

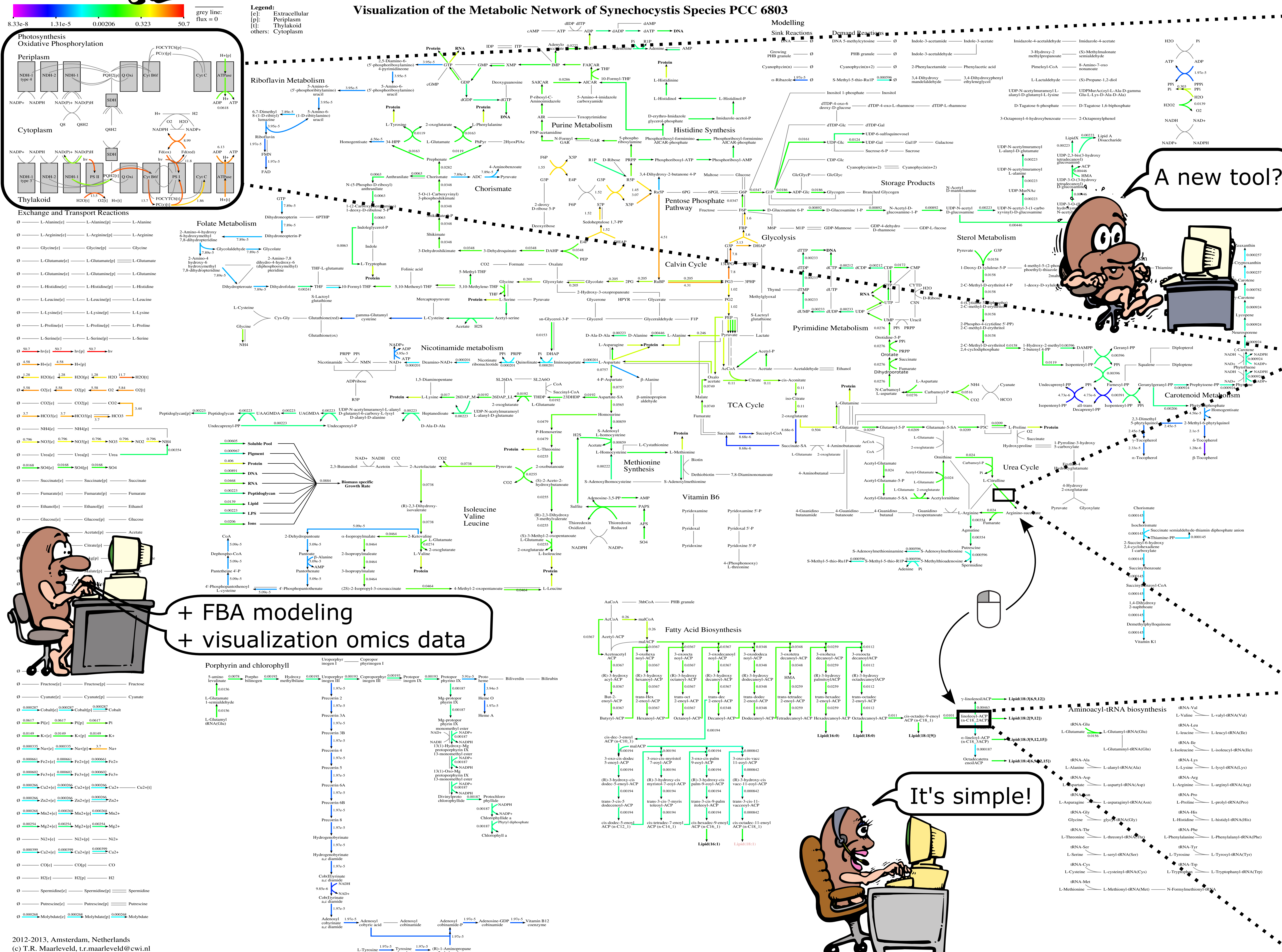
Modeling is too difficult

# Making Genome-scale Modeling Simple

Timo R. Maarleveld<sup>1,2</sup>, J. Boele<sup>2</sup>, F.J. Bruggeman<sup>2</sup>, B. Teusink<sup>2</sup>  
1 - Centrum Wiskunde & Informatica, 2 - VU University Amsterdam



