Metabolic model integration of the bibliome, genome, metabolome, and reactome of *Aspergillus niger* — Supplementary information

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Suppl. Figure 1: Map of *A. niger* metabolism in scalable vector graphics. EC numbers are shown for all reactions where a such is defined. A list of abbreviations for the metabolite-names is available in Suppl. Table 2.
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Suppl. Figure 2: Map of transcription on glucose/ammonium medium. Based Present/Absent calls from transcription data from Pel et al. (2007) (Pel et al., 2007). A red box denotes the transcription of at least one of the genes assigned to the reaction, green denotes a complete absence of transcription of all isoenzymes and subunits. A gray box is indicative of a process with no assigned ORF.
The figure is available as a separate PDF-file due to the size of it

Suppl. Table I: *Aspergillus niger* reconstructed metabolic network. Abbreviations of the names of the metabolites are found in Suppl. Table 2. For each reaction the following information is noted where it is known: The EC-number and enzyme name. A list of references discussing or indicating the presence of the reaction (If a reaction is found in another Aspergillus sp or inferred based on observations in A.niger, it will be written as Hondmann (1994, A.nidulans) or Morozova et al. (2002, Inferred) respectively). ORF/gene numbers from the A. niger CBS 513.88 and ATCC 1015-genome sequences (Columns CBS and ATCC respectively). The column named "Model" shows which other Aspergillus models the reaction is present in. ANID: A. nidulans iHD666, ANIG, A. niger iHD20, ANEW: The reaction is only present in A. niger iMA871. An $*$ indicates that an enzyme-complex catalyses this reaction.

ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
Conversions								
NE1	:	DGLCe ⇆ 0.33 GLCe + 0.67 bDGLCe	Non enzymatic step	Non enzymatic reaction	David et al. (2003)	ANIG, ANID		
NE2	:	DGLC ⇆ 0.33 GLC + 0.67 bDGLC	Non enzymatic step	Non enzymatic reaction	Kinoshita et al. (1981)	ANIG, ANID		
r1	:	GLC ⇆ bDGLC	5.1.3.3	Aldose 1-epimerase	Kinoshita et al. (1981)	ANIG, ANID	An02g09090; An11g10890	55604; 56084
r2	:	GLAC ⇆ bGLAC	5.1.3.3	aldose-1-epimerase	Kinoshita et al. (1981)	ANEW	An02g09090; An11g10890	55604; 56084
r3	:	LARAB ⇆ bLARAB	5.1.3.3	aldose-1-epimerase	Kinoshita et al. (1981)	ANEW	An02g09090; An11g10890	55604; 56084
r4	:	bFRU ⇆ FRU	5.1.3.3	aldose-1-epimerase	Kinoshita et al. (1981)	ANEW	An02g09090; An11g10890	55604; 56084
Gluconeogenesis & Glycolysis Embden-Meyerhoff-Parnas Pathway								
r5	:	ATP + GLC ⇒ ADP + G6P	2.7.1.1	Hexokinase (hxk)	Jagannathan and Singh (1953); Muller (1986); Martinelli and Kinghorn (1994); Panneman et al. (1998); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001)	ANIG, ANID	An02g14380; An06g00380; An13g00510	55651; 134301; 50817
r6	:	ATP + bDGLC ⇒ ADP + bDG6P	2.7.1.2	Glucokinase (glkA)	Panneman et al. (1996); Karaffa et al. (2001)	ANIG, ANID	An12g08610	201877
