SECTION 1: Algorithm to Compute Isotopomer Mapping Matrices (IMM)

The original algorithm to compute IMM was described in Schmidt *et al,* 1997. However, these are the cases that were not accounted for by that algorithm.

Case 1: Either the reactant or the product molecule is symmetric

SUCOAS1m: CoA + GTP + succinate <==> GDP + P_i + succinyl-CoA

$$AMM^{1}_{succ->succoa} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad AMM^{2}_{succ->succoa} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Since C_1 and C_4 are equivalent, and C_2 and C_3 are equivalent in the reactant molecule (succ), we swapped the columns 1 and 4, and 2 and 3 in $AMM^{1}_{succ->succoa}$ to produce $AMM^{2}_{succ->succoa}$. The following IMMs are computed with respect to its corresponding AMMs.

$IMM^{1}_{succ->succoa} =$

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

$IMM^{1}_{succ->succoa} =$

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Assuming an equal weighing between the two isomers of succinate

$IMM_{succ->succoa} = (IMM^{1}_{succ->succoa} + IMM^{2}_{succ->succoa})/2 =$

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0.5	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0
0	0	0.5	0	0.5	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0.5	0	0	0	0	0	0	0	0	0.5	0	0	0
0	0	0.5	0	0.5	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0.5	0	0	0	0	0.5	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0.5	0
0	0.5	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	0	0	0	0.5	0	0	0	0	0.5	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0.5	0	0.5	0	0
0	0	0	0.5	0	0	0	0	0	0	0	0	0.5	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0.5	0	0.5	0	0
0	0	0	0	0	0	0	0.5	0	0	0	0	0	0	0.5	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Case 2: Reactions with multiple reactants, at least one product molecule is partially symmetric

CSm: acetyl-CoA + H_2O + oxaloaceate --> citrate + CoA + H

This is only used as an example to illustrate the rules on computing IMMs for partially symmetric compounds. In the model, citrate was actually treated as a prochiral molecule (Stryer). The asymmetric enzyme (citrate synthase) can distinguish between citrate's two identical groups.

$$AMM^{1}_{accoa->cit} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad AMM^{2}_{accoa->cit} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$AMM^{1}_{oaa->cit} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad AMM^{2}_{oaa->cit} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

The IMM^1 and IMM^2 are constructed based on the corresponding AMMs. The isotopomer balance equation should include both IMMs

$$\frac{d[IDV_{cit}]}{dt} = \ldots + \{(IMM^{1}_{accoa->cit} * IDV_{accit} \otimes IMM^{1}_{oaa->cit} * IDV_{oaa}) + (IMM^{2}_{accoa->cit} * IDV_{accit} \otimes IMM^{2}_{oaa->cit} * IDV_{oaa})\} / 2 * v(CSm)\ldots$$

$\otimes$ signifies an elementary-wise product of two vectors

$IMM^{1}_{accoa->cit} =$

1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1
1	0	0	0
1	0	0	0
0	0	1	0
0	0	1	0
0	1	0	0
0	1	0	0
0	0	0	1
0	0	0	1

$IMM^{1}_{oaa->cit} =$

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

$IMM^{2}_{accoa->cit}$

1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
1	0	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	1	0	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	1	0
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1
0	0	0	1

$IMM^{2}_{oaa->cit}$

1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Case 3: Reactions with multiple reactants and/or multiple products of the same species
ACACT1rm [m] : (2) acetyl-CoA <==> acetoacetyl-CoA + CoA

$$AMM_{accoa1->aacoa} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad AMM_{accoa1->aacoa} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$IMM_{accoa1->aacoa} = \begin{matrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{matrix} \qquad IMM_{accoa2->aacoa} = \begin{matrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{matrix}$$

In general, for a reaction of the form

A + B = C

The following equality holds

$IMM_{C->A}=(IMM_{C->A})^T$

$IMM_{C->B}=(IMM_{C->B})^T$

However, for this particular case, since both of the reactants molecules are of the same species, we have to modify the IMM such that every turn of this reaction produces two different sources of acety-CoA: one from C1 and C2 or acetoacetyl-CoA (aacoa) and the other from C3 and C4 of aacoa.

$$IMM_{aacoa->accoa} = IMM_{accoa1->aacoa} + IMM_{accoa2->aacoa} =$$

$$\begin{matrix} 2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 2 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 2 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 2 \end{matrix}$$

SECTION 2: Isotopomer balance equations

See Section 1 for the definitions of IMMs; particular those that have superscripts. The abbreviation vF() and vR( ) signify the forward and reverse fluxes of the reaction in the parentheses.

The below are isotopomer balance equation examples for symmetric compounds (succinate) and compounds that have non-unity coefficients in reactions.

