

NADH to Oxygen steady state expression, MatLab program.

This is an research program and also calculates the concentrations of intermediates of cytochrome c oxidase.

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Ke = 6.4 * 10^11;
k1 = 5*10^10;
k1r = 5*10^8;
k2 = 3.5*10^8;
k2r = 1*10^1;
K3 = 2*10^6;
K5 = 1*10^25;
k4a = 2.4*10^8;
k4b = 8*10^7;
a3t = 1*10^-6;           % cytochrome a3 concentration
ct = 2*10^-6;           % cytochrome c concentration (2 x cyt a3t)
NADt = 2 * 10^-5;      % total concentration of NAD (NADH + NAD+)
x = (1:100)';          % used to generate levels for energy state Q
for q = 1:6;           % used to set oxygen concentration
    W = 7.1;           % W = pH of the medium
    H = 10^-W;         % H = hydrogen ion concentration
    N = 0.1;           % N = intramitochondrial [NAD+]/[NADH]
    Q = 0.270 + x.*0.0005; % energy state in volts
    O = q.*1.*10.^-5; % O is the oxygen concentration
    G = Q .* 46.183;   % Gibb's free energy in kcal for 2 electron transfer
    S = Q./0.059;     % coupling value for energy conservation
    z = 10.^S;         % used to couple rate and equilibrium constants to the energy state
    kf1 = k1 ./z.^0.5; % couples k1 to energy state
    kr1 = k1r .*z.^0.5; % couples k1r to energy state
    D = N.^0.5 .*z.^2.*(H./Ke).^0.5; % expression D in steady state
    co = D.*ct./(1 + D); % co is oxidized cytochrome c
    cr = ct - co;      % cr is reduced cytochrome c
    A = (k2r + k4a.*cr + k4b.*cr.* K3.*H)./(k2.*O); % calculates value of expression A
    B = (k2.*O.*A + kr1.*co.* A -k2r)./(kf1 .* cr); % calculates value of expression B
    C = K5.^-1 .* (1/H)^2.*(co./cr).^2 .* z.^2 .* B; % calculates value of expression C
    III = a3t./(1 + K3.*H + A + B + C); % concentration of intermediate III
    I = B .* III;      % concentration of intermediate I
    II = A .* III;     % concentration of intermediate II
    IV = K3 .*H.* III; % concentration of intermediate IV
    V = C.*III;        % concentration of intermediate V
    y(q,x) = (k4a.*cr + k4b.*cr.*K3.*H) .* III .*4./ct; % rate as cyt c TN
end
plot (x,y) % plots cyt c TN (y) vs x value
axis([0 100 0 40]) % sets graph x and y axis limits
```