r7	:	G6P ⇆ F6P	5.3.1.9	Glucose-6-phosphate isomerase	Jagannathan and Singh (1953); Martinelli and Kinghorn (1994); Ruijter and Visser (1999); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An16g05420	210433
r8	:	bDG6P ⇆ F6P	5.3.1.9	Glucose-6-phosphate isomerase	Jagannathan and Singh (1953); Ruijter and Visser (1999); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An16g05420	210433
r9	:	G6P ⇆ bDG6P	5.3.1.9	Glucose-6-phosphate isomerase	Jagannathan and Singh (1953); Ruijter and Visser (1999); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An16g05420	210433
r10	:	ATP + F6P ⇒ ADP + FDP	2.7.1.11	6-phosphofructokinase (Phosphofructokinase I, pfkA)	Jagannathan and Singh (1953); Habison et al. (1983); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001)	ANIG, ANID	An18g01670	54093
r11	:	FDP + H2O ⇒ F6P + PI	3.1.3.11	Fructose-2,6-bisphosphatase	Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An04g05300	214375

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r12	:	FDP ⇆ T3P2 + T3P1	4.1.2.13	Fructose-bisphosphate aldolase	Jagannathan and Singh (1953); Jagannathan et al. (1956); Muller (1986); Martinelli and Kinghorn (1994)	ANIG, ANID	An02g07470; An05g02040; An14g04410; An16g00110	55586; 43928; 211172; N/A
r13	:	T3P2 ⇆ T3P1	5.3.1.1	Triosephosphate isomerase (tpiA)	Inoue et al. (1988); Martinelli and Kinghorn (1994)	ANIG, ANID	An02g02920; An14g04920	206602; 56602
r14	:	T3P1 + PI + NAD ⇆ 13PDG + NADH	1.2.1.12	Glyceraldehyde 3-phosphate dehydrogenase (gpdA)	Muller (1986); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An16g01830	56485
r15	:	ADP + 13PDG ⇆ ATP + 3PG	2.7.2.3	Phosphoglycerate kinase	David et al. (2003)	ANIG, ANID	An08g02260	208318
r16	:	3PG ⇆ 2PG	5.4.2.1	Phosphoglycerate mutase	Jagannathan and Singh (1953); Muller (1986)	ANIG, ANID	An16g02990; An16g06010	210655; 40937
r17	:	2PG ⇆ PEP + H2O	4.2.1.11	Phosphopyruvate hydratase (enolase)	Jagannathan and Singh (1953); Muller (1986); Martinelli and Kinghorn (1994)	ANIG, ANID	An18g06250	202692
r18	:	ADP + PEP ⇒ ATP + PYR	2.7.1.40	Pyruvate kinase (pkiA)	Patil and Ramakrishnan (1966); Perl (1982); Meixner-Monori et al. (1984); Muller (1986); Kubicek et al. (1988); de Graaff et al. (1992); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000)	ANIG, ANID	An07g08990	56137
r19	:	ATP + PYR + H2O + CO2 ⇒ ADP + PI + OA	6.4.1.1	Pyruvate carboxylase (pyc)	Tachibana (1964); Bercovitz et al. (1990); Martinelli and Kinghorn (1994); Jaklitsch et al. (1991); Pel et al. (2007)	ANIG, ANID	An04g02090	213185
r20	:	ATPm + PYRm + H2Om + CO2m ⇒ ADPm + PIm + OAm	6.4.1.1	Pyruvate carboxylase	Tachibana (1964); Ma et al. (1981); Bercovitz et al. (1990); Martinelli and Kinghorn (1994); Jaklitsch et al. (1991); Pel et al. (2007)	ANID	An15g02820	129399
r21	:	ATP + OA ⇒ ADP + PEP + CO2	4.1.1.49	Phosphoenolpyruvate carboxykinase (ATP)	Woronick and Johnson (1960); Patil and Ramakrishnan (1966)	ANIG, ANID	An11g02550	208685
Pentose-Phosphate Shunt								
r22	:	G6P + NADP ⇒ D6PGL + NADPH	1.1.1.49	Glucose 6-phosphate 1-dehydrogenase (gsdA)	McDonough and Martin (1958); Muller (1985); Jaklitsch et al. (1991); Wennekes et al. (1993); van den Broek et al. (1995); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Kirimura et al. (2000)	ANIG, ANID	An02g12140	55633
