# Issues

August 9, 2023

## 1 ALD

Is it on purpose that there is a term missing ($\frac{aq}{KaKiq}$)?
vALD: F16BP → GLYCERAL3P + DHAP

$$v_{\mathrm{ALD}} = p.\mathrm{FBA\_ExprsCor} \cdot \frac{\left(\frac{p.\mathrm{FBA1\_kcat} \cdot f.\mathrm{FBA1}}{p.\mathrm{FBA1\_Kf16bp}} \cdot \frac{F16BP - (\mathrm{GLYCERAL3P} \cdot \mathrm{DHAP})}{p.\mathrm{FBA1\_Keq}}\right)}{(1 + \frac{F16BP}{p.\mathrm{FBA1\_Kf16bp}} + (1 + \frac{\mathrm{GLYCERAL3P}}{p.\mathrm{FBA1\_Kglyceral3p}}) \cdot (1 + \frac{\mathrm{DHAP}}{p.\mathrm{FBA1\_Kdhap}}) - 1)}$$

**Aldolase: ALD**

Aldolase is generally assumed to follow an ordered uni-bi mechanism, with Gra*P* binding after glycerone phosphate [27,74]. The equation is:

$$v_{\mathrm{ALD}} = V^{+} \frac{\frac{a}{K_{\mathrm{a}}}\left(1 - \frac{\Gamma}{K_{\mathrm{eq}}}\right)}{1 + \frac{a}{K_{\mathrm{a}}} + \frac{p}{K_{\mathrm{p}}} + \frac{q}{K_{\mathrm{q}}} + \frac{aq}{K_{\mathrm{a}}K_{\mathrm{iq}}} + \frac{pq}{K_{\mathrm{p}}K_{\mathrm{q}}}} \qquad \text{(A4)}$$

where $a$ represents [F1,6b$P_2$], $p$ represents [glycerone phosphate] and $q$ represents [Gra$P$]. The kinetic parameters are scarce, but all agree on the $K_{\mathrm{m}}$ for F1,6b$P_2$: around 0.3 mM [47–49]. Not many studies have been performed on the

Source: Tesuink et al., 2000

# 2 PGM, ENO (corrected)

Michaelis-Menten uni-uni, but incorrect denominator!

## APPENDIX 1: ENZYME KINETICS

In this Appendix the rate equations, experimental kinetic data and an overview of the biochemical knowledge concerning the glycolytic enzymes are given. Derivations follow established practice [32,59]. One substrate, one product reversible Michaelis–Menten kinetics was used to describe the enzymes PGI, PGM and ENO:

$$v = V^{+}\frac{\frac{a}{K_a}\left(1-\frac{\Gamma}{K_{eq}}\right)}{1+\frac{a}{K_a}+\frac{p}{K_p}} \qquad \text{(A1)}$$

Source: Tesuink et al., 2000

# 3 PFK (corrected)

Addition instead of multiplication! $PFK_{nom} = (p.PFK_kcat.*f.PFK.*p.PFK_gR.*(F6P./p.PFK_Kf6p).*(ATP./p.PFK_Katp).*(1+(\mathbf{F6P./p.PFK_Kf6p}) + (\mathbf{ATP./p.PFK_Katp})+p.PFK_gR.*((F6P./p.PFK_Kf6p).*(ATP./p.PFK_Katp))))$;
$PFK_{denom} = (1+\mathbf{F6P./p.PFK_Kf6p} + \mathbf{ATP./p.PFK_Katp}+(p.PFK_gR.*(F6P./p.PFK_Kf6p).*(ATP./p.PFK_Katp))).^2+...p.PFK_L.*...((1+p.PFK_Ciatp.*(ATP./p.PFK_Kiatp))./(1+ATP./p.PFK_Kiatp)).^2.*...((1+p.PFK_Camp.*(AMP./p.PFK_Kamp))./(1+AMP./p.PFK_Kamp)).^2.*...((1+((p.PFK_Cf26bp*F26BP)./(p.PFK_Kf26bp))+((p.PFK_Cf16bp.*F16BP)./(p.PFK_Kf16bp)))./(1+(F26BP./p.PFK_Kf26bp)+(F16BP./p.PFK_Kf16bp))).^2.*...(1+p.PFK_Catp.*(ATP./p.PFK_Katp)).^2$; $v_PFK = p.PFK_ExprsCor.*(PFK_nom./PFK_denom)$;