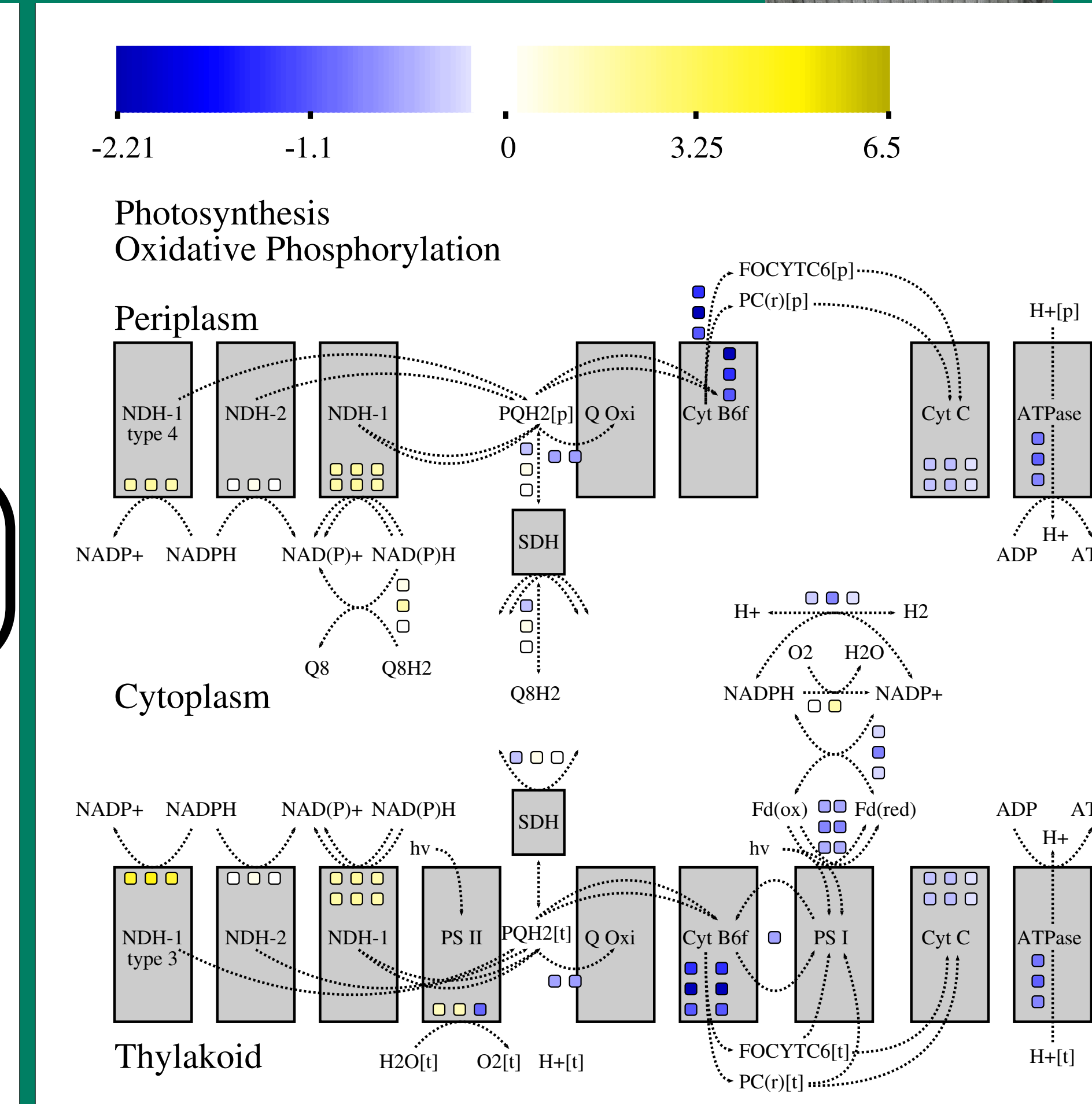
E-mail: t.r.maarleveld@cwi.nl



A new tool?

It's simple!

+ FBA modeling  
+ visualization omics data



REACTION: R01954

Entry	R01954	Reaction
Name		L-Citrulline:L-aspartate ligase (AMP-forming)
Definition		ATP + L-Citrulline + L-Aspartate <=> AMP + Diphosphate + N-(L-Arginino)succinate
Equation		C00002 + C00327 + C00049 <=> C00020 + C00013 + C03406
Chemical		<chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem> + <chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem> + <chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem> <=> <chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem> + <chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem> + <chem>C1=NC2=C(NC(=O)N2)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N</chem>
RPair	RP00008 RP00009 RP01870 RP01871	C00002 C00020 ligase C00002 C00013 ligase C00049 C03406 main C00327 C03406 main
Enzyme	6.3.4.5	
Pathway	rn00250 rn00330 rn01100 rn01110 rn01230	Alanine, aspartate and glutamate metabolism Arginine and proline metabolism Metabolic pathways Biosynthesis of secondary metabolites Biosynthesis of amino acids
Orthology	K01940	argininosuccinate synthase [EC:6.3.4.5]

FAME

Target species: M\_octe\_9\_12\_ACP\_c (linoleoyl-ACP (n-C18\_2ACP))

Total flux through metabolic: 0.0101443200492

Click here to toggle species IDs and names

Producing reactions	Rate	Consuming reactions	Rate
R_DES_122_M_h_c1	0.0010100463	2 M_h_c1 M_h2_c1	0.0010100463
M_o2_c1		M_octe_9_12_ACP_c	
M_octe_9_ACP_c		2 M_fdo_2_2_c	
2 M_fdo_2_2_c			
		M_octe_9_12_ACP_c	0.0025
		M_octe_9_12_ACP_c	0.0025
		1 M_octe_9_12_ACP_c	0.0005172
		2 M_octe_9_12_ACP_c	0.0005172
		M_octe_9_12_ACP_c	0.0005172
		M_octe_9_12_ACP_c	0.0005172

© 2011-2013, Timo R. Maarleveld / VU University Amsterdam. All rights reserved. Last update: May 2nd, 2013.