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***Supplementary Material:*****Article TitleA verified Petri model for the metabolism of *Arabidopsis thaliana*: application of network decomposition and network reduction**

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## 1 SUPPLEMENTARY TABLES

**Supplementary Table 1.** Metabolites of the complete PN model. *Name* corresponds to the metabolite's name. *No.* gives the number of the corresponding place.

No.	Name	No.	Name	No.	Name
1	ornithine	46	D-ribose 5-phosphate	91	acetyl-L-serine
2	glutamate	47	coumaroyl-CoA	92	acetyl-CoA
3	$\gamma$ -aminobutyric acid (GABA)	48	sinapyl alcohol	93	coenzyme A (CoA)
4	succinate	49	$\beta$ -D-glucose 6-phosphate	94	citrulline
5	succinyl-CoA	50	$\alpha$ -D-glucose 1-phosphate	95	3-dehydroshikimate
6	fumarate	51	$\beta$ -D-glucose	96	shikimate 3-phosphate
7	feruloyl-CoA	52	D-ribulose 5-phosphate	97	5-enolpyruvyl-shikimate-3-phosphate
8	malate	53	6-phosphogluconate	98	L-arogenate
9	$\alpha$ -ketoglutarate)	54	D-glucono-1,5-lactone 6-phosphate	99	homogentisate
10	isocitrate	55	Sinapate	100	coumaroyl shikimic acid
11	citrate	56	$\alpha$ -D-glucose 6-phosphate	101	quinate
12	oxalacetate	57	$\alpha$ -D-glucose	102	shikimate
13	glyoxylate	58	ADP-glucose	103	chorismate
14	glycerate	59	starch	104	coumaroyl quinic acid
15	hydroxypyruvate	60	D-ribulose 1,5-bisphosphate	105	prephenate
16	serine	61	maltose	106	4-hydroxy-phenylpyroavate
17	coniferyl aldehyde	62	sorbitol	107	tyrosine
18	glycine	63	D-fructose	108	caffeooyl-CoA
19	coniferyl alcohol	64	2-phospho glycolate	109	phenylalanine
20	pyruvate	65	sedoheptulose 7-phosphate	110	trans-cinnamate
21	L-alanine	66	sucrose	111	caffeooyl quinic acid
22	not modeled	67	sedoheptulose 1,7-biphosphate	112	p-coumaric acid
23	L-aspartate	68	Dihydroxyacetone phosphate	113	cysteine
24	uracil	69	1L-myo-inositol-1-phosphate	114	acetaldehyde
25	urea	70	raffinose	115	uridine diphosphate (UDP)
26	asparagine	71	stachyose	116	carbamoyl phosphate
27	L-arginino-succinate	72	galactinol	117	carbamoyl aspartate
28	arginine	73	D-galactose	118	dihydroorotate
29	ammonia	74	D-myo-inositol	119	orotic acid
30a,b	lignin	75	galactane	120	orotidine 5'-monophosphate
31	hydroxyconiferyl alcohol	76	$\alpha$ -D-Galactose 1-phosphate	121	5-phosphoribosyl 1-phosphate
32	D-erythrose 4-phosphate	77	UDP-galactose	122	cytidine triphosphate
33	glutamine	78	L-galactono 1,4-lactone	123	cytidine monophosphate (CMP)
34	phosphoenolpyruvate	79	succinate semialdehyde	124	dihydouracil
35	glycolate	80	uridine 5'-phosphate (UMP)	125	$\beta$ -ureidopropionate
36	7-phospho-2-dehydro-3-deoxy-D-arabinohexonate	81	amylopectin	126	uridine
37	3-dehydroquinate	82	UDP-glucose	127	cytidine
38	acetate	83	trehalose	128	cytidine diphosphate (CDP)
39	glycerate 2-phosphate	84	trehalose 6-phosphate	129	uridine triphosphate (UTP)
40	glycerate 3-phosphate	85	UDP-D-glucuronate	130	L-galactonate
41	glycerate 1,3-biphosphophosphate	86	amylose	131	UDP-D-Galacturonate
42	glyceraldehyde 3-phosphate	87	D-galacturonate	132	D-galacturonate 1-phosphate
43	$\beta$ -D-fructose 1,6-phosphate	88	UDP-xylose	133	hydroxyconiferyl aldehyde
44	$\beta$ -D-fructose 6-phosphate	89	heteroglycan		
45	D-xylulose 5-phosphate	90	caffeooyl shikimic acid		