1) Isotopomer balance for mitochondrial succinate

OCOAT1m	[m] acac + succoa <==> aacoa + succ
SUCCt2m	pi[m] + succ[c] <==> pi[c] + succ[m]
SUCD1m	[m] fad + succ <==> fadh2 + fum
SUCOAS1m	[m] coa + gtp + succ <==> gdp + pi + succoa

$$\frac{d[IDV_{succ}]}{dt} = IMM_{succoa->succ} * IDV_{succoa} * vF(OCOAT1m) - IDV_{succ} * vR(OCOAT1m) +$$
$$IDV_{succ\_C} * vF(SUCCt2m) - IDV_{succ} * vR(SUCCt2m) - IDV_{succ} * vF(SUCD1m) + IDV_{fum} * vR(SUCD1m)$$
$$- IMM_{succ->succoa} * IDV_{succ} * vF(SUCOAS1m) + IMM^{T}_{succ->succoa} IDV_{fum} * vR(SUCOAS1m) = 0$$

$IMM^{T}_{succ->succoa}$ is the transpose of $IMM_{succ->succoa}$

The IMMs in reactions SUCCt2m and SUCD1m are removed because they are transport reactions, where IMMs are identity matrices.

2) Isotopomer balance for mitochondrial acetyl-CoA

ACACT1rm	[m] (2) accoa <==> aacoa + coa
ACCOACm	[m] accoa + atp + hco3 --> adp + h + malcoa + pi
ACSm	[m] ac + atp + coa --> accoa + amp + ppi
CSNATm	[m] acrn + coa <==> accoa + crn
CSm	[m] accoa + h2o + oaa --> cit + coa + h
FAOXC160	[m] (7) coa + (7) fad + (7) h2o + (7) nad + pmtcoa --> (8) accoa + (7) fadh2 + (7) h + (7) nadh
FAOXC180	[m] coa + fad + h2o + nad + stcoa --> accoa + fadh2 + h + nadh + pmtcoa
FAOXC181	[m] coa + h2o + nad + odecoa --> accoa + h + nadh + pmtcoa
FAOXC182	[m] (8) coa + (6) fad + (8) h2o + (8) nad + ocdycacoa --> (9) accoa + (6) fadh2 + (8) h + (8) nadh
FAOXC204	[m] c204coa + (9) coa + (5) fad + (9) h2o + (9) nad --> (10) accoa + (5) fadh2 + (9) h + (9) nadh

FAOXC226 [m] c226coa + (10) coa + (4) fad + (10) h2o + (10) nad --> (11) accoa + (4) fadh2 + (10) h + (10) nadh
FAOXC80 [m] (3) coa + (3) fad + (3) h2o + (3) nad + occoa --> (4) accoa + (3) fadh2 + (3) h + (3) nadh
HMGCOASm [m] coa + h + hmgcoa <==> aacoa + accoa + h2o
HMGLm [m] hmgcoa --> acac + accoa
MCD [m] h + malcoa --> accoa + co2
PDHm [m] coa + nad + pyr --> accoa + co2 + nadh

$$\frac{d[IDV_{accoa}]}{dt} = -2 * IDV_{accoa} * vF(ACACT1rm) + IMM_{aacoa->accoa} * IDV_{aacoa} * vR(ACACT1rm) - IDV_{accoa} * vR(ACCOACm)$$
$$IDV_{ac} * v(ACSm) - IDV_{accoa} * v(CSm) + IMM^{final}_{occoa->accoa} * IDV_{occoa} * v(FAOXC80) +$$
$$IMM_{hmgcoa->accoa} * IDV_{hmgcoa} * v(HMGCOASm) - IDV_{accoa} * vR(HMGCOASm) +$$
$$IMM_{hmgcoa->accoa} * IDV_{hmgcoa} * v(HMGLm) + IMM_{malcoa->accoa} * IDV_{malcoa} * v(MCD) + IMM_{pyr->.accoa} * IDV_{pyr} * v(PDHm) +$$
$$IDV^{fixed}_{accoa} * (8 * v(FAOXC160) + v(FAOXC180) + v(FAOXC181) + 9 * v(FAOXC182) + 10 * v(FAOXC204) + 11 * v(FAOXC226)) +$$
$$IDV^{fixed}_{accoa}(vF(CSNATm) - v(CSNATm)) = 0$$

See Supplemental data S2 for the definition of $IMM_{aacoa->accoa}$.
$IMM^{final}_{occoa->accoa}$ is the sum of all four IMMs, each corresponds to a particular acetyl-CoA product.
IDV^{fixed}_{accoa} is the vector $(1, 0, 0, 0)^T$, which accounts for the fact that the acetyl-CoA contributed from fatty acids C16:0, C18:0, C18:1, C18:2, C20:4, C22:6 are not labeled in any carbon because these fatty acids are not labeled in the experiments.