$$v_{\mathrm{PFK}} = V^{+}\frac{g_{\mathrm{R}}\lambda_1\lambda_2 R}{R^2 + LT^2}$$

$$\lambda_1 = [\mathrm{F6}P]/K_{\mathrm{R,\,F6}P}$$

$$\lambda_2 = [\mathrm{ATP}]/K_{\mathrm{R,\,ATP}}$$

$$R = 1 + \lambda_1\lambda_2 + g_{\mathrm{R}}\lambda_1\lambda_2$$

$$T = 1 + c_{\mathrm{ATP}}\lambda_2$$

Source: Tesuink et al., 2000

# 4 PYK (corrected)

Incorrect power? h instead of h-1!!
$v_{PYK} = p.PYK_Exprs Cor.*((((p.PYK1_kcat.*(f.PYK1+f.PYK2))./(p.PYK1_Kadp.*p.PYK1_Kpep).*ADP.*PEP)./...((1+ADP./p.PYK1_Kadp).*(1+PEP./p.PYK1_Kpep))).*...((PEP./p.PYK1_Kpep+1).^{p.PYK1_hill}./(p.PYK1_L.*((ATP./p.PYK1_Katp+1)./(F16BP./p.PYK1_Kf16bp+1)).^{p.PYK1_hill}+(PEP./p.PYK1_Kpep+1).^{p.PYK1_hill})));$

$$v_{\mathrm{PYK}} = p_{\mathrm{PYK\_ExprsCor}} \cdot \frac{p_{\mathrm{PYK1\_kcat}} \cdot (f_{\mathrm{PYK1}} + f_{\mathrm{PYK2}})}{p_{\mathrm{PYK1\_Kadp}} \cdot p_{\mathrm{PYK1\_Kpep}}} \cdot$$

$$\frac{ADP \cdot PEP}{(1 + \frac{ADP}{p_{\mathrm{PYK1\_Kadp}}}) \cdot (1 + \frac{PEP}{p_{\mathrm{PYK1\_Kpep}}})}$$

$$\cdot \frac{(PEP/p_{\mathrm{PYK1\_Kpep}} + 1)^{p_{\mathrm{PYK1\_hill}}}}{p_{\mathrm{PYK1\_L}} \cdot \left(\frac{ATP}{p_{\mathrm{PYK1\_Katp}}} + 1\right) \cdot \left(\frac{F16BP}{p_{\mathrm{PYK1\_Kf16bp}}+1}\right)^{p_{\mathrm{PYK1\_hill}}} + \left(\frac{PEP}{p_{\mathrm{PYK1\_Kpep}}} + 1\right)^{p_{\mathrm{PYK1\_hill}}}}$$

$$v_{\mathrm{pyk}} = \frac{v_{\mathrm{max.pyk}} \cdot \frac{\mathrm{PEP}}{k_{\mathrm{PEP}}} \left(\frac{\mathrm{PEP}}{k_{\mathrm{PEP}}} + 1\right)^{n-1}}{k_{\mathrm{PEP}} \left( L_{0,PYK} \left( \frac{\frac{\mathrm{ATP}}{k_{\mathrm{ATP}}} + 1}{\frac{\mathrm{FBP}}{k_{\mathrm{FBP}}} + 1} \right)^{n} + \left( \frac{\mathrm{PEP}}{k_{\mathrm{PEP}}} + 1 \right)^{n} \right)} \frac{\mathrm{ADP}}{(\mathrm{ADP} + k_{\mathrm{ADP}})}$$

Source: van Heerden et al., 2014

# 5 Pnp1 (not corrected)

Missing Pi?