**Supplementary Table 2.** Reactions of the complete PN model. The column *Transitions* gives the reaction names. The reactions are named a combination of letters and numbers. A reaction name is represented by  $Ex$ , where  $x$  stands for an integer, which is random. Forward and backward reactions are indicated by  $Ex\_f$  and  $Ex\_b$ , respectively.  $IN_x$  stands for input reactions, where  $x$  denotes the supplied metabolite, and  $OUT_x$  for an output input reactions, where  $x$  denotes the removed metabolite. *Biochemical Pathway* denotes the biochemical pathways the reaction is participating. *Enzyme name* gives the name of the enzyme catalyzing the reaction. *References* refers to the publications where the reaction is described. *Reactions* describes the reactions' formulae and adds comments for special treatments. The metabolites' numbers are encoded in Table 1.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E1_44_b E1_44_f	1. ribose degradation 2. pentose phosphate pathway (non-oxidative branch)	transketolase	Buchanan et al. (2000)	1. $45 + 46 \rightarrow 42 + 65$ 2. $45 + 46 \rightarrow 42 + 65 \& 32 + 45 \rightarrow 42 + 44$
E1_46_b E1_46_f	3. Calvin-Benson-Bassham cycle 4. Rubisco shunt			3. $42 + 65 \rightarrow 45 + 46$ 4. $42 + 44 \rightarrow 32 + 45 \& 42 + 65 \rightarrow 45 + 46$
E2_f E2_b	aspartate biosynthesis	aspartate transaminase	Wilkie and Warren (1998) Graindorge et al. (2010)	$2 + 12 \rightarrow 23 + 9$ $23 + 9 \rightarrow 2 + 12$
E3_f E3_b	1. ribose degradation 2. pentose phosphate pathway (non-oxidative branch) 3. Calvin-Benson-Bassham cycle 4. Rubisco shunt	ribose-5-phosphate isomerase	Berg et al. (2002) Buchanan et al. (2000)	1. $46 \rightarrow 52$ 2. $52 \rightarrow 46$ 3. $46 \rightarrow 52$ 4. $46 \rightarrow 52$
E4	pentose phosphate pathway (oxidative branch)	phosphogluconate dehydrogenase	Dey and Harborne (1997)	$53 \rightarrow 52$
E5	pentose phosphate pathway (oxidative branch)	6-phosphogluconolactonase	Dey and Harborne (1997)	$54 \rightarrow 53$
E6_f E6_b	pentose phosphate pathway (oxidative branch)	glucose-6-phosphate 1-dehydrogenase	Dey and Harborne (1997)	$49 \rightarrow 54$ $54 \rightarrow 49$
E7	Calvin-Benson-Bassham cycle	sedoheptulose-bisphosphatase	Lefebvre et al. (2005)	$67 \rightarrow 65$
E8	1. starch biosynthesis 2. gluconeogenesis 3. sucrose degradation III 4. glycolysis I (plastidic)	spontaneous	Nelson and Cox (2000)	$1. 49 \rightarrow 56$ $2. 56 \rightarrow 49$ $3. 49 \rightarrow \leftarrow 56$ $4. 49 \rightarrow \leftarrow 56$
E9_b E9_f	1. starch degradation 2. starch biosynthesis 3. sucrose biosynthesis 4. UDP-glucose biosynthesis (from glucose 6-phosphate) 5. sucrose degradation III 6. superpathway of sucrose and starch metabolism I (non-photosynthetic tissue)	phosphoglucomutase	Reiter (2008)	$1. 50 \rightarrow 56$ $2. 56 \rightarrow 50$ $3. 56 \rightarrow 50$ $4. 56 \rightarrow 50$ $5. 50 \rightarrow 56$ $6. 50 \rightarrow 56$
E10_56 E10_49	1. starch degradation 2. sucrose degradation III	hexokinase/ glucokinase	Lu and Sharkey (2006) Guy et al. (2008)	$57 \rightarrow 56$ $51 \rightarrow 49$

