$$v = \frac{V_f\, \alpha - V_r\, \pi}{1 + \alpha + \pi}$$

12. **Reversible Michaelis-Menten with Haldane Substitution (3.23)**

$$v = \frac{V_f \alpha (1 - \rho)}{1 + \alpha + \pi}$$

13. **Michaelis-Menten with Product Inhibition (4.5)**

$$v = \frac{V_f \alpha}{1 + \alpha + \pi}$$

14. **Membrane Transport Carrier Model: Iso Uni-Uni**

$$v = \frac{V_f \alpha (1 - \rho)}{1 + \alpha + \pi + \alpha P / K_{ii}}$$

Inhibition Rate Laws

16. **Irreversible Competitive Inhibition (4.3)**

$$v = \frac{V_f \, \alpha}{1 + \alpha + \iota}$$

17. **Reversible Competitive Inhibition (4.4)**

$$v = \frac{V_f \alpha - V_r \pi}{1 + \alpha + \pi + \iota}$$

18. **Irreversible Uncompetitive Inhibition (4.9)**

$$v = \frac{V_f \alpha}{1 + \alpha \, (1 + \iota)}$$

19. **Reversible Uncompetitive Inhibition (4.10)**

$$v = \frac{V_f \alpha - V_r \pi}{1 + (\alpha + \pi)(1 + \iota)}$$

20. Irreversible Noncompetitive Inhibition (4.13)

$$v = \frac{V_f \alpha}{(1 + \alpha)(1 + \iota)}$$

21. Reversible Noncompetitive Inhibition (4.14)

$$v = \frac{V_f \alpha - V_r \pi}{(1 + \alpha + \pi)(1 + \iota)}$$

22. Irreversible Mixed Inhibition (4.11)

$$v = \frac{V_f \alpha}{(1 + \iota) + \alpha(1 + f \, \iota)}$$

23. Reversible Mixed Inhibition

$$v = \frac{V_f \alpha - V_r \pi}{(1 + \iota) + (\alpha + \pi)(1 + f \, \iota)}$$

24. Irreversible Mixed Partial Inhibition (4.1)

$$v = \frac{V_m \dfrac{S}{K_m}\left(1 + b\dfrac{I}{a\,K_i}\right)}{1 + \dfrac{S}{K_m} + \dfrac{I}{K_i} + \dfrac{S\,I}{a\,K_i\,K_m}}$$

Cooperative and Allosteric Rate Laws

16. Hill Equation using Dissociation constant, K_d (6.3)

$$v = \frac{V_f S^h}{K_d + S^h}$$

17. Hill Equation using Half Maximal activity, K_s (6.4)

$$v = \frac{V_f S^h}{K_s^h + S^h}$$

18. Adair Equation for a Dimer (6.13)

$$v = V_f \frac{K_1 S + 2 K_1 K_2 S^2}{2(1 + K_1 S + K_1 K_2 S^2)}$$

19. Adair Equation for a Trimer

$$v = V_f \frac{K_1 S + 2 K_1 K_2 S^2 + 3 K_1 K_2 K_3 S^3}{3(1 + K_1 S + K_1 K_2 S^2 + K_1 K_2 K_3 S^3)}$$

20. MWC Cooperative Model (6.14)

$$v = V_f \frac{\alpha (1 + \alpha)^{n-1}}{(1 + \alpha)^n + L}$$

21. Allosteric MWC Model with Inhibitor, ι (7.2)

$$v = V_f \frac{\alpha (1 + \alpha)^{n-1}}{(1 + \alpha)^n + L (1 + \iota)^n}$$

22. Allosteric MWC Model with Activator, μ (7.3)

$$v = V_f \frac{\alpha (1 + \alpha)^{n-1}}{(1 + \alpha)^n + L \dfrac{1}{(1 + \mu)^n}}$$

23. Simplified Reversible MWC Model (6.20)

$$v = \frac{V_f \alpha (1 - \rho) (1 + \alpha + \pi)^{n-1}}{L + (1 + \alpha + \pi)^n}$$

24. **Simplified Reversible MWC Model with inhibitor ι**

$$v = \frac{V_f \alpha \, (1 - \rho) \, (1 + \alpha + \pi)^{n-1}}{L(1 + \iota)^n + (1 + \alpha + \pi)^n}$$

25. **Reversible Hill Equation (6.6)**

$$v = \frac{V_f \alpha \, (1 - \rho) \, (\alpha + \pi)^{h-1}}{1 + (\alpha + \pi)^h}$$

26. **Reversible Hill with One Modifier, μ (7.7)**

$$v = \frac{V_f \alpha \, (1 - \rho) \, (\alpha + \pi)^{h-1}}{\dfrac{1 + \mu^h}{1 + \sigma \mu^h} + (\alpha + \pi)^h}$$

μ acts as an inhibitor when $\sigma < 1$ and an activator when $\sigma > 1$.

