

Descriptions of MATLAB Codes and Data Files for “Computer Modeling of Mitochondrial Tricarboxylic Acid Cycle, Oxidative Phosphorylation, Metabolite Transport, and Electrophysiology” (Wu et al., *J. Biol. Chem.*, 2007)

Version 1.4 (Updated on 10/27/08)

File Names	Descriptions *
<i>Main driver programs</i>	
state_2_LaNoueData.m	simulating LaNoue et al. state-2 experiments and (as shown in Figure 2)
state_3_LaNoueData.m	simulating LaNoue et al. state-3 experiments and (as shown in Figure 3)
state_2_BoseData.m	simulating Bose et al. state-2 experiments (shown in Figure 4 in the full text via “plot_BoseData.m”)
state_3_BoseData.m	simulating Bose et al. state-3 experiments (shown in Figure 4 in the full text via “plot_BoseData.m”)
<i>Functions</i>	
IsoMito_dXdT.m	computing time derivatives of state variables in the model
fluxes.m	computing reaction fluxes in the model
define_global.m	defining global variables
default_IC_vitro.m	including initial conditions of state variables for the <i>in vitro</i> simulations
plot_BoseData.m	plotting simulations of Bose et al.’s experiments (as shown in Figure 4)
<i>Data files</i>	
param10.mat	model parameters
state4con.mat	data points of LaNoue et al.’s state-2 experiments (as shown in Figure 2A, C-E in Wu et al.’s paper)
state3con.mat	data points of LaNoue et al.’s state-3 experiments (as shown in Figure 3A-E in Wu et al.’s paper)
fig3gluaspl.mat	data points of LaNoue et al.’s state-2 and -3 experiments on ASP and GLU (as shown in Figure 2F and 3F)
fig7cit.mat	data points of LaNoue et al.’s state-2 experiments on CIT (as shown in Figure 2B)
Pi_exp_r.mat	data points of Bose et al.’s state-2 experiments on PI
d_Psi_exp_r.mat	data points of Bose et al.’s state-2 experiments on membrane potentials (as shown in Figure 4E)
NADH_exp_r.mat	data points of Bose et al.’s state-2 experiments on relative NADH levels (as shown in Figure 4A)
Pi_exp_a.mat	data points of Bose et al.’s state-3 experiments on PI (as shown in Figure 4)
d_Psi_exp_a.mat	data points of Bose et al.’s state-3 experiments on membrane potentials (as shown in Figure 4)
NADH_exp_a.mat	data points of Bose et al.’s state-3 experiments on relative NADH levels (as shown in Figure 4A)
JO2_exp_a.mat	data points of Bose et al.’s state-3 experiments on oxygen consumption rate (as shown in Figure 4B)

* LaNoue et al.’s experiments refer to those measuring state-2 and state-3 time courses of TCA intermediates (LaNoue et al., *J. Biol. Chem.*, 1970). Bose et al.’s experiments refer to those reported in their work (Bose et al., *J. Biol. Chem.*, 2003). In parentheses are listed correspondingly produced figures or tables in the full text (Wu et al., *J. Biol. Chem.*, 2007).