**Supplementary Table 3.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E11_b E11_f	Calvin-Benson-Bassham cycle	aldolase	Buchanan et al. (2000)	$32 + 68 \rightarrow 67$ $67 \rightarrow 32 + 68$
E12	sucrose degradation III	fructokinase	Guy et al. (2008)	$63 \rightarrow 44$
E13_b E13_f	1. glycolysis IV (plant cytosol) 2. Calvin-Benson-Bassham cycle 3. glycolysis I (plastidic)	triose-phosphate isomerase	Berg et al. (2002)	$42 \rightarrow 68$ $68 \rightarrow 42$
E14_f E14_b	1. Gluconeogenesis 2. Calvin-Benson-Bassham cycle 3. glycolysis I (plastidic)	fructose-bisphosphate aldolase	Guy et al. (2008)	$43 \rightarrow 42 + 68$ $44 + 68 \rightarrow 43$
E15	1. Gluconeogenesis 2. Calvin-Benson-Bassham cycle 3. glycolysis I (plastidic)	fructose-1,6-bisphosphatase	Guy et al. (2008)	$43 \rightarrow 44$
E16	1. glycolysis I (plastidic) 2. glycolysis IV (plant cytosol)	6-phosphofructokinase	Dey and Harborne (1997)	$44 \rightarrow 43$
E17	1. galactose degradation II 2. galactose degradation III 3. sucrose biosynthesis 4. UDP-glucose biosynthesis (from glucose 6-phosphate) 5. sucrose degradation III 6. superpathway of sucrose and starch metabolism I (non-photosynthetic tissue) 7. superpathway of sucrose and starch metabolism II (photosynthetic tissue)	UDP-glucose pyrophosphorylase UDP-D-galactose phosphorylase	Guy et al. (2008) Reiter (2008)	$50 + 129 \rightarrow 82$ $76 + 129 \rightarrow 77$
E18_f E18_b	1. galactose degradation III 2. sucrose biosynthesis 3. UDP-glucose biosynthesis (from sucrose) 4. sucrose degradation III	sucrose synthase	Guy et al. (2008)	$66 + 115 \rightarrow 63 + 82$ $63 + 82 \rightarrow 66 + 115$
E19	1. galactose degradation III 2. UDP-D-xylose biosynthesis	UDP-D-glucose dehydrogenasae	Reiter (2008)	$82 \rightarrow 85$
E20_b E20_f	1. galactose degradation II 2. galactose degradation III 3. UDP-galactose biosynthesis 4. galactose degradation I (Leloir pathway)	UDP-glucose 4-epimerase	Guy et al. (2008)	$1.77 \rightarrow 82$ $2.82 \rightarrow 77$ $3.77 \rightarrow \leftarrow 82$ $4.77 \rightarrow 82$
E21	Non-enzymatic $H_2O_2$ interaction	Non-enzymatic	Cousins et al. (2008)	$15 \rightarrow 35$
E22	1. galactose degradation II 2. galactose degradation III 3. galactose degradation I (Leloir pathway)	D-galactokinase	Reiter (2008)	$73 \rightarrow 76$

**Supplementary Table 4.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E23	UDP-D-xylose biosynthesis	UDP-D-glucuronate decarboxylase	Reiter (2008)	$85 \rightarrow 88$
E24_f E24_b	galactose degradation I (Leloir pathway)	ADP glucose-1-phosphate adenylyltransferase	Berg et al. (2002)	$76 + 82 \rightarrow 50 + 77$ $77 + 50 \rightarrow 82 + 76$
E25	ascorbate biosynthesis I (L-galactose pathway)	L-galactose dehydrogenase	Davey et al. (1999)	$73 \rightarrow 78$
E26_f E26_b	no pathway assigned in AraCyc	UDP-galacturonate pyrophosphatase	Litterer et al. (2006)	$131 \rightarrow 132 + 129$ $132 + 129 \rightarrow 131$
E27	stachyose biosynthesis	galactinol synthase	Guy et al. (2008)	$74 + 77 \rightarrow 72 + 115$
E28	stachyose biosynthesis	raffinose synthase	Guy et al. (2008)	$72 + 66 \rightarrow 74 + 70$
E29	stachyose biosynthesis	stachyose synthase	Guy et al. (2008)	$70 + 72 \rightarrow 71 + 74$
E30	trehalose biosynthesis I	trehalose phosphate synthatase	Paul et al. (2008)	$56 + 82 \rightarrow 84 + 115$
E31	trehalose biosynthesis I	trehalose phosphate phosphatase	Paul et al. (2008)	$84 \rightarrow 83$
E32	trehalose biosynthesis I	trehalase	Paul et al. (2008)	$83 \rightarrow 51 + 57$
E33	myo-inositol biosynthesis	myo-inositol 1-phosphate monophosphatase	Guy et al. (2008)	$69 \rightarrow 74$
E34_f E34_b	1D-myo-inositol hexakisphosphate biosynthesis III ( <i>Spirodela polyrrhiza</i> )	myo-inositol-1-phosphate synthase	Guy et al. (2008)	$56 \rightarrow 69$ $69 \rightarrow 56$
E35	pyrimidine salvage pathway	uracil phosphoribosyltransferase	Zrenner et al. (2006)	$24 + 121 \rightarrow 80$
E36_f E36_b	No pathway assigned	unknown	Berg et al. (2002)	$51 + 73 \rightarrow 75$ $75 \rightarrow 73 + 51$
E37	sucrose degradation III	vacuolar invertase	Tymowska-Lalanne and Kreis (1998)	$66 \rightarrow 51 + 63$
E38	uridine-5-phosphate biosynthesis	carbamoylphosphatesynthetase	Zrenner et al. (2006)	$33 \rightarrow 2 + 116$
E39	No pathway assigned	aldose 6-phosphate reductase	hypothetical reaction Nosarzewski et al. (2012) enzyme name and reaction Negm and Loescher (1981)	$49 \rightarrow 62$
E40	citrulline biosynthesis arginine biosynthesis I arginine biosynthesis II (acetyl cycle)	ornithine transcarbamoylase	Tischner et al. (2007)	$1 + 116 \rightarrow 94$

