H^+ Consumption and Release Stoichiometry

H^+ binding or release are not singular during chemical reactions involving H^+ as substrates or products.

To understand H^+ balance during chemical reactions, fractional H^+ binding must be understood and computed.

Accurate computations of factional H^+ binding require adjustments for competitive binding of metabolites with other cations.

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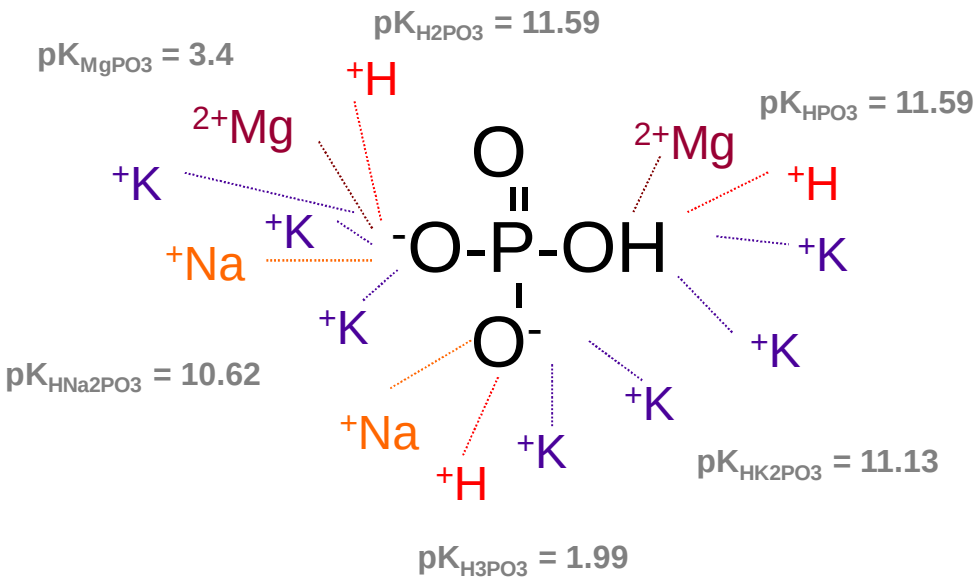
Competitive Cation Binding



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Methods

Latest electronic version of the NIST data base.

$pK_{L\text{-}M+}$ data were identified for as many metabolite cation complexes of non-mitochondrial energy metabolism as possible.

Data not in the NIST date base were obtained from prior research.

21 metabolites, 104 $L^{-}M^{+}$ complexes, 17 reactions

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Reaction	Enzyme	ΔH^+
HCrP + ADP + H^+ ↔ Cr + ATP	Creatine kinase	+1
ADP + ADP ↔ ATP + AMP	Adenylate kinase	0
AMP + H^+ ↔ IMP + NH_4	AMP deaminase	+1
ATP + H_2O ↔ ADP + Pi +H^+	ATPase	-1
Glycogen(n) + HPi ↔ Glycogen(n-1) + G1P	Phosphorylase	0
G1P ↔ G6P	Phosphogluco mutase	0
Glucose + ATP ↔ G6P + ADP + H^+	Hexokinase	-1
G6P ↔ F6P	Glucose-6-phosphate isomerase	0
F6P + ATP ↔ F1,6P + ADP + H^+	Phosphofructokinase	-1
F1,6P ↔ DHP + G3P	Aldolase	0
DHP ↔ G3P	Phosphofructokinase	0
G3P + HPi + NAD+ ↔ 1,3BPG + NADH + H^+	Glyceraldehyde-3-phosphate dehydrogenase	-1
1,3BPG + ADP ↔ 3PG + ATP	Phosphoglycerate kinase	0
3PG ↔ 2PG	Phosphoglycerate mutase	0
2PG + ADP ↔ PEP	Enolase	0
PEP + ADP + H+ ↔ Pyr + ATP	Pyruvate kinase	+1
Pyr + NADH + H^+ ↔ La + NAD^+	Lactate dehydrogenase	+1