SECTION 3: Criteria for reversible reactions which forward and reverse fluxes need not to be tracked explicitly.

Example 1

$$I \xrightarrow{v_1} A \xleftrightarrow{v_2} B \xrightarrow{v_3} O$$

I_X: isotopomer distribution vector of metabolite X; IMM_{AB}: isotopomer mapping matrix from reactant A to product B; vF: $v^{forward}$; vR: $v^{reverse}$

IDV balance for A

$$\frac{dI_A}{dt} = I_I \cdot v_1 - I_A \cdot v_2 F + IMM_{AB}^T \cdot I_B \cdot v_2 R = 0 \qquad \text{(Eq. 1)}$$

Case 1: $v_2^{net} \geq 0$

$$\frac{dI_A}{dt} = I_I \cdot v_1 - I_A \cdot v_2^{net} = 0 \qquad \text{(Eq. 2)}$$

Condition to be satisfied for Eq. 1 and 2 to be equivalent

$$-I_A \cdot v_2 F + IMM_{AB}^T \cdot I_B \cdot v_2 R = -I_A (v_2 F - v_2 R)$$

Or $\quad IMM_{AB}^T \cdot I_B = I_A \qquad$ (Eq. 3)

Case 2: $v_2^{net} < 0$

$$\frac{dI_A}{dt} = I_I \cdot v_1 - IMM_{AB}^T \cdot I_B \cdot v_2^{net} = 0 \qquad \text{(Eq. 4)}$$

Condition to be satisfied for Eq. 1 and 4 to be equivalent

$$-I_A \cdot v_2 F + IMM_{AB}^T \cdot I_B \cdot vR = -IMM_{AB}^T \cdot I_B (v_2 F - v_2 R)$$

Or $\quad I_A = IMM_{AB}^T \cdot I_B$, which is the same condition as in Eq. 3.

IDV balance for B

$$\frac{dI_B}{dt} = IMM_{AB} \cdot I_A \cdot v_2 F - I_B \cdot v_2 R - I_B \cdot v_3 = 0 \qquad \text{(Eq. 5)}$$

$$IMM_{AB} \cdot I_A \cdot v_2 F = I_B (v_2 R + v_3)$$

Flux balance yields $\quad v_2 F = v_2 R + v_3$

Thus we obtain

$$IMM_{AB} \cdot I_A = I_B \qquad \text{(Eq. 6)}$$

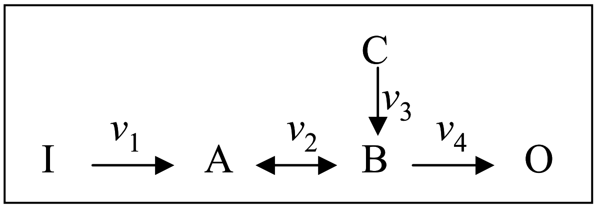
Substitute this expression for I_B (Eq. 6) into the condition stated by Eq. 3, we get

$$IMM_{AB}^T \cdot IMM_{AB} \cdot I_A = I_A$$

Or $\quad \boxed{IMM_{AB}^T \cdot IMM_{AB} = I} \qquad$ (Eq. 7)

Thus this is the condition for which one can replace $v^{forward}$ and $v^{reverse}$ by v^{net} for a reversible reaction.

Example 2



IDV balance for A

$$\frac{dI_A}{dt} = I_I \cdot v_1 - I_A \cdot v_2F + IMM_{AB}^T \cdot I_B \cdot v_2R = 0 \qquad \text{(Eq. 1)}$$

Similar to Example 1, we derive the following condition

$$IMM_{AB}^T \cdot I_B = I_A \qquad \text{(Eq. 2)}$$

IDV balance for B

$$\frac{dI_B}{dt} = IMM_{AB} \cdot I_A \cdot v_2F - I_B \cdot v_2R + IMM_{CB} \cdot I_C \cdot v_3 - I_B \cdot v_4 = 0 \qquad \text{(Eq. 3)}$$

Thus

$$IMM_{AB} \cdot I_A \cdot v_2F + IMM_{CB} \cdot I_C \cdot v_3 = I_B \cdot (v_2R + v_4)$$

Since flux balance on B yields $v_2R + v_4 = v_2F + v_3$, we get

$$IMM_{AB} \cdot I_A + IMM_{CB} \cdot I_C = I_B$$

Substituting this expression for I_B into the condition in Eq. 2

$$IMM_{AB}^T \cdot IMM_{AB} \cdot I_A + IMM_{AB}^T \cdot IMM_{CB} \cdot I_C = I_A$$

But this equality does not hold in general because I_C is a variable.