**Supplementary Table 5.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E41	no pathway assigned			
E42	uridine-5-phosphate biosynthesis	aspartate transcarbamoylase	Zrenner et al. (2006)	$23 + 116 \rightarrow 117$
E43	uridine-5-phosphate biosynthesis	dihydroorotase	Zrenner et al. (2006)	$117 \rightarrow 118$
E44	uridine-5-phosphate biosynthesis	dihydroorotate dehydrogenase	Zrenner et al. (2006)	$118 \rightarrow 119$
E45_73 E45_66	no pathway assigned	alpha-galactosidase	Gross and Pharr (1982)	$71 \rightarrow 70 + 73$   $70 \rightarrow 66 + 73$
E46	starch biosynthesis	ADP-glucose pyrophosphorylase	Kossmann and Lloyd (2000)	$50 \rightarrow 58$
E47	not assigned			
E48	not assigned			
E49	not assigned			
E50	not assigned			
E51	not assigned			
E52	not assigned			
E53	not assigned			
E54_b E54_f	connection of glycolysis and pentosephosphate pathway	transaldolase	Berg et al. (2002)	$32 + 44 \rightarrow 42 + 65$   $65 + 42 \rightarrow 44 + 32$
E55	not assigned			
E56	not assigned			
E57	not assigned			
E58	not assigned			
E59	not assigned			
E60	not assigned			
E61_119 E61_80	uridine-5-phosphate biosynthesis	UMP synthase (orotate phosphoribosyl-transferase)	Zrenner et al. (2006)	$119 + 121 \rightarrow 120$   $120 \rightarrow 80$
E62_u E62_c	pyrimidine ribonucleotides interconversion	uridylylate/cytidylate kinase	Zrenner et al. (2006)	$80 \rightarrow 115$   $123 \rightarrow 128$

**Supplementary Table 6.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E63_b E63_f	glycolysis	enolase	Plaxton (1996)	$39 \rightarrow 34$ $34 \rightarrow 39$
E64	chorismate biosynthesis	3-deoxy-arabino-heptulonate 7-phosphate (DAHP) synthase	Herrmann (1995)	$32 + 34 \rightarrow 36$
E65	chorismate biosynthesis	3-dehydroquinate synthase	Herrmann (1995)	$36 \rightarrow 37$
E66_95_b E66_95_f E66_101_f E66_101_b	chorismate biosynthesis	1. 3-dehydroquinate dehydratase 2. quinate hydrolyase	Herrmann (1995)	$1. 37 \rightarrow 95$ $1. 95 \rightarrow 37$ $2. 101 \rightarrow 102$ $2. 102 \rightarrow 101$
E67_101_f E67_101_b E67_95_f E67_95_b	chorismate biosynthesis	1. quinate dehydrogenase 2. shikimate dehydrogenase 3. shikimate kinase	Herrmann (1995)	$1. 37 \rightarrow 101$ $1. 101 \rightarrow 37$ $2. 95 \rightarrow 102$ $2. 102 \rightarrow 95$ $3. 102 \rightarrow 96$
E68	chorismate biosynthesis	5-enolpyruylshikimate 3-phosphate (EPSP) synthase	Herrmann (1995)	$34 + 96 \rightarrow 97$
E69	chorismate biosynthesis	chorismate synthase	Herrmann (1995)	$97 \rightarrow 103$
E70	chorismate biosynthesis	chorismate mutase	Strawn et al. (2006)	$103 \rightarrow 105$
E71_f E71_b	phenylalanine biosynthesis II tyrosine biosynthesis II	prephenate amino-transferase	Graindorge et al. (2010)	$2 + 105 \rightarrow 9 + 98$ $9 + 98 \rightarrow 2 + 105$
E72_107 E72_106	tyrosine biosynthesis II	1. arogenate dehydrogenase 2. prephenate dehydrogenase	1. Rippert and Matringe (2002) 2. hypothetical Rippert and Matringe (2002)	$1. 98 \rightarrow 107$ $2. 105 \rightarrow 106$
E73	phenylalanine biosynthesis II	arogenate dehydratase	Cho et al. (2007)	$98 \rightarrow 109$
E74	tyrosine degradation I	4-hydroxyphenylpyruvate dioxygenase	Garcia et al. (1999)	$106 \rightarrow 99$
E75_f E75_b	tyrosine biosynthesis I	tyrosine amino-transferase	Tao et al. (2008) Holländer-Czytko et al. (2005)	$9 + 107 \rightarrow 2 + 106$ $2 + 106 \rightarrow 9 + 107$
E76	Not assigned			
E77	phenylpropanoid biosynthesis	phenylalanine ammonialyase	Humphreys and Chapple (2002)	$109 \rightarrow 110 + 29$
E78	phenylpropanoid biosynthesis	phenylalanine ammonialyase	Humphreys and Chapple (2002)	$109 \rightarrow 110 + 29$

