

**Updates in the MATLAB Code Package “Code\_TCAv4.zip” Implementing “Computer Modeling of Mitochondrial Tricarboxylic Acid Cycle, Oxidative Phosphorylation, Metabolite Transport, and Electrophysiology” (Wu et al., JBC, 2007)**

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The following updates have been made in the files of “IsoMito\_dXdT.m” and “fluxes.m”.

- 1) The following dissociation constants ( $T = 298.15$  K and  $I = 0.17$  M) were updated:
  - a.  $\text{pK}(\text{KATP}^{3-}) = 1.013$ ;
  - b.  $\text{pK}(\text{KADP}^{2-}) = 0.8820$ ;
  - c.  $\text{pK}(\text{KAMP}^-) = 0.6215$ ;
  - d.  $\text{pK}(\text{KSUC}^-) = 0.3525$ ;
  - e.  $\text{pK}(\text{MgOAA}^+) = 0.8629$ .
- 2) Typos in flux expressions of succinyl-CoA synthetase were corrected.
  - a.  $V_{mf} * K_m Q * K_{ir} * A * B * Q \rightarrow V_{mf} * K_m Q * K_{ir} * A * B * P$ ;
  - b.  $V_{mf} * K_m A * B * C * Q * R \rightarrow V_{mr} * K_m A * B * C * Q * R$ ;
  - c.  $V_{mf} * K_m A * B * C * P * Q * R \rightarrow V_{mr} * K_m A * B * C * P * Q * R$ .

The updated model is re-parameterized. The new parameter set is named as “param14.mat” and included in the package. The comparison between “param10.mat” and “param14.mat” is listed in Table 1.

**Table1: Comparison between “param10.mat” and “param14.mat”**

No.	Parameters	param10.mat	param14.mat	Relative Difference (%)
1	X_pdh	1.22E-01	2.05E-01	68.35
2	X_cits	1.16E+01	9.83E+00	15.15
3	X_acon	3.21E-02	2.77E-02	13.77
4	X_isod	4.25E-01	4.92E-01	15.84
5	X_akgd	7.70E-02	8.76E-02	13.81
6	X_scoas	5.82E-01	4.49E-01	22.96
7	X_sdh	6.23E-02	8.58E-02	37.71
8	X_fum	7.12E-03	7.08E-03	0.57
9	X_mdh	6.94E-02	7.71E-02	10.99
10	X_ndk	2.65E-02	2.55E-02	3.75
11	X_got	7.96E+00	4.55E+00	42.79
12	X_PYRH	4.12E+08	3.00E+08	27.22
13	X_GLUH	3.26E+08	2.73E+08	16.38
14	X_CITMAL	7.31E+01	8.04E+01	9.98
15	X_AKGMAL	3.46E-01	2.82E-01	18.44
16	N/A	N/A	N/A	N/A
17	X_MALPI	1.58E+01	1.61E+01	1.43
18	X_ASPGLU	7.48E-05	5.87E-05	21.58
19	N/A	N/A	N/A	N/A
20	N/A	N/A	N/A	N/A
21	X_SUCMAL	9.54E+01	9.70E+01	1.70
22	N/A	N/A	N/A	N/A
23	Km_akgd	6.04E-07	6.01E-07	0.44
24	N/A	N/A	N/A	N/A
25	X_HK	1.19E-01	1.07E-01	9.67
26	N/A	N/A	N/A	N/A
27	N/A	N/A	N/A	N/A
28	N/A	N/A	N/A	N/A
29	N/A	N/A	N/A	N/A
30	N/A	N/A	N/A	N/A
31	X_C1	2.47E+04	3.24E+04	31.13
32	X_C3	6.65E-01	7.91E-01	18.91
33	X_C4	9.93E-05	1.08E-04	8.32
34	X_F1	5.95E+03	8.12E+03	36.39
35	X_ANT	7.27E-03	7.52E-03	3.50
36	X_PIH	2.01E+07	3.34E+07	65.55
37	Km_PIH	1.01E-03	1.61E-03	59.75
38	X_KH	5.65E+06	4.76E+06	15.78
39	X_Hle	3.05E+02	3.02E+02	0.99
40	Km_C3_Pi1	2.81E-05	3.25E-05	15.48
41	Km_C3_Pi2	3.14E-03	3.47E-03	10.74