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// -- Begin Antimony block converted from wolf2001.xml
// Created by libAntimony v2.9.1
model *wolf2001()

// Compartments and Species:
compartment c0, c1, c2;
species $sul_ex in c0, $eth_ex in c0, $oxy_ex in c0, oxy in c2, $H2O in c2;
species A3c in c1, aps in c1, $PPi in c1, pap in c1, sul in c1, eth in c1;
species $A2c in c1, hyd in c1, cys in c1, N2 in c1, $N1 in c1, aco in c1;
species oah in c1, S1 in c2, $S2 in c2, $C1 in c2, $C2 in c2, $A2m in c2;
species A3m in c2, $Ho in c1, $Hm in c2;

// Assignment Rules:
A2c := Ac - A3c;
N1 := N - N2;
S2 := S - S1;
A2m := Am - A3m;

// Reactions:
v1: $sul_ex => sul; c0*k_v0/(1 + (cys/Kc)^n);
v13: $eth_ex => eth; c0*k_v13;
v2: sul + A3c => aps + $PPi; c1*k2*sul*A3c;
v10: $oxy_ex => oxy; c0*k_v10;
v14: oxy => $oxy_ex; c2*k14*oxy;
v3: aps + A3c => pap + $A2c; c1*k3*aps*A3c;
v4: pap + 3N2 => hyd + 3$N1; c1*k4*pap*N2;
v5: hyd + oah => cys; c1*k5*hyd*oah;
v6: cys => ; c1*k6*cys;
v7: eth + 2$N1 => aco + 2N2; c1*k7*eth*N1;
v15: aco => oah; c1*k15*aco;
v17: hyd => ; c1*k17*hyd;
v18: oah => ; c1*k18*oah;
v8: $S2 + aco => S1; c2*k8*aco*S2;
v9: S1 + 4$N1 => $S2 + 4N2; c2*k9*S1*N1;
v11a: $C1 + $Hm + N2 => $C2 + $Ho + $N1; c2*k11*N2*oxy/((a*N2 + oxy)*(1 +
(hyd/Kh)^m));
v11a2: $C2 + oxy => $C1 + $H2O; c2*k11*N2*oxy/((a*N2 + oxy)*(1 + (hyd/Kh)^m));
v16: $A2c + A3m => $A2m + A3c; c2*k16*A3m*A2c;
v11b: $Ho + $A2m => $Hm + A3m; (c2*3*k11*N2*oxy/((a*N2 + oxy)*(1 +
(hyd/Kh)^m)))*A2m/(Ka + A2m);
vLEAK: $Ho => $Hm; 0;
v12: A3c => $A2c; c1*k12*A3c;

// Species initializations:
sul_ex = 0;
eth_ex = 0;
oxy_ex = 0;
oxy = 7;
oxy has substance_per_volume;
H2O = 0;
A3c = 1.5;
A3c has substance_per_volume;
aps = 0.5;
aps has substance_per_volume;
PPi = 0;
pap = 0.4;
pap has substance_per_volume;
sul = 0.4;
sul has substance_per_volume;
eth = 4;
eth has substance_per_volume;
A2c has substance_per_volume;
hyd = 0.5;
hyd has substance_per_volume;
cys = 0.3;
cys has substance_per_volume;
N2 = 2;
N2 has substance_per_volume;
N1 has substance_per_volume;
aco = 0.3;
aco has substance_per_volume;
oah = 1.5;
oah has substance_per_volume;
S1 = 1.5;
S1 has substance_per_volume;
S2 has substance_per_volume;
C1 = 0;
C2 = 0;
A2m has substance_per_volume;
A3m = 1.5;
A3m has substance_per_volume;
Ho = 0;
Hm = 0;

// Compartment initializations:
c0 = 1;
c1 = 1;
c2 = 1;

// Variable initializations:
Ac = 2;
N = 2;
S = 2;
Am = 2;
k_v0 = 1.6;
Kc = 0.1;
n = 4;
k_v13 = 4;
k2 = 0.2;
k_v10 = 80;
k14 = 10;
k3 = 0.2;
k4 = 0.2;
k5 = 0.1;
k6 = 0.12;
k7 = 10;
k15 = 5;
k17 = 0.02;
k18 = 1;
k8 = 10;
k9 = 10;
k11 = 10;
a = 0.1;
Kh = 0.5;
m = 4;
k16 = 10;
Ka = 1;
k12 = 5;

// Other declarations:
const c0, c1, c2, Ac, N, S, Am, k_v0, Kc, n, k_v13, k2, k_v10, k14, k3;
const k4, k5, k6, k7, k15, k17, k18, k8, k9, k11, a, Kh, m, k16, Ka, k12;

// Unit definitions:
unit substance_per_volume = mole / litre;
unit substance = mole;

// Display Names:
c0 is "external";
c1 is "cytosol";
c2 is "mitochondria";
sul_ex is "S04_ex";
eth_ex is "EtOH_ex";
oxy_ex is "O2_ex";
oxy is "O2";
A3c is "ATP";
aps is "APS";
pap is "PAPS";
sul is "S04";
eth is "EtOH";
A2c is "ADP";
hyd is "H2S";
cys is "CYS";
N2 is "NADH";
N1 is "NAD";
aco is "AcCoA";
oah is "OAH";
A2m is "ADP_mit";
A3m is "ATP_mit";
v11a is "vET1";
v11a2 is "vET2";
v11b is "vSYNT";
end
// -- End Antimony block

// -- Begin PhraSEDML block converted from main.xml
// Created by libphrasedml v1.0.5
// Models
model_m_1 = model "wolf2001" with m=1
model_m_2 = model "wolf2001" with m=2
model_m_4 = model "wolf2001" with m=4
model_m_8 = model "wolf2001" with m=8

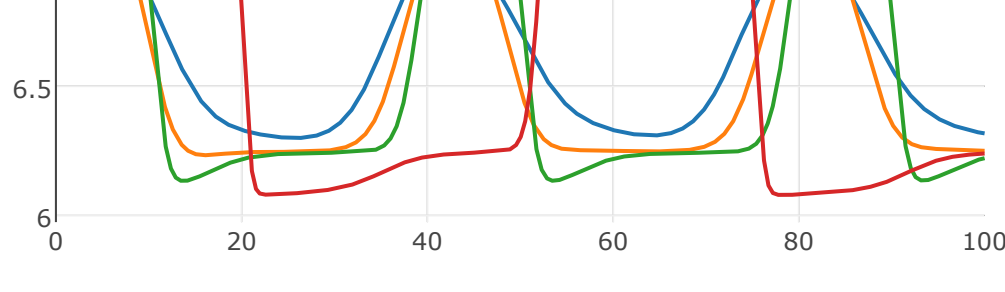
// Simulations
sim1 = simulate uniform(0, 100, 5000)
sim2 = simulate uniform(0, 200, 5000)

// Tasks
task1_100 = run sim1 on model_m_1
task2_100 = run sim1 on model_m_2
task4_100 = run sim1 on model_m_4
task8_100 = run sim1 on model_m_8

task1_200 = run sim2 on model_m_1
task2_200 = run sim2 on model_m_2
task4_200 = run sim2 on model_m_4
task8_200 = run sim2 on model_m_8

// Outputs
plot "Oxygen (100 min)" task1_100.time vs task1_100.oxy, task2_100.oxy, task4_100.oxy,
task8_100.oxy
plot "Oxygen (200 min)" task1_200.time vs task1_200.oxy, task2_200.oxy, task4_200.oxy,
task8_200.oxy

// -- End PhraSEDML block
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Oxygen (200 min)