**Supplementary Table 7.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E79	phenylpropanoid biosynthesis	cinnamate 4-hydroxylase	Humphreys and Chapple (2002)	110 → 112
E80	phenylpropanoid biosynthesis	4-(hydroxy)cinnamoyl CoA ligase	Humphreys and Chapple (2002)	112 + 93 → 47
E81_111 E81_104	phenylpropanoid biosynthesis	1. hydroxycinnamoyl CoA:quinate hydroxycinnamoyltransferase 2. hydroxycinnamoyl CoA:shikimate hydroxycinnamoyltransferase	Humphreys and Chapple (2002)	1, 93 + 111 → 101 + 108 & 47 + 101 → 93 + 104
E81_90 E81_100				2, 90 + 93 → 102 + 108 & 47 + 102 → 93 + 100
E82_90 E82_111	phenylpropanoid biosynthesis	p-coumarate 3-hydroxylase	Humphreys and Chapple (2002)	100 → 90 104 → 111
E83	phenylpropanoid biosynthesis	caffeyl CoA O-methyltransferase	Humphreys and Chapple (2002)	108 → 7
E84	phenylpropanoid biosynthesis	cinnamoyl CoA reductase	Humphreys and Chapple (2002)	7 → 17 + 93
E85	phenylpropanoid biosynthesis	cinnamyl alcohol dehydrogenase / sinapyl alcohol dehydrogenase	Humphreys and Chapple (2002)	17 → 19
E86_31 E86_133	phenylpropanoid biosynthesis	ferulate 5-hydroxylase	Humphreys and Chapple (2002)	19 → 31 & 17 → 133
E87_48 E87_134	phenylpropanoid biosynthesis	caffeyc acid/5-hydroxyferulic acid Omethyltransferase	Humphreys and Chapple (2002)	31 → 48 & 133 → 134
E88_19 E88_48	phenylpropanoid biosynthesis		Humphreys and Chapple (2002)	19 → 30a & 48 → 30b (two different kinds of lignin)
E89_f E89_b	1. glycolysis IV (plant cytosol) 2. gluconeogenesis 3. glycolysis I (plastidic) 4. rubisco shunt	phosphoglyceromutase	Plaxton (1996)	1. 40 → 39  2. 39 → 40 3. 39 → 40  4. 40 → 39
E90_f E90_b	1. glycolysis IV (plant cytosol) 2. gluconeogenesis 3. Calvin-Benson-Bassham cycle 4. glycolysis I (plastidic)	3-PGA kinase	Plaxton (1996)	1. 41 → 40  2. 40 → 41 3. 40 → 41  4. 40 → 41
E91_b E91_f	1. Calvin-Benson-Bassham cycle 2. gluconeogenesis	NAD-dependent GAPDH (phosphorylating)	Plaxton (1996)	1. 41 → 42  2. 41 → 42

**Supplementary Table 8.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E92	CO <sub>2</sub> fixation into oxaloacetate glutamine biosynthesis III	phosphoenolpyruvate carboxylase	Dey and Harborne (1997)	34 → 12
E93	gluconeogenesis superpathway of glyoxylate cycle	phosphoenolpyruvate carboxylase	Cornah et al. (2004)	12 → 34
E94_f E94_b	TCAcycle glyoxylate cycle	malate dehydrogenase	Berg et al. (2002) Cornah et al. (2004)	8 → 12 12 → 8
E95	sinapate ester biosynthesis	hydroxycinnamaldehyde dehydrogenase	Fraser and Chapple (2011)	134 → 55
E96_b E96_f	TCAcycle	fumarate hydratase	Berg et al. (2002) Cornah et al. (2004)	6 → 8 8 → 6
E97_f E97_b	TCAcycle	succinate dehydrogenase	Berg et al. (2002) Cornah et al. (2004)	4 → 6 6 → 4
E98	TCAcycle glyoxylate cycle	citrate synthase	Berg et al. (2002) Cornah et al. (2004)	12 + 92 → 11 + 93
E99	TCAcycle glyoxylate cycle	aconitase	Berg et al. (2002) Cornah et al. (2004)	11 → 10
E100	TCAcycle	isocitrate dehydrogenase	Berg et al. (2002) Cornah et al. (2004)	10 → 9
E101	TCAcycle	a-ketoglutarate dehydrogenase	Berg et al. (2002) Aubert et al. (2001)	9 + 93 → 5
E102_f E102_b	TCAcycle	succinate-CoA ligase	Berg et al. (2002) Cornah et al. (2004)	5 → 4 + 93 4 + 93 → 5
E103	glutamate degra degradation IV 4-aminobutyrate degradation IV	succinic semialdehyde dehydrogenase	Bouché and Fromm (2004)	79 → 4
E104_f E104_b	glutamate degra degradation IV 4-aminobutyrate degradation IV	gamma-aminobutyric acid transaminase	Bouché and Fromm (2004)	3 + 20 → 21 + 79
E105	glutamate degradation IV 4-aminobutyrate degradation IV	glutamate decarboxylase	Bouché and Fromm (2004)	2 → 3
E106_f E106_b	glutamate degradation I	glutamate dehydrogenase	Aubert et al. (2001)	9 + 29 → 2 2 → 29 + 9