Alternatively,

$$\frac{dI_B}{dt} = IMM_{AB} \cdot I_A \cdot v_2F - I_B \cdot v_2R + IMM_{CB} \cdot I_C \cdot v_3 - I_B \cdot v_4 = 0 \qquad \text{(Eq. 4)}$$

If v_{net} can replace both vF and vR in reaction 2

$$\frac{dI_B}{dt} = IMM_{AB} \cdot I_A \cdot v_2^{net} + IMM_{CB} \cdot I_C \cdot v_3 - I_B \cdot v_4 = 0 \qquad \text{if } v_2^{net} \geq 0 \qquad \text{(Eq. 5)}$$

Or

$$\frac{dI_B}{dt} = I_B \cdot v_2^{net} + IMM_{CB} \cdot I_C \cdot v_3 - I_B \cdot v_4 = 0 \qquad \text{if } v_2^{net} < 0 \qquad \text{(Eq. 6)}$$

Eq. 4, 5, and 6 are equivalent only if

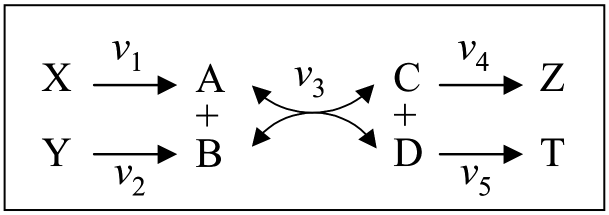
$$IMM_{AB} \cdot I_A \cdot v_2F - I_B \cdot v_2R = IMM_{AB} \cdot I_A \cdot v_2^{net}$$

$$IMM_{AB} \cdot I_A = I_B$$

$$IMM_{AB} \cdot I_A = IMM_{AB} \cdot I_A + IMM_{BC} \cdot I_C \qquad \text{(Eq. 7)}$$

But Eq. 6 does not hold in general because I_C is not necessary in the null space of IMM_{BC}.

Example 3



IDV balance for A

$$\frac{dI_A}{dt} = I_X \cdot v_1 - I_A \cdot v_3 F + IMM_{AC}^T \cdot I_C \cdot v_3 R = 0 \qquad \text{(Eq. 1)}$$

If v_{net} can replace both *vF* and *vR* in reaction 2

$$\frac{dI_A}{dt} = I_X \cdot v_1 - I_A \cdot v_3^{net} = 0 \qquad \text{(Eq. 2)}$$

Eq. 1 and 2 are equivalent only if

$$-I_A \cdot v_3 F + IMM_{AC}^T \cdot I_C \cdot v_3 R = -I_A \cdot v_3^{net}$$

Or $$I_A = IMM_{AC}^T \cdot I_C \qquad \text{(Eq. 3)}$$

IDV balance for C

$$\frac{dI_C}{dt} = IMM_{AC} \cdot I_A \cdot v_3 F - I_C \cdot v_3 R - I_C \cdot v_4 = 0$$

$$IMM_{AC} \cdot I_A \cdot v_3 F = I_C (v_3 R + v_4)$$

$$IMM_{AC} * I_A = I_C \qquad \text{(Eq. 4)}$$

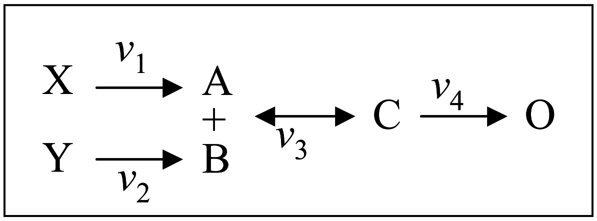
Substitute Eq. 4 into the condition in Eq. 3

$$I_A = IMM_{AC}^T * IMM_{AC} * I_A = I_A$$

Or $$\boxed{IMM_{AC}^T * IMM_{AC} = I} \qquad \text{(Eq. 7)}$$

The same proof works for the pair of reactant B-product D.
Thus this is the condition for c

Example 4



IDV balance for A

$$\frac{dI_A}{dt} = I_X \cdot v_1 - I_A \cdot v_3F + IMM_{AC}^T \cdot I_C \cdot v_3R = 0 \qquad \text{(Eq. 1)}$$

If v_{net} can replace both vF and vR in reaction 2

$$\frac{dI_A}{dt} = I_X \cdot v_1 - I_A \cdot v_3^{net} = 0 \qquad \text{(Eq. 2)}$$

Eq. 1 and 2 are equivalent only if

$$-I_A * v_3F + IMM_{AB}^T * I_C * v_3R = -I_A * v_3^{net}$$

Or $I_A = IMM_{AC}^T * I_C$ (Eq. 3)