r23	:	D6PGL + H2O ⇒ D6PGC	3.1.1.31	6-Phosphogluconolactonase	Martinelli and Kinghorn (1994)	ANIG, ANID	An01g05150	206051
r24	:	D6PGC + NADP ⇒ RL5P + CO2 + NADPH	1.1.1.44	Phosphogluconate dehydrogenase (decarboxylating)	McDonough and Martin (1958); Muller (1985); Martinelli and Kinghorn (1994)	ANIG, ANID	An11g06120	178461
r25	:	RL5P ⇆ XUL5P	5.1.3.1	Ribulose-phosphate 3-epimerase	Martinelli and Kinghorn (1994); Muller (1985); de Groot et al. (2003)	ANIG, ANID	An09g03450	50154
r26	:	R5P ⇆ RL5P	5.3.1.6	Ribose-5-phosphate isomerase	Lakshminarayana et al. (1969b); Martinelli and Kinghorn (1994); Muller (1985); de Groot et al. (2003)	ANIG, ANID	An02g02930	206607

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r27	:	R5P + XUL5P ⇆ S7P + T3P1	2.2.1.1	Transketolase	Martinelli and Kinghorn (1994); de Groot et al. (2003)	ANIG, ANID		An02g06430; An08g06570	197387; 207951
r28	:	E4P + XUL5P ⇆ F6P + T3P1	2.2.1.1	Transketolase	Martinelli and Kinghorn (1994); de Groot et al. (2003)	ANIG, ANID		An02g06430; An08g06570	197387; 207951
r29	:	S7P + T3P1 ⇆ E4P + F6P	2.2.1.2	Transaldolase	Martinelli and Kinghorn (1994); de Groot et al. (2003)	ANIG, ANID		An07g03160; An07g03850	40065; 209713
Tricarboxylic Acid Cycle									
r31	:	ACCOAm + H2Om + OAm ⇆ CITm + COAm	2.3.3.1	Citrate synthase (citA)	Muller (1975b, 1986); Bercovitz et al. (1990); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Kubicek et al. (1988); Pel et al. (2007)	ANIG, ANID		An01g09940; An08g10920; An09g06680	35756; 176409; 202801
r32	:	CITm ⇆ ACOm + H2Om	4.2.1.3	Aconitate hydratase	Muller (1975b); Neilson (1955); Muller (1986); Alvarez-Vasquez et al. (2000); Kirimura et al. (2000); Karaffa et al. (2001)	ANIG, ANID		An02g11040; An08g10530; An09g03870; An16g05760	130186; 52568; 212582; 48916
r33	:	ACOm + H2Om ⇆ ICITm	4.2.1.3	Aconitate hydratase	Muller (1975b); Neilson (1955); Muller (1986); Alvarez-Vasquez et al. (2000); Kirimura et al. (2000); Karaffa et al. (2001)	ANIG, ANID		An02g11040; An08g10530; An09g03870; An16g05760	130186; 52568; 212582; 48916
r34	:	ICITm + NADPm ⇒ AKGm + CO2m + NADPHm	1.1.1.42	Isocitrate dehydrogenase (icdA) (NADP+)	Patil and Ramakrishnan (1966); Muller (1975b, 1986); Meixner-Monori et al. (1986); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001); Jaklitsch et al. (1991); Pel et al. (2007)	ANIG, ANID		An02g12430	47151
r30	:	ICITm + NADm ⇒ AKGm + CO2m + NADHm	1.1.1.41	Isocitrate dehydrogenase (NAD+)	Muller (1975b); Jaklitsch et al. (1991); Pel et al. (2007)	ANIG, ANID	*	An08g05580; An18g06760	208051; 212289
r35	:	ICIT + NADP ⇒ AKG + CO2 + NADPH	1.1.1.42	Isocitrate dehydrogenase (NADP+)	Patil and Ramakrishnan (1966); Muller (1975b, 1986); Meixner-Monori et al. (1986); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001); Jaklitsch et al. (1991); Pel et al. (2007)	ANIG, ANID		An02g12430	47151
r36a	:	AKGm + TDPE1m ⇒ AKGE1m + CO2m	1.2.4.2	alpha-ketoglutarate dehydrogenase	Muller (1975b); Meixner-Monori et al. (1985); Martinelli and Kinghorn (1994)	ANIG, ANID	*	An04g04750; An06g00390	212992; 47240