**Supplementary Table 9.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E107	glutamate biosynthesis V ammonia assimilation cycle II glutamine biosynthesis III	glutamate synthase	Forde and Lea (2007)	$9 + 33 \rightarrow 2x2$
E108	glutamate biosynthesis V ammonia assimilation cycle II glutamine biosynthesis III	glutamate synthase	Forde and Lea (2007)	$9 + 33 \rightarrow 2x2$
E109	ammonia assimilation cycle II glutamine biosynthesis I glutamine biosynthesis III	glutamine synthetase	Forde and Lea (2007)	$2 + 29 \rightarrow 33$
E110	glutamine biosynthesis III	pyruvate, orthophosphate dikinase	Matsuoka (1995)	$20 \rightarrow 34$
E111	glycolysis IV (plant cytosol) glycolysis I (plastidic) rubisco shunt	pyruvate kinase	Andre et al. (2007)	$34 \rightarrow 20$
E112	sucrose degradation to ethanol and lactate (anaerobic) pyruvate fermentation to ethanol II acetaldehyde biosynthesis I	pyruvate decarboxylase	Ismond et al. (2003)	$20 \rightarrow 114$
E113.b	1. alanine degradation III 1. alanine biosynthesis II 2. glycine biosynthesis 2. photorespiration	1. alanine aminotransferase 2. glyoxylate aminotransferase	Igarashi et al. (2003)	$1. 2 + 20 \rightarrow 9 + 21$ $9 + 21 \rightarrow 2 + 20$ $2. 2 + 13 \rightarrow 9 + 18$
E114	ethanol degradation II (cytosol) ethanol degradation IV (peroxisomal)	acetate-CoA ligase	Lin and Oliver (2008)	$38 + 93 \rightarrow 92$
E115	oxidative ethanol degradation III oxidative ethanol degradation I	aldehyde dehydrogenase	Wei et al. (2007)	$114 \rightarrow 38$
E116	cysteine biosynthesis I	O-acetylserine (thiol) lyase	Wirtz and Hell (2006)	$91 \rightarrow 38 + 113$

**Supplementary Table 10.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E117	cysteine biosynthesis I	serine acetyltransferase	Wirtz and Hell (2006)	$16 + 92 \rightarrow 91 + 93$
E118	glycine biosynthesis	serine hydroxymethyltransferase	Berg et al. (2002)	$16 + 29 \rightarrow 2x18$
E119	glycine biosynthesis photorespiration	serine hydroxymethyltransferase	Goyer et al. (2005)	$2x18 \rightarrow 16 + 29$
E120_u E120_c	pyrimidine salvage pathway	pyrimidine specific 5-nucleotidase	Zrenner et al. (2006)	$80 \rightarrow 126$ $123 \rightarrow 127$
E121	glycine biosynthesis photorespiration	glyoxylate aminotransferase	Liepmann and Olsen (2001)	$13 + 16 \rightarrow 15 + 18$
E122	photorespiration	hydroxypyruvate reductase	Cousins et al. (2008)	$15 \rightarrow 14$
E123	photorespiration	glycerate kinase	Liepmann and Olsen (2003)	$14 \rightarrow 40$
E124	Not assigned			
E125	glyoxylate cycle	isocitrate lyase	Cornah et al. (2004)	$10 \rightarrow 4 + 13$
E126	glycolate and glyoxylate degradation II	glycolate oxidase	Liepmann and Olsen (2003)	$35 \rightarrow 13$
E127	uridine-5-phosphate biosynthesis	5-phosphoribosyl-1-pyrophosphate synthase	Zrenner et al. (2006)	$46 \rightarrow 121$
E128	photorespiration	phosphoglycolate phosphatase	Linka and Weber (2005)	$64 \rightarrow 35$
E129	photorespiration ribulose Rubisco shunt/ Calvin-Benson-Bassham cycle	1,5-bisphosphate carboxylase / oxygenase (Rubisco)	Linka and Weber (2005)	$60 \rightarrow 40 + 64$ $3x60 \rightarrow 6x40$
E130	Calvin-Benson-Bassham cycle rubisco shunt	phosphoribulo-kinase	Berg et al. (2002)	$52 \rightarrow 60$
E131	pyrimidine salvage pathway pyrimidine ribonucleosides degradation II	uridine nucleosidase (+ ribokinase for ribose $\rightarrow 46$ )	Zrenner et al. (2006)	$126 \rightarrow 24 + 46$
E132	uracil degradation (reductive)	dihydrouracil dehydrogenase	Zrenner et al. (2006)	$24 \rightarrow 124$
E133_f E133_b	citrulline biosynthesis arginine biosynthesis I arginine biosynthesis II (acetyl cycle) urea cycle	argininosuccinate lyase	Tischner et al. (2007)	$27 \rightarrow 6 + 28$ $6 + 28 \rightarrow 27$