27. **Reversible Hill with Two Modifiers, μ_a and μ_b (7.8)**

$$v = \frac{V_f \alpha \, (1 - \rho) \, (\alpha + \pi)^{h-1}}{D}$$

$$D = (\alpha + \pi)^h + \left(\frac{1 + \mu_1^h}{1 + \sigma_1 \mu_1^h} \right) \left(\frac{1 + \mu_2^h}{1 + \sigma_2 \mu_2^h} \right)$$

σ_1 and σ_2 represent the factors that determine whether μ_1 and μ_2 are activators or inhibitors (See above). This equation assumes that both modifiers bind independently.

Two Substrate Rate Laws

25. **Random Order Bi-Uni Rate Law (8.10)**

$$v = \frac{V_f \alpha_1 \alpha_2 \, (1 - \rho)}{1 + \alpha_1 + \alpha_2 + \alpha_1 \alpha_2 + \pi_1}$$

26. Random Order Uni-Bi Rate Law (8.11)

$$v = \frac{V_f \alpha \, (1 - \rho)}{1 + \alpha + \pi_1 + \pi_1 \pi_2 + \pi_2}$$

27. Alberty Two Substrate Irreversible (5.3)

$$v = \frac{V_f S_1 S_2}{K_{S2} S_1 + K_{S1} S_2 + S_1 S_2 + K_{iS_1} K_{S2}}$$

28. Random Order Bi-Bi Rate Law (8.9)

$$v = \frac{V_f \, \alpha_1 \alpha_2 \, (1 - \rho)}{(1 + \alpha_1 + \pi_2)(1 + \alpha_2 + \pi_1)}$$

29. Ordered Bi-Uni Rate Law

$$v = \frac{V_f \alpha_1 \alpha_2 \, (1 - \rho)}{1 + \alpha_1 + \alpha_2 + \alpha_1 \alpha_2 + \alpha_1 \pi_1 + \pi_1}$$

30. Ordered Bi-Bi Rate Law (5.1)

$$v = \frac{V_f \, AB \, (1 - \rho)}{D}$$

where

$$D = K_{ia} K_b + K_b A + K_a B + AB + \frac{K_b K_q AP}{K_p K_{iq}} + \frac{K_b K_{ia} PQ}{K_p K_{iq}}$$

$$+ \frac{K_b K_{ia} BPQ}{K_p K_{iq} K_{ib}} + \frac{ABP}{K_{ip}} + \frac{K_a BQ}{K_{iq}} + \frac{K_q K_b K_{ia} P}{K_p K_{iq}} + \frac{K_b K_{ia} Q}{K_{iq}}$$

$$\text{(B.1)}$$

Generalized Rate Laws

1. Bi-Bi Enzyme with Cooperativity (8.13)

$$v = \frac{V_f \alpha_1 \alpha_2 \left(1 - \frac{\Gamma}{K_{eq}}\right) (\alpha_1 + \pi_1)^{h-1} (\alpha_2 + \pi_2)^{h-1}}{\left(1 + (\alpha_1 + \pi_1)^h\right)\left(1 + (\alpha_2 + \pi_2)^h\right)}$$

2. Uni-Bi Enzyme with Cooperativity (8.15)

$$v = \frac{V_f \alpha \left(1 - \frac{\Gamma}{K_{eq}}\right) (\alpha + \pi \rho)^{h-1}}{1 + (\alpha + \pi)^h + (\alpha + \rho)^h + (\alpha + \pi \rho)^h - 2\alpha^h}$$