r36b	:	AKGE1m + LPSE2m ⇒ AKGE2m + TDPE1m	2.3.1.61	Dihydrolipoamide S-succinyl transferase	Meixner-Monori et al. (1985); Martinelli and Kinghorn (1994)	ANIG, ANID		An11g11280	56101
r36c	:	AKGE2m + COAm + NADm ⇆ LPSE2m + SUCCOAm + NADHm	1.8.1.4	Dihydrolipoamide dehydrogenase	Meixner-Monori et al. (1985); Martinelli and Kinghorn (1994)	ANIG, ANID		An07g06840	53232
r38	:	GDPm + PIm + SUCCOAm ⇆ GTPm + SUCCm + COAm	6.2.1.4	Succinate CoA ligase (GDP forming)	David et al. (2003)	ANIG, ANID	*	An08g02970; An08g02980	176118; 176118
r39	:	SUCCm + Qm ⇆ FUMm + QH2m	1.3.5.1	Succinate dehydrogenase (ubiquinone)	Martinelli and Kinghorn (1994); Karaffa et al. (2001)	ANIG, ANID	*	An14g04395; An14g04400; An02g07600; An02g12770; An07g03170	201642; 201642; 130857; 55637; 40064
r40	:	FUMm + FADH2m ⇒ SUCCm + FADm	1.3.99.1	Succinate dehydrogenase	Muller (1975b); Kirimura et al. (2000); Karaffa et al. (2001)	ANIG, ANID		An01g13930; An02g05410	51710; 52233

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r41	:	FUM + FADH2m ⇒ SUCC + FADm	1.3.99.1	Succinate dehydrogenase		ANID	An16g07150	205005
r42	:	FUMm + H2Om ⇆ MALm	4.2.1.2	Fumarate hydratase	David et al. (2003)	ANIG, ANID	An12g07850	56673
r43	:	MAL ⇆ FUM + H2O	4.2.1.2	Fumarate hydratase	Muller (1975a, 1986)	ANID	An12g07850	56673
r44	:	MALm + NADm ⇆ OAm + NADHm	1.1.1.37	Malate dehydrogenase	Muller (1975b); Ma et al. (1981); Bercovitz et al. (1990); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001); Pel et al. (2007)	ANIG, ANID	An16g00120	N/A
r45	:	MAL + NAD ⇆ OA + NADH	1.1.1.37	Malate dehydrogenase	Muller (1975b); Ma et al. (1981); Muller (1986); Bercovitz et al. (1990); Jaklitsch et al. (1991); Martinelli and Kinghorn (1994); Alvarez-Vasquez et al. (2000); Karaffa et al. (2001); Pel et al. (2007)	ANIG, ANID	An11g07190; An15g00070; An12g00160	48047; 183145; 212768
Anaplerotic reactions (besides Gluconeogenesis)								
Glyoxylate Shunt					Martinelli and Kinghorn (1994)			
r46	:	ICITm ⇒ SUCCm + GLXm	4.1.3.1	Isocitrate lyase	Shah and Ramakrishnan (1963); Sahasrabudhe et al. (1986)	ANIG, ANID	An01g09270	196237
r47	:	ACCOAm + H2Om + GLXm ⇒ MALm + COAm	4.1.3.2	Malate synthase	David et al. (2003)	ANIG, ANID	An15g01860	48680
Oxidation of malate to pyruvate								
r48c	:	MAL + NADP ⇒ PYR + CO2 + NADPH	1.1.1.40	Malate dehydrogenase (NADP-specific) (malic enzyme)	Jernejc and Legisa (2002)	ANIG, ANID	An05g00930	211661
r48m	:	MALm + NADPm ⇒ PYRm + CO2m + NADPHm	1.1.1.40	Malate dehydrogenase (NADP-specific) (malic enzyme)		ANID	An12g00160	212768
TCA intermediates metabolism								
r50	:	ATP + CIT + COA ⇒ ADP + PI + ACCOA + OA	2.3.3.8	ATP:citrate oxaloacetate-lyase ((pro-3S)-CH2COO- ->acetyl-CoA) (ATP-dephosphorylating)	Pel et al. (2007); Pfitzner et al. (1987)	ANIG, ANID	An11g00530	199043
r50m	:	ATPm + CITm + COAm ⇒ ADPm + PIm + ACCOAm + OAm	2.3.3.8	ATP:citrate oxaloacetate-lyase ((pro-3S)-CH2COO- ->acetyl-CoA) (ATP-dephosphorylating) mitochondrial	Pel et al. (2007); Pfitzner et al. (1987)	ANIG, ANID	An11g00510	208547