IDV balance for C

$$\frac{dI_C}{dt} = (IMM_{AC} \cdot I_A \otimes IMM_{BC} \cdot I_B) \cdot v_3F - I_C \cdot v_3R - I_C \cdot v_4 = 0 \qquad \text{(Eq. 4)}$$

where ⊗ signifies an elementary-wise product of two vectors

Flux balance on C yields

$$v_3F = v_3R + v_4$$

Thus Eq. 4 can be simplified to

$$(IMM_{AC} * I_A \otimes IMM_{BC} * I_B) = I_C \qquad \text{(Eq. 5)}$$

Substitute the left hand side in Eq. 5 into Eq. 3 for I_C, we derive the condition that must be satisfied before one can replace $v^{forward}$ and $v^{reverse}$ by v^{net}

$$I_A = IMM_{AC}^T * (IMM_{AC} * I_A \otimes IMM_{BC} * I_C)$$

This condition does not hold in general.

A similar proof can be shown for the pair of reactant B-product C.

SECTION 4: List of metabolites in the network

Num. of Carbon column:

Digit: the number of carbon atoms, whose labeling patterns are tracked in the model

DE: metabolites are dead ends in the network

Number	Abbr.	Name	Compartment	Num of Carbon
1	12dgr(c)	1,2-Diacylglycerol	Cytosol	NA
2	13dpg(c)	3-Phospho-D-glyceroyl phosphate	Cytosol	3
3	2pg(c)	D-Glycerate 2-phosphate	Cytosol	3
4	3pg(c)	3-Phospho-D-glycerate	Cytosol	3
5	5aop(c)	5-Amino-4-oxopentanoate	Cytosol	5
6	ac(c)	Acetate	Cytosol	2
7	acac(c)	Acetoacetate	Cytosol	4
8	accoa(c)	Acetyl-CoA	Cytosol	eff DE
9	acrn(c)	O-Acetylcarnitine	Cytosol	DE
10	adp(c)	ADP	Cytosol	NA
11	akg(c)	2-Oxoglutarate	Cytosol	5
12	ala-L(c)	L-Alanine	Cytosol	3
13	amp(c)	AMP	Cytosol	NA
14	arachd(c)	arachidonic acid	Cytosol	NA
15	arachdcoa(c)	C20:4-CoA	Cytosol	NA
16	arachdcrn(c)	C20:4 carnitine	Cytosol	NA
17	arg-L(c)	L-Arginine	Cytosol	DE
18	asp-L(c)	L-Aspartate	Cytosol	4
19	atp(c)	ATP	Cytosol	NA
20	bhb(c)	(R)-3-Hydroxybutanoate	Cytosol	4
21	bilirub(c)	Bilirubin	Cytosol	NA
22	biliverd(c)	Biliverdin	Cytosol	NA
23	c226coa(c)	cervonyl coenzyme A	Cytosol	NA
24	c226crn(c)	cervonyl carnitine	Cytosol	NA
25	cdp(c)	CDP	Cytosol	NA
26	cdpchol(c)	CDPcholine	Cytosol	NA
27	chol(c)	Choline	Cytosol	NA
28	cholp(c)	Choline phosphate	Cytosol	NA
29	cit(c)	Citrate	Cytosol	6
30	citr-L(c)	L-Citrulline	Cytosol	6
31	cmp(c)	CMP	Cytosol	NA
32	co(c)	Carbon monoxide	Cytosol	eff DE
33	co2(c)	CO2	Cytosol	1
34	coa(c)	Coenzyme A	Cytosol	NA
35	cpppg3(c)	Coproporphyrinogen III	Cytosol	NA
36	crn(c)	L-Carnitine	Cytosol	NA
37	crvnc(c)	cervonic acid	Cytosol	NA
38	ctp(c)	CTP	Cytosol	NA
39	cys-L(c)	L-Cysteine	Cytosol	DE
40	dhap(c)	Dihydroxyacetone phosphate	Cytosol	3
41	f6p(c)	D-Fructose 6-phosphate	Cytosol	6
42	fdp(c)	D-Fructose 1,6-bisphosphate	Cytosol	6
43	fe2(c)	Fe2+	Cytosol	NA
44	fum(c)	Fumarate	Cytosol	DE
45	g3p(c)	Glyceraldehyde 3-phosphate	Cytosol	3
46	g6p(c)	D-Glucose 6-phosphate	Cytosol	6
47	gdp(c)	GDP	Cytosol	NA
48	glc-D(c)	D-Glucose	Cytosol	6
49	gln-L(c)	L-Glutamine	Cytosol	5
50	glu-L(c)	L-Glutamate	Cytosol	5
51	glucys(c)	gamma-L-Glutamyl-L-cysteine	Cytosol	NA