**Supplementary Table 11.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E134	citrulline biosynthesis arginine biosynthesis I arginine biosynthesis II (acetyl cycle) urea cycle	argininosuccinate synthetase	Tischner et al. (2007)	$23 + 94 \rightarrow 27$
E135	citrulline biosynthesis arginine biosynthesis I arginine biosynthesis II (acetyl cycle) urea cycle arginine degradation VI (arginase 2 pathway)	arginase	Tischner et al. (2007)	$28 \rightarrow 1 + 25$
E136	urea degradation II	urease	Sirko and Brodzik (2000)	$25 \rightarrow 2x29$
E137	uracil degradation (reductive)	dihydropyrimidinase	Zrenner et al. (2006)	$124 \rightarrow 125$
E138	uracil degradation (reductive)	b-ureidopropionase	Zrenner et al. (2006)	$125 \rightarrow 29$ beta-alanine not modeled, reaction only recycles bound NH3, which would be set free in the reaction to beta-alanine
E139_u_dtom E139_c_dtom E139_u_ttod E139_c_ttod	pyrimidine ribonucleotides interconversion	1. nucleoside di-phosphate phosphatase 2. nucleoside tri-phosphate phosphatase	Zrenner et al. (2006)	1. $115 \rightarrow 80$ $128 \rightarrow 123$ 2. $129 \rightarrow 115$ $122 \rightarrow 128$
E140	asparagine biosynthesis I	asparagine synthetase	Lam et al. (1994)	$23 + 33 \rightarrow 2 + 26$
E141	asparagine degradation I	asparaginase	Bruneau et al. (2006)	$26 \rightarrow 23 + 29$
E142	Not assigned			
E143_f E143_b	No pathway assigned	aldonolactonase	Ishikawa and Shigeoka (2008)	$130 \rightarrow 78$ $78 \rightarrow 130$
E144_u E144_c	pyrimidine ribonucleotides interconversion	nucleoside diphosphate kinase	Zrenner et al. (2006)	$115 \rightarrow 129$ $128 \rightarrow 122$
E145_u E145_c	pyrimidine ribonucleotides interconversion	apyrase	Zrenner et al. (2006)	$129 \rightarrow 80$ $122 \rightarrow 123$
E146	pyrimidine ribonucleotides interconversion	CTP synthase	Zrenner et al. (2006)	$33 + 129 \rightarrow 2 + 122$