r37	:	CITm ⇒ OAm + ACm	4.1.3.6	Mitochondrial citrate lyase	Pel et al. (2007)	ANIG, ANID	An01g08610	51845
Oxalic acid					Rymowicz and Lenart (2003)			
r51	:	OA + H2O ⇒ OXAL + AC	3.7.1.1	Oxaloacetate acetylhydrolase (oahA)	Muller (1975a); Lenz et al. (1976); Muller (1986); Kubicek et al. (1988); Ruijter and Visser (1999); Pedersen et al. (2000a); Hjort and Pedersen (2000)	ANIG, ANID	An10g00820	57241
r52	:	OXAL ⇒ FOR + CO2	4.1.1.2	Oxalate decarboxylase	Emiliani and Riera (1968)	ANIG, ANID	An15g03980	182700
r56	:	OXALe ⇒ FORe + CO2e	4.1.1.2	Oxalate decarboxylase		ANEW	An03g01140	214686
Methanol								

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r53	:	METHOL + NAD ⇆ FALD + NADH	1.1.1.1	Alcohol dehydrogenase (adhA)	Lusta et al. (1991, A. terreus)	ANID		An12g09810; An17g01530; An01g12170; An01g14590; An02g02060; An02g02870; An03g01350; An04g02690; An08g09750; An09g03140; An11g04150; An11g04290; An12g09950; An13g00950; An13g03330; An14g02160; An14g07180; An16g00010; An16g00400; An16g06240	46038; 204476; 205557; 170152; 206534; 174157; 194416; 190222; 177276; 43351; 179042; 39027; 195091; 44729; 134944; N/A; 42017; 41439; 41421; 40925
Formic acid									
r54	:	FALD + NAD + H2O ⇆ FOR + NADH	1.2.1.46	Formaldehyde dehydrogenase	Lusta et al. (1991, A. terrerus)	ANID		An10g00230	44975
r55	:	FOR + O2 ⇒ H2O2 + CO2	1.2.1.2	Formate oxidase	Hauge (1957)	ANEW		An15g00410	124156
r61	:	FALD + RGT + NAD ⇆ FGT + NADH	1.2.1.1	Formaldehyde dehydrogenase (glutathione)	Lusta et al. (1991, A. terreus)	ANID		An02g00080	173994
Pyruvate metabolism									
r56a	:	PYRm + LIPOm ⇒ ADHLIPOm + CO2m	1.2.4.1	Pyruvate dehydrogenase (lipoamide)	Alvarez-Vasquez et al. (2000); Karaffa and Kubicek (2003); Pel et al. (2007)	ANIG, ANID	*	An01g00100; An07g09530; An11g04550	55510; 209315; 125186
r56b	:	COAm + ADHLIPOm + NADm ⇆ ACOAm + LIPOm + NADHm	2.3.1.12	Dihydrolipoamide S-acetyltransferase and lipoamide dehydrogenase	Pel et al. (2007)	ANIG, ANID	*	An07g02180; An07g06840; An02g11910	53338; 53232; 197817
r58	:	PYR ⇒ ACAL + CO2	4.1.1.1	Pyruvate decarboxylase	David et al. (2003)	ANIG, ANID		An02g06820; An01g01590; An09g01030; An13g03320	55573; 125264 and 170782; 189097; 192165
r59	:	PYR + PI + O2 + H2O ⇒ ACTP + CO2 + H2O2	1.2.3.3	Pyruvate oxidase	Patil and Ramakrishnan (1966)	ANEW			
r60	:	ATP + AC ⇒ ADP + ACTP	2.7.2.1	Acetate kinase	Pel et al. (2007)	ANIG, ANID		An02g06420	206885
Methylglyoxal bypass									
r62	:	T3P2 ⇒ MTHGXL + PI	4.2.3.3	Methylglyoxal synthase or non-enzymatic	Martinelli and Kinghorn (1994)	ANIG			
r63	:	T3P1 ⇒ MTHGXL + PI	No EC	chemical reaction	Martinelli and Kinghorn (1994)	ANEW			
r64	:	MTHGXL + NADPH ⇆ LACAL + NADP	1.1.1.78	D-Lactaldehyde dehydrogenase (Methylglyoxal reductase) (MGR I)	Inoue et al. (1988); Martinelli and Kinghorn (1994)	ANIG, ANID			
r65	:	LACAL + NAD + H2O ⇒ LAC + NADH	1.2.1.22	Lactaldehyde dehydrogenase	Inoue et al. (1988)	ANIG, ANID			

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r66	:	LAC + NAD ⇆ PYR + NADH	1.1.1.28	D-lactate dehydrogenase	David et al. (2003)	ANIG	An01g09780	51812