52	gly(c)	Glycine	Cytosol		2
53	glyc(c)	Glycerol	Cytosol		3
54	gthrd(c)	Reduced glutathione	Cytosol	NA	
55	gtp(c)	GTP	Cytosol	NA	
56	h(c)	H+	Cytosol	NA	
57	h2o(c)	H2O	Cytosol	NA	
58	hdca(c)	Hexadecanoate (n-C16:0)	Cytosol	NA	
59	hdcea(c)	Hexadecenoate (n-C16:1)	Cytosol	NA	
60	hdcecrn(c)	Hexadecenoyl-CoA (nC16:1)	Cytosol	NA	
61	hdcoa(c)	Hexadecenoyl-CoA (n-C16:1CoA)	Cytosol	NA	
62	hmbil(c)	Hydroxymethylbilane	Cytosol	NA	
63	k(c)	potassium	Cytosol	NA	
64	lac-L(c)	L-Lactate	Cytosol		3
65	mal-L(c)	L-Malate	Cytosol		4
66	na1(c)	Sodium	Cytosol	NA	
67	nad(c)	Nicotinamide adenine dinucleotide	Cytosol	NA	
68	nadh(c)	Nicotinamide adenine dinucleotide - reduced	Cytosol	NA	
69	nadp(c)	Nicotinamide adenine dinucleotide phosphate	Cytosol	DE	
70	nadph(c)	Nicotinamide adenine dinucleotide phosphate - reduced	Cytosol	DE	
71	nh4(c)	Ammonium	Cytosol	NA	
72	o2(c)	O2	Cytosol	NA	
73	oaa(c)	Oxaloacetate	Cytosol		4
74	occoa(c)	Octanoyl-CoA (n-C8:0CoA)	Cytosol	NA	
75	ocdca(c)	octadecanoate (n-C18:0)	Cytosol	NA	
76	ocdcea(c)	octadecenoate (n-C18:1)	Cytosol	NA	
77	ocdcya(c)	octadecadienoate (n-C18:2)	Cytosol	NA	
78	ocdycacoa(c)	Octadecynoyl-CoA (n-C18:2CoA)	Cytosol	NA	
79	ocdycrn(c)	octadecynoyl carnitine	Cytosol	NA	
80	octa(c)	octanoate (n-C8:0)	Cytosol	NA	
81	odecoa(c)	Octadecenoyl-CoA (n-C18:1CoA)	Cytosol	NA	
82	odecrn(c)	octadecenoyl carnitine	Cytosol	NA	
83	oh1(c)	hydroxide ion	Cytosol	DE	
84	orn(c)	Ornithine	Cytosol		5
85	pc(c)	Phosphatidylcholine	Cytosol	NA	
86	pep(c)	Phosphoenolpyruvate	Cytosol		3
87	pheme(c)	Protoheme	Cytosol	NA	
88	pi(c)	Phosphate	Cytosol	NA	
89	pmtcoa(c)	Palmitoyl-CoA (n-C16:0CoA)	Cytosol	NA	
90	pmtcrn(c)	L-Palmitoylcarnitine	Cytosol	NA	
91	ppa(c)	Propionate (n-C3:0)	Cytosol		3
92	ppbng(c)	Porphobilinogen	Cytosol	NA	
93	ppi(c)	Diphosphate	Cytosol	NA	
94	pppg9(c)	Protoporphyrinogen IX	Cytosol	NA	
95	ps(c)	Phosphatidylserine	Cytosol	NA	
96	pyr(c)	Pyruvate	Cytosol		3
97	stcoa(c)	Stearoyl-CoA (n-C18:0CoA)	Cytosol	NA	
98	stcrn(c)	stearoylcarnitine	Cytosol	NA	
99	succ(c)	Succinate	Cytosol		4
100	uppg3(c)	Uroporphyrinogen III	Cytosol	NA	
101	12dgr(e)	1,2-Diacylglycerol	Extracellular	NA	
102	ac(e)	Acetate	Extracellular		2
103	acac(e)	Acetoacetate	Extracellular		4
104	ala-L(e)	L-Alanine	Extracellular		3
105	arachd(e)	arachidonic acid	Extracellular	NA	
106	bhb(e)	(R)-3-Hydroxybutanoate	Extracellular		4
107	bilirub(e)	Bilirubin	Extracellular	NA	
108	chol(e)	Choline	Extracellular	NA	