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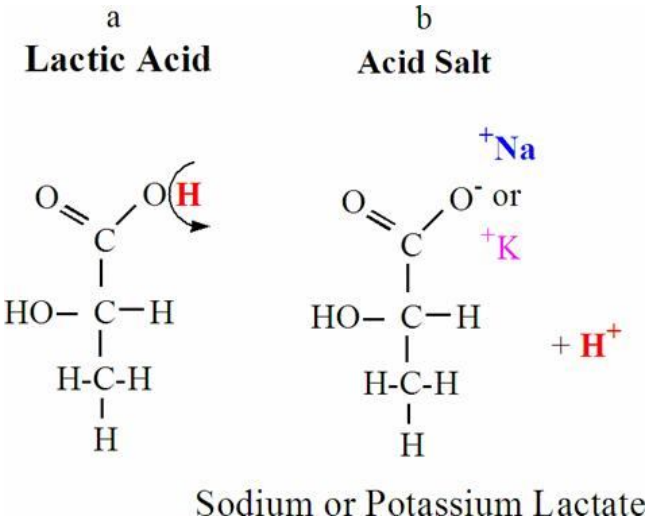
Association and Dissociation Constants



Sodium or Potassium Lactate

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$$Association\ constant = K_a = \frac{[HA]}{[H^-][A^-]}$$

$$-\log K_a = -\log\left(\frac{[HA]}{[H^-][A^-]}\right);\ for\ lactic\ acid\ with\ a\ Ka = 2.13796 \times 10^{-4}$$

$$pK_a = -\log\left(2.13796 \times 10^{-4}\right) = -\log 0.000213796 = -(-3.67) = 3.67$$

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$$Dissociation\ constant = K_d = \frac{[H^+][A^-]}{[HA]}$$

$$K_d\ (lactic\ acid) = \frac{[La^-]\times[H^+]}{[LaH]} = 4677.3514\ ;\ where\ \log_{10}\ 4677.3514 = 3.67$$

$$\log_{10} K_d\ (lactic\ acid) = 3.67$$

$$when\ [A^-] = [AH];\ \log 10\ \frac{[A^-]}{[AH]} = 0$$

$$then\ pH = pKa + 0\ or\ pKa = pH$$

$$pH = pKa + \log 10\ \frac{[A^-]}{[AH]}\ ;\ where\ pKa = pH - \log 10\ \frac{[A^-]}{[AH]}$$

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$$H_2CO_3 \Leftrightarrow H^+ + HCO_3^-\ ;\ K_1 = \frac{[H^+][HCO_3^-]}{H_2CO_3}$$

$$CO_2(d) + H_2O \Leftrightarrow H_2CO_3\ ;\ K_2 = \frac{[H_2CO_3]}{[CO_2(d)]+[H_2O]}$$

The dissociation constants for almost al metabolites in biological systems have been researched and compiled in a data base – NIST database.

See NIST data base
See Excel spreadsheet

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Analytical Chemistry

$$K_H = \frac{[HL^{1-n}]}{[H^+][L^{n-}]} \qquad K_{AH} = \frac{[AHL^{1+a-n}]}{[A^{a+}][H^+][L^{n-}]} \qquad K_{AAH} = \frac{[A_2HL^{1+a-n}]}{[A^{a+}]^2[H^+][L^{n-}]}$$

$$L_{tot} = [L^{n-}] + K_H[H^+][L^{n-}] + K_{Hn}[H^+]^n[L^{n-}] + K_A[A^{a+}][L^{n-}] + K_{AH}[A^{a+}][H^+][L^{n-}] + ...$$

$$\alpha_{-n} = \frac{[L^{n-}]}{L_{tot}} = \frac{1}{1 + K_H[H^+] + ... + K_{Hn}[H^+]^n + K_A[A^{a+}] + K_{AH}[A^{a+}][H^+] + ..}$$

$$[L^{n-}] = \alpha_{n-} L_{tot}$$

$$K_A[A^{a+}][L^{n-}] = [AL^{a-n}]$$

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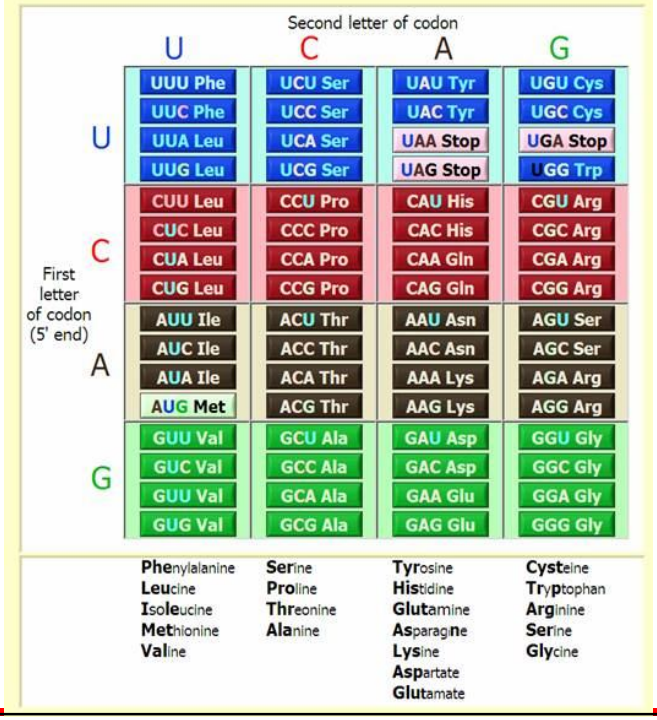
Amino Acids