r67	:	RGT + MTHGXL ⇆ LGT	4.4.1.5	Lactoylglutathione lyase (glyoxylase I)	Inoue et al. (1987, 1988); Martinelli and Kinghorn (1994)	ANIG, ANID	An08g09300; An11g02860; An02g05670	37996; 38904; 52241
r68	:	LGT + H2O ⇒ LAC + RGT	3.1.2.6	Hydroxyacylglutathione hydrolase (glyoxylase II)	Inoue et al. (1988)	ANIG, ANID	An04g07220; An11g07320; An14g06340	214187; 48052; 184532
Methylcitrate pathway					Sealy-Lewis and Fairhurst (1998); Kanehisa et al. (2002)			
r69	:	PROPAL + NAD + H2O ⇆ PROP + NADH	1.2.1.3	Aldehyde dehydrogenase (NAD+)	Kazimirova and Novotel'nov (1956)	ANEW	An04g03400; An01g15170; An08g07290; An08g10820; An10g00850; An15g05890; An18g04130	57028; N/A; 55742; 37719; 57243; 40734; 187856
r70	:	ATPm + PROPm + COAm ⇆ AMPm + PPIm + PROPCOAm	6.2.1.17	Propanoate:CoA ligase (AMP-forming)	Sealy-Lewis and Fairhurst (1998)	ANIG, ANID		
r85	:	ATP + PROP + COA ⇆ AMP + PPI + PROPCOA	6.2.1.17	Propanoate:CoA ligase (AMP-forming)	Sealy-Lewis and Fairhurst (1998)	ANEW		
r71	:	PROPCOAm + H2Om + OAm ⇆ 2MCITm + COAm	2.3.3.5	2-Methylcitrate synthase	Miyakoshi et al. (1987); Sealy-Lewis and Fairhurst (1998)	ANIG, ANID	An15g01920	48684
r72	:	2MCITm ⇆ 2MACOm + H2Om	4.2.1.79	2-methylcitrate hydrolyase	Sealy-Lewis and Fairhurst (1998, Inferred)	ANIG	An15g01780	53423
r73	:	2MACOm + H2Om ⇆ 2MICITm	4.2.1.99	2-methylisocitrate dehydratase	Sealy-Lewis and Fairhurst (1998, Inferred)	ANIG		
r74	:	2MICITm ⇆ PYRm + SUCCm	4.1.3.30	2-methylisocitrate lyase	Miyakoshi et al. (1987)	ANIG	An12g07630	42171
4-aminobutyrate (GABA) shunt								
r75	:	GLUm ⇒ GABAm + CO2m	4.1.1.15	Glutamate decarboxylase	Kumar et al. (2000)	ANID	An02g06860; An08g08840; An15g04770	173821; 52600; 210245
r76	:	GABAm + AKGm ⇒ SUCCSALm + GLUm	2.6.1.19	4-Aminobutyrate transaminase	David et al. (2003)	ANIG, ANID	An17g00910	57265
r77	:	SUCCSALm + NADm + H2Om ⇒ SUCCm + NADHm	1.2.1.16	Succinate-semialdehyde dehydrogenase (NAD(P)+)	Kumar and Punekar (1998)	ANIG, ANID	An15g01740; An04g02610; An14g02870	56305; 57046; 56568
ONE CARBON -METABOLISM								
Folate biosynthesis								
r78	:	GTP + 2 H2O ⇒ FOR + AHTD	3.5.4.16	GTP cyclohydrolase I	Cossins and Chen (1997, Inferred)	ANID	An09g05310	212481
r79	:	AHTD ⇒ DHP + 3 PI	3.1.3.1	Glycerophosphatase, alkaline phosphatase; nucleoside triphosphatase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID	An07g07520	209506
r80	:	DHP ⇒ AHHMP + GLAL	4.1.2.25	Dihydroneopterin aldolase		ANID	An16g03880	49007
r991	:	GLAL + NAD + H2O ⇆ GLYA + NADH	1.2.1.21	Glycolaldehyde dehydrogenase		ANEW		
r992	:	GLYA + O2 ⇒ GLX + H2O2	1.1.3.15	Glycolate oxidase		ANEW	An01g14530; An12g10140	46259; 46010
r81	:	AHHMP + ATP ⇒ AMP + AHHMD	2.7.6.3	6-Hydroxymethyl-7,8 dihydropterin pyrophosphokinase		ANID	An16g05350	183733

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r82	:	CHOR + GLN ⇒ ADCHOR + GLU	6.3.5.8	Aminodeoxychorismate synthase		ANID		
r83	:	ADCHOR ⇒ PYR + PABA	4.1.3.38	Aminodeoxychorismate lyase		ANID		
r84	:	PABA + AHHMD ⇒ PPI + DHPT	2.5.1.15	Dihydropteroate synthase	Cossins and Chen (1997, Inferred)	ANID	An16g03880	49007
r86	:	DHPT + ATP + GLU ⇒ ADP + PI + DHF	6.3.2.12	Dihydrofolate synthase	Iwai et al. (1977)	ANID		