**Supplementary Table 12.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
E147	pyrimidine ribonucleotides interconversion	cytidine deaminase	Zrenner et al. (2006)	$127 \rightarrow 29 + 126$
E148_b E148_f	1. pentose phosphate pathway (non-oxidative branch) 2. Calvin-Benson-Bassham cycle 3. Rubisco shunt	ribulose-phosphate 3-epimerase	Berg et al. (2002) Dey and Harborne (1997)	1. $52 \rightarrow 45$
				2. $45 \rightarrow 52$
E149	no pathway assigned	sorbitol dehydrogenase	Nosarzewski et al. (2012)	$62 \rightarrow 63$
E150	no pathway assigned	UDP-glucuronate 4-epimerase	Ishikawa and Shigeoka (2008)	$85 \rightarrow 131$
E151	no pathway assigned	UDP-galacturonate pyrophosphatase	Ishikawa and Shigeoka (2008)	$132 \rightarrow 87$
E152	no pathway assigned	D-galacturonate reductase	Ishikawa and Shigeoka (2008)	$87 \rightarrow 130$
E153	phenylpropanoid biosynthesis	hydroxycinnamaldehyde dehydrogenase	Fraser and Chapple (2011)	$134 \rightarrow 48$
E154	glycolysis	lipoate acetyl-transferase	Buchanan et al. (2000)	$20 + 93 \rightarrow 92$
E155	glyoxylate cycle	malate synthase	Buchanan et al. (2000)	$13 + 92 \rightarrow 8 + 93$
IN_18	glycine		Jander et al. (2004) Joshi et al. (December 2006)	$\rightarrow 18$
IN_29	ammonia		von Wirén et al. (2000) Morgan and Jackson (1988)	$\rightarrow 29$
IN_63	D-fructose		Sauer et al. (1990)	$\rightarrow 63$
IN_73	D-galactose		Sauer et al. (1990)	$\rightarrow 73$
IN_92	acetyl-CoA		Fulda et al. (2002)	$\rightarrow 92$
IN_93	CoA		Kupke et al. (2001)	$\rightarrow 93$
IN_94	citrulline		Ludwig (1993)	$\rightarrow 94$
OUT_29	ammonia		Morgan and Jackson (1988)	$29 \rightarrow$
OUT_30a	lignin		Buchanan et al. (2000)	$30a \rightarrow$
OUT_30b	lignin		Buchanan et al. (2000)	$30b \rightarrow$
OUT_50	Alpha-D-glucose 1-phosphate		Wolucka and Montagu (2007)	$50 \rightarrow$

**Supplementary Table 13.** Reactions of the complete PN model. For the legend see Table 2.

Transition	Biochemical pathway	Enzyme name	Reference	Reactions
OUT_51	Beta-D-glucose		AraCyc (2012)	51 →
OUT_62	sorbitol		Noiraud et al. (2001)	62 →
OUT_66	sucrose		Sauer and Stoltz (1994)	66 →
OUT_71	stachyose		AraCyc (2012)	71 →
OUT_74	D-myo-inositol		Reiter (2008)	74 →
OUT_78	L-galactono-1,4-lactone		Davey et al. (1999)	78 →
OUT_82	UDP-glucose		Dean and Delaney (2008)	82 →
OUT_88	UDP-xylose		Buchanan et al. (2000)	88 →
OUT_92	acetyl-CoA		external metabolite	92 →
OUT_93	CoA		external metabolite	93 →
OUT_94	citrulline		external metabolite	94 →
OUT_99	homogentisate		Collakova and DellaPenna (2001)	99 →
OUT_103	chorismate		Strawn et al. (2006)	103 →
OUT_106	4-hydroxy-phenylpyruvate		AraCyc (2012)	106 →
OUT_113	cysteine		Buchanan et al. (2000)	113 →
OUT_115	uridine diphosphate (UDP)		Buchanan et al. (2000)	115 →
OUT_122	CTP		Zrenner et al. (2006)	122 → ( <i>RNA synthesis</i> )
OUT_129	UTP		Zrenner et al. (2006)	129 → ( <i>RNA synthesis</i> )
R1	starch degradation	phosphoglucan, water dikinase	Guy et al. (2008)	59 → 61
R2	starch degradation	glucan, water dikinase	Fettke et al. (2009)	59 → 2x57
R3	starch synthesis	starch branching enzyme	Kossmann and Lloyd (2000)	81 + 86 → 59
R4_b R4_f	starch degradation	disproportionating isozyme 2	Fettke et al. (2009)	61 → 57 + 89 57 + 89 → 61
R5_1	starch synthesis	1. R5 1: granule bound starch synthase	Kossmann and Lloyd (2000)	1. 58 → 86
R5_2		2. R5 2: starch synthase		2. 58 → 81
R6_b R6_f	starch degradation	phosphorylase isozyme	Fettke et al. (2009)	89 → 50 50 → 89

**Supplementary Table 14.** Output reactions of the PN ordered by the subnetwork and increasing place numbers.

Place number	Metabolite	Subnetwork
29	ammonia	citrate
92	acetyl-CoA	citrate
93	CoA	citrate
94	citrulline	citrate
113	cysteine	citrate
30a	lignin	phenyl
30b	lignin	phenyl
99	homogentisate	phenyl
103	chorismate	phenyl
106	4-hydroxy-phenylpyruvate	phenyl
115	uridine diphosphate (UDP)	UTP
122	cytosine triphosphate (CTP)	UTP
129	uridine triphosphate (UTP)	UTP
50	$\alpha$ -D-glucose 1-phosphate	sucrose
51	$\beta$ -D-glucose	sucrose
62	sorbitol	sucrose
66	sucrose	sucrose
71	stachyose	sucrose
74	D-myo-inositol	sucrose
78	L-galactono-1,4-lactone	sucrose
82	UDP-glucose	sucrose
88	UDP-xylose	sucrose

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