109	cit(e)	Citrate	Extracellular		6
110	co(e)	Carbon monoxide	Extracellular	eff DE	
111	co2(e)	CO2	Extracellular		1
112	coa(e)	Coenzyme A	Extracellular	NA	
113	crvnc(e)	cervonic acid	Extracellular	NA	
114	fe2(e)	Fe2+	Extracellular	NA	
115	glc-D(e)	D-Glucose	Extracellular		6
116	gln-L(e)	L-Glutamine	Extracellular		5
117	glu-L(e)	L-Glutamate	Extracellular		5
118	gly(e)	Glycine	Extracellular		2
119	glyc(e)	Glycerol	Extracellular		3
120	h(e)	H+	Extracellular	NA	
121	h2o(e)	H2O	Extracellular	NA	
122	hdca(e)	Hexadecanoate (n-C16:0)	Extracellular	NA	
123	hdcea(e)	Hexadecenoate (n-C16:1)	Extracellular	NA	
124	k(e)	potassium	Extracellular	NA	
125	lac-L(e)	L-Lactate	Extracellular		3
126	na1(e)	Sodium	Extracellular	NA	
127	nh4(e)	Ammonium	Extracellular	NA	
128	o2(e)	O2	Extracellular	NA	
129	ocdca(e)	octadecanoate (n-C18:0)	Extracellular	NA	
130	ocdcea(e)	octadecenoate (n-C18:1)	Extracellular	NA	
131	ocdcya(e)	octadecadienoate (n-C18:2)	Extracellular	NA	
132	octa(e)	octanoate (n-C8:0)	Extracellular	NA	
133	pi(e)	Phosphate	Extracellular	NA	
134	ppa(e)	Propionate (n-C3:0)	Extracellular		3
135	ps(e)	Phosphatidylserine	Extracellular	NA	
136	pyr(e)	Pyruvate	Extracellular		3
137	succ(e)	Succinate	Extracellular		4
138	12dgr(m)	1,2-Diacylglycerol	Mitochondria	NA	
139	1ag3p(m)	1-Acyl-sn-glycerol 3-phosphate	Mitochondria	NA	
140	5aop(m)	5-Amino-4-oxopentanoate	Mitochondria		5
141	aacoa(m)	Acetoacetyl-CoA	Mitochondria		4
142	ac(m)	Acetate	Mitochondria		2
143	acac(m)	Acetoacetate	Mitochondria		4
144	accoa(m)	Acetyl-CoA	Mitochondria		2
145	acrn(m)	O-Acetylcarnitine	Mitochondria	eff DE	
146	adp(m)	ADP	Mitochondria	NA	
147	akg(m)	2-Oxoglutarate	Mitochondria		5
148	amp(m)	AMP	Mitochondria	NA	
149	arachdcoa(m)	C20:4-CoA	Mitochondria	NA	
150	arachdcrn(m)	C20:4 carnitine	Mitochondria	NA	
151	arg-L(m)	L-Arginine	Mitochondria	DE	
152	asn-L(m)	L-Asparagine	Mitochondria	DE	
153	asp-L(m)	L-Aspartate	Mitochondria		4
154	atp(m)	ATP	Mitochondria	NA	
155	bhb(m)	(R)-3-Hydroxybutanoate	Mitochondria		4
156	c226coa(m)	cervonyl coenzyme A	Mitochondria	NA	
157	c226crn(m)	cervonyl carnitine	Mitochondria	NA	
158	cdp(m)	CDP	Mitochondria	DE	
159	cdpdag(m)	CDPdiacylglycerol	Mitochondria	NA	
160	cdpea(m)	CDPethanolamine	Mitochondria	DE	
161	chol(m)	Choline	Mitochondria	DE	
162	cit(m)	Citrate	Mitochondria		6
163	citr-L(m)	L-Citrulline	Mitochondria		6
164	clpn(m)	Cardiolipin	Mitochondria	NA	
165	cmp(m)	CMP	Mitochondria	NA	