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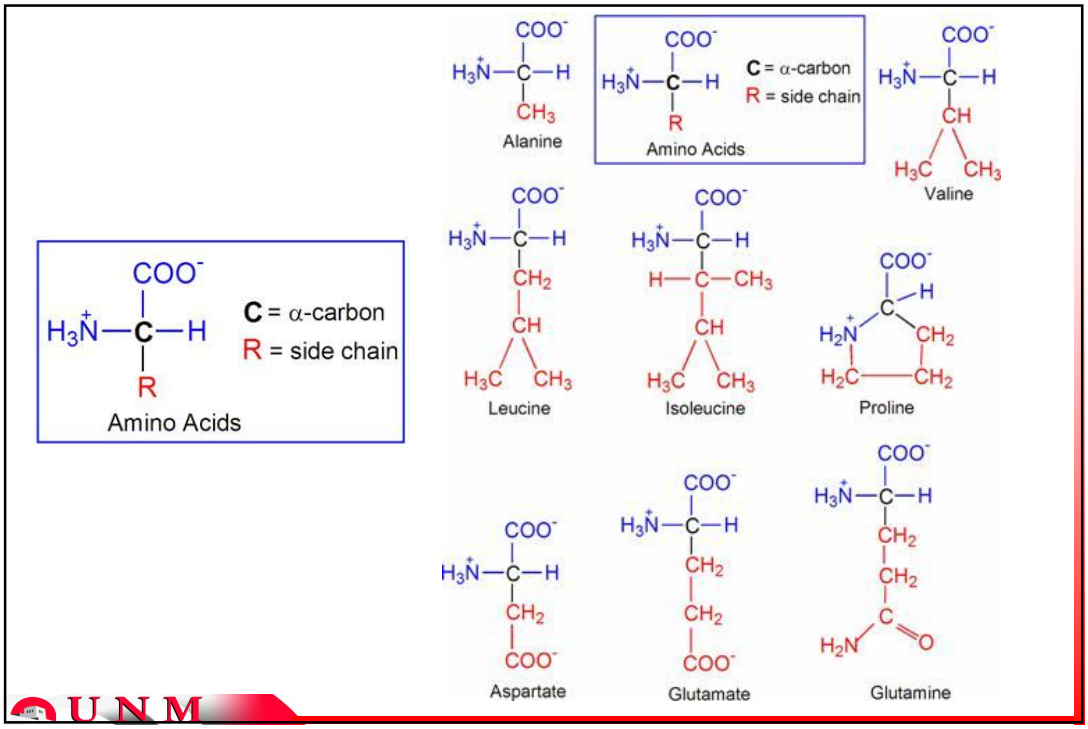
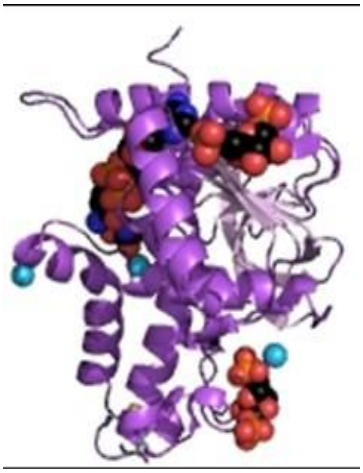
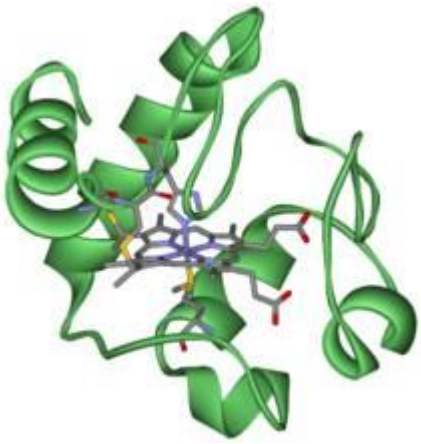




Lactate Dehydrogenase



Cytochrome-C