3. Bi-Uni Enzyme with Cooperativity (8.16)

$$v = \frac{V_f \alpha \beta \left(1 - \frac{\Gamma}{K_{eq}}\right) (\alpha \beta + \pi)^{h-1}}{1 + (\alpha + \pi)^h + (\beta + \pi)^h + (\alpha \beta + \pi)^h - 2\pi^h}$$

4. Common Modular (8.19)

$$v = V_f \frac{\prod \alpha_i^{n_i} \left(1 - \frac{\Gamma}{K_{eq}}\right)}{\prod_i (1 + \alpha_i)^{h n_i} + \prod_i (1 + \pi_i)^{h n_i} - 1}$$

5. Direct Binding (8.20)

$$v = V_f \frac{\prod \alpha_i^{n_i} \left(1 - \frac{\Gamma}{K_{eq}}\right)}{1 + \prod \alpha_i^{h n_i} + \prod \pi_i^{h n_i}}$$

Gene Expression

30. Gene Expression Activation (9.16)

$$v = \frac{V_f S^h}{K_s + S^h}$$

31. **Gene Expression Inhibition (9.17)**

$$v = \frac{V_f}{K_s + S^h}$$

In all the following examples, cooperativity can be included by raising the species with an appropriate Hill coefficient.

32. **Gene Expression AND Function (9.8)**

$$v = V_f \frac{K_1 K_2 A \cdot B}{1 + K_1 A + K_2 B + K_1 K_2 A \cdot B}$$

33. **Gene Expression AND Function with Cooperativity ($h = 4$)**

$$v = V_f \frac{K_1 K_2 A^4 \cdot B^4}{1 + K_1 A^4 + K_2 B^4 + K_1 K_2 A^4 \cdot B^4}$$

34. **Gene Expression OR Function (9.6)**

$$v = V_f \frac{K_1\,A + K_2\,B}{1 + K_1\,A + K_2\,B}$$

35. **Gene Expression NOR Function (9.9)**

$$v = V_f \frac{1}{1 + K_1 A + K_2 B + K_3 A \cdot B}$$

36. **Gene Expression NAND Function (9.10)**

$$v = V_f \frac{1 + K_1 A + K_2 B}{1 + K_1 A + K_2 B + K_3 A \cdot B}$$

37. **Gene Expression XOR Function (9.11)**

$$v = V_f \frac{K_1 A + K_2 B}{1 + K_1 A + K_2 B + K_3 A \cdot B}$$

38. **Gene Expression EQ Function (9.12)**

$$v = V_f \frac{1 + K_1 A \cdot B}{1 + K_1 A + K_2 B + K_3 A \cdot B}$$

39. **Counter Regulation (Non-Competitive Model (9.13))**

$$v = V_f \frac{K_1 A}{1 + K_1 A + K_2 R + K_3 A \cdot R}$$

where A is the activator and R the repressor.

40. **Counter Regulation (Competitive Model (9.14))**

$$v = V_f \frac{K_1 A}{1 + K_1 A + K_2 R + K_3 A \cdot R}$$

where A is the activator and R the repressor.

Abbreviations for Appendix B:

S_i	Substrate i concentration
P_i	Product i concentration
I	Inhibitor concentration
A	Activator concentration
M	Modifier concentration
M_x	Modifier x concentration
α	Effect of M, if $M < 1$: Inhibitor; $M > 1$: Activator
V_f	Forward V_{max}
V_r	Reverse V_{max}
K_{eq}	Equilibrium constant
Γ	Mass-action ratio
k_i	Rate constant
K_S	Concentration of substrate at half-maximal velocity
K_P	Concentration of product at half-maximal velocity
K_X	Concentration of modifier at half-maximal velocity
K_d	Dissociation constant
K_i	Microscopic association constant
α	Abbreviation for S/K_S
π	Abbreviation for P/K_P
ι	Abbreviation for I/K_I
μ	Abbreviation for M/K_M
Γ	Abbreviation for P/S
ρ	Abbreviation for Γ/K_{eq}
σ	Modifier action in reversible Hill equation
ε_S^v	Elasticity of rate, v, with respect to species S
n_i and m_i	Stoichiometric amounts
h	Hill coefficient
n	Number of binding sites
L	Allosteric constant
v_o	Reference reaction rate for approximate rate laws
S_i^o	Reference concentration for approximate rate laws
e_o	Reference enzyme activity for approximate rate laws