166	co2(m)	CO2	Mitochondria		1
167	coa(m)	Coenzyme A	Mitochondria	NA	
168	creat(m)	Creatine	Mitochondria	DE	
169	crn(m)	L-Carnitine	Mitochondria	NA	
170	ctp(m)	CTP	Mitochondria	NA	
171	dhap(m)	Dihydroxyacetone phosphate	Mitochondria	DE	
172	facoa_hg(m)	Weighted average acyl group of HepG2 cell phospholipid	Mitochondria	NA	
173	fad(m)	Flavin adenine dinucleotide oxidized	Mitochondria	NA	
174	fadh2(m)	Flavin adenine dinucleotide reduced	Mitochondria	NA	
175	fe2(m)	Fe2+	Mitochondria	NA	
176	ficytC(m)	Ferricytochrome c	Mitochondria	NA	
177	focytC(m)	Ferrocytochrome C	Mitochondria	NA	
178	fum(m)	Fumarate	Mitochondria		4
179	gdp(m)	GDP	Mitochondria	NA	
180	gln-L(m)	L-Glutamine	Mitochondria		5
181	glu-L(m)	L-Glutamate	Mitochondria		5
182	gly(m)	Glycine	Mitochondria		2
183	glyc(m)	Glycerol	Mitochondria		3
184	glyc3p(m)	Glycerol 3-phosphate	Mitochondria		3
185	gthox(m)	Oxidized glutathione	Mitochondria	NA	
186	gthrd(m)	Reduced glutathione	Mitochondria	NA	
187	gtp(m)	GTP	Mitochondria	NA	
188	h(m)	H+	Mitochondria	NA	
189	h2co3(m)	carbonic acid	Mitochondria	DE	
190	h2o(m)	H2O	Mitochondria	NA	
191	h2o2(m)	Hydrogen peroxide	Mitochondria	NA	
192	hco3(m)	Bicarbonate	Mitochondria		1
193	hdcecrn(m)	Hexadecenoyl-CoA (nC16:1)	Mitochondria	NA	
194	hdcoa(m)	Hexadecenoyl-CoA (n-C16:1CoA)	Mitochondria	NA	
195	hmgcoa(m)	Hydroxymethylglutaryl-CoA	Mitochondria		6
196	icit(m)	Isocitrate	Mitochondria		6
197	lac-L(m)	L-Lactate	Mitochondria		3
198	mal-L(m)	L-Malate	Mitochondria		4
199	malcoa(m)	Malonyl-CoA	Mitochondria		3
200	mmcoa-R(m)	(R)-Methylmalonyl-CoA	Mitochondria		4
201	mmcoa-S(m)	(S)-Methylmalonyl-CoA	Mitochondria		4
202	nad(m)	Nicotinamide adenine dinucleotide	Mitochondria	NA	
203	nadh(m)	Nicotinamide adenine dinucleotide - reduced	Mitochondria	NA	
204	nadp(m)	Nicotinamide adenine dinucleotide phosphate	Mitochondria	NA	
205	nadph(m)	Nicotinamide adenine dinucleotide phosphate - reduced	Mitochondria	NA	
206	nh4(m)	Ammonium	Mitochondria	NA	
207	o2(m)	O2	Mitochondria	NA	
208	o2s(m)	Superoxide anion	Mitochondria	NA	
209	oaa(m)	Oxaloacetate	Mitochondria		4
210	occoa(m)	Octanoyl-CoA (n-C8:0CoA)	Mitochondria	NA	
211	ocdycacoa(m)	Octadecynoyl-CoA (n-C18:2CoA)	Mitochondria	NA	
212	ocdycrn(m)	octadecynoyl carnitine	Mitochondria	NA	
213	odecoa(m)	Octadecenoyl-CoA (n-C18:1CoA)	Mitochondria	NA	
214	odecrn(m)	octadecenoyl carnitine	Mitochondria	NA	
215	orn(m)	Ornithine	Mitochondria		5
216	pa(m)	Phosphatidate	Mitochondria	NA	
217	pc(m)	Phosphatidylcholine	Mitochondria	NA	
218	pcreat(m)	Phosphocreatine	Mitochondria	DE	
219	pcrn(m)	propionyl-carnitine	Mitochondria	DE	
220	pe(m)	Phosphatidylethanolamine	Mitochondria	NA	
221	pep(m)	Phosphoenolpyruvate	Mitochondria		3

222	pg(m)	Phosphatidylglycerol	Mitochondria	NA	
223	pgp(m)	Phosphatidylglycerophosphate	Mitochondria	NA	
224	pheme(m)	Protoheme	Mitochondria	NA	
225	pi(m)	Phosphate	Mitochondria	NA	
226	pmtcoa(m)	Palmitoyl-CoA (n-C16:0CoA)	Mitochondria	NA	
227	pmtcrn(m)	L-Palmitoylcarnitine	Mitochondria	NA	
228	ppa(m)	Propionate (n-C3:0)	Mitochondria		3
229	ppcoa(m)	Propanoyl-CoA	Mitochondria		3
230	ppi(m)	Diphosphate	Mitochondria	NA	
231	ppp9(m)	Protoporphyrin	Mitochondria	NA	
232	pppg9(m)	Protoporphyrinogen IX	Mitochondria	NA	
233	ps(m)	Phosphatidylserine	Mitochondria	NA	
234	pyr(m)	Pyruvate	Mitochondria		3
235	q10(m)	Ubiquinone-10	Mitochondria	NA	
236	q10h2(m)	Ubiquinol-10	Mitochondria	NA	
237	stcoa(m)	Stearoyl-CoA (n-C18:0CoA)	Mitochondria	NA	
238	stcrn(m)	stearoylcarnitine	Mitochondria	NA	
239	succ(m)	Succinate	Mitochondria		4
240	succoa(m)	Succinyl-CoA	Mitochondria		4