r87	:	DHF + NADPH ⇒ NADP + THF	1.5.1.5	Dihydrofolate reductase	Balinska and Paszewski (1979, A. nidulans)	ANIG, ANID	An02g12420	47150
r88	:	THF + ATP + GLU ⇆ ADP + PI + THFG	6.3.2.17	Tetrahydrofolylpolyglutamat synthase	Lewandowska et al. (1996, A. nidulans)	ANID	An02g02950; An04g01120; An04g02490; An04g09750	174911; 50605; 54580; 122883
Folate one-carbon pool					Cossins and Chen (1997); Kanehisa et al. (2002)			
r89	:	ATPm + FORm + THFm ⇒ ADPm + PIm + FTHFm	6.3.4.3	Formate-dihydrofolate ligase (10-Formyltetrahydrofolate synthetase, FTHFS) (Trifunctional)	Cossins and Chen (1997, Inferred)	ANID	An02g12420	47150
r90	:	FTHFm ⇆ METHFm + H2Om	3.5.4.9	Methenyltetrahydrofolate cyclohydrolase (Trifunctional)	Cossins and Chen (1997, Inferred)	ANID	An02g12420	47150
r91	:	METHFm + NADPHm + Hm ⇆ METHFm + NADPm	1.5.1.5	Methylenetetrahydrofolate dehydrogenase (NADP+) (Trifunctional)	Cossins and Chen (1997, Inferred)	ANID	An02g12420	47150
r92	:	METTHFm + NADPHm + Hm ⇒ MTHFm + NADPm	1.5.1.20	Methylenetetrahydrofolate reductase (NADPH)		ANID	An02g03270	55539
r93	:	METTHF + NAD ⇒ METHF + NADH	1.5.1.15	Methylenetetrahydrofolate dehydrogenase (NAD+)	Lewandowska et al. (1996, A. nidulans)	ANID	An16g07400	214561
r94	:	METHF + H2O ⇆ FTHF	3.5.4.9	Methenyltetrahydrofolate cyclohydrolase		ANID	An02g12420	47150
r95	:	FTHF + H2O ⇒ FOR + THF	3.5.1.10	5-formyltetrahydrofolate deformylase		ANEW	An01g11650	196101
r96	:	METTHF + NADPH ⇒ MTHF + NADP	1.5.1.20	Methylenetetrahydrofolate reductase (NADPH)	Balinska and Paszewski (1979, A. nidulans)	ANIG	An09g05860	50057
Coenzyme A and pantothenate biosynthesis								
r97	:	OIVALm + METTHF + H2O ⇒ AKP + THF	2.1.2.11	Ketopentoate hydroxymethyl transferase		ANID		
r98	:	AKP + NADPH ⇒ NADP + PANT	1.1.1.169	Ketopantoate reductase (2-dehydropantoate 2-reductase)		ANID	An09g01130; An18g01140; An11g09950	56955; 42642; 178804
r99	:	AKPm + NADPHm ⇒ NADPm + PANTm	1.1.1.169	Ketopantoate reductase (2-dehydropantoate 2-reductase)		ANID	An09g01130; An11g09950	56955; 178804
r100	:	PANT + bALA + ATP ⇒ AMP + PPI + PNTO	6.3.2.1	Pantoate-B-alanine ligase	Shimizu et al. (1974)	ANID	An18g01970	49810
r101	:	PNTO + ATP ⇒ ADP + 4PPNTO	2.7.1.33	Pantothenate kinase	Shimizu et al. (1974)	ANID	An02g13550	37546
r102	:	4PPNTO + CTP + CYS ⇒ CMP + PPI + 4PPNCYS	6.3.2.5	Phosphopantothenate-cysteine ligase	Shimizu et al. (1974)	ANID		
r103	:	4PPNCYS ⇒ CO2 + 4PPNTE	4.1.1.36	Phosphopantothenate-cysteine decarboxylase	Shimizu et al. (1974)	ANID		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r104	:	4PPNTE + ATP ⇒ PPI + DPCOA	2.7.7.3	Phospho-pantethiene adenylyltransferase (Bifunctional with 2.7.1.24)	Shimizu et al. (1974)	ANID		
r105	:	DPCOA + ATP ⇒ ADP + COA	2.7.1.24	DephosphoCoA kinase (Bifunctional with 2.7.7.3)	Shimizu et al. (1974)	ANID		
Biotin biosynthesis					Parry and Kunitani (1979); Parry and Naidu (1980)			
r107	:	3 MALCOA + 4 NADPH ⇒ 4 NADP + CHCOA + 2 CO2 + 2 COA + 2 H2O	6.4.1.2; 6.3.4.1; 4 2.3.1.85;1.1.1	B-ketoacyl-ACP synthase (c10,0), fatty acyl CoA synthase	Parry and Naidu (1980, Inferred)	ANEW		
r108	:	ALA + CHCOA ⇆ CO2 + COA + AONA	2.3.1.47	8-Amino-7-oxononanoate synthase	Parry and Naidu (1980, Inferred)	ANID	An04g01140; An11g05560; An12g00920; An15g01980	190614; 179151; 189889; 200589
r109	:	AONA + SAM ⇆ DAONA + SAMOB	2.6.1.62	adenosyl:methionine-8-amino-7-oxononanoate aminotransferase	Parry and Naidu (1980, Inferred)	ANEW	An15g01990	48688
r110	:	DAONA + ATP + CO2 ⇆ ADP + PI + DTB	6.3.3.3	dethiobiotin synthetase	Parry and Naidu (1980, Inferred)	ANEW		
r111	:	DTB + S ⇆ BT	2.8.1.6	Biotin synthase	Tepper et al. (1966); Parry and Kunitani (1979); Parry and Naidu (1980)	ANID	An15g02000	51633
OTHER CARBOHYDRATES, ALCOHOLS AND ORGANIC ACIDS C2 METABOLISM								
Acetate/Acetaldehyde/Ethanol metabolism					Martinelli and Kinghorn (1994)			
r113	:	ETH + NAD ⇆ ACAL + NADH	1.1.1.1	Alcohol dehydrogenase (adhA)	Martinelli and Kinghorn (1994)	ANIG, ANID	An12g09810; An17g01530; An01g12170; An01g14590; An02g02060; An02g02870; An03g01350; An04g02690; An08g09750; An09g03140; An11g04150; An11g04290; An12g09950; An13g00950; An13g03330; An14g02160; An14g07180; An16g00010; An16g00400; An16g06240	46038; 204476; 205557; 170152; 206534; 174157; 194416; 190222; 177276; 43351; 179042; 39027; 195091; 44729; 134944; N/A; 42017; 41439; 41421; 40925
r114	:	ETH + NADP ⇆ ACAL + NADPH	1.1.1.2	Alcohol dehydrogenase (Catalysed by Glycerol dehydrogenase II (NADP+) EC 1.1.1.72)	David et al. (2003)	ANIG	An05g02070; An10g00010; An16g02510	190030; N/A; 184073

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r115	:	ACAL + NAD + H2O ⇒ AC + NADH	1.2.1.3	Aldehyde dehydrogenase (NAD+) (aldA)	O'Connell and Kelly (1988, 1989, 1992); Martinelli and Kinghorn (1994)	ANIG, ANID	An04g03400; An01g15170; An08g07290; An08g10820; An10g00850; An15g05890; An18g04130	57028; N/A; 55742; 37719; 57243; 40734; 187856
r116	:	AC + COA + ATP ⇒ AMP + PPI + ACCOA	6.2.1.1	Acetyl-CoA synthase (acuA)	Sealy-Lewis and Fairhurst (1998)	ANIG, ANID	An04g05620	214348
r117	:	ACCOA + H2O ⇒ COA + AC	3.1.2.1	Acetyl-CoA hydrolase	Ramakrishnan and Raina (1958); Ramakrishnan et al. (1959)	ANIG, ANID	An16g07110	214587
r118	:	ETHm + NADm ⇆ ACALm + NADHm	1.1.1.1	Alcohol dehydrogenase		ANID	An12g09810; An17g01530; An01g12170; An01g14590; An02g02060; An02g02870; An03g01350; An04g02690; An08g09750; An09g03140; An11g04150; An11g04290; An12g09950; An13g00950; An13g03330; An14g02160; An14g07180; An16g00010; An16g00400; An16g06240	46038; 204476; 205557; 170152; 206534; 174157; 194416; 190222; 177276; 43351; 179042; 39027; 195091; 44729; 134944; N/A; 42017; 41439; 41421; 40925
r119	:	ACALm + NADm + H2Om ⇒ ACm + NADHm	1.2.1.3	Aldehyde dehydrogenase (NAD+) (adhA)		ANID	An04g03400; An01g15170; An08g07290; An08g10820; An10g00850; An15g05890; An18g04130	57028; N/A; 55742; 37719; 57243; 40734; 187856
r120	:	ACm + COAm + ATPm ⇒ AMPm + PPIm + ACCOAm	6.2.1.1	Acetyl-CoA synthase	Pel et al. (2007)	ANIG, ANID	An05g00390	185892
r121	:	ACCOAm + H2Om ⇒ COAm + ACm	3.1.2.1	Acetyl-CoA hydrolase	David et al. (2003)	ANIG, ANID	An16g07110	214587
C3 METABOLISM								
Glycerol metabolism								
r122	:	GL + NAD ⇒ GLYN + NADH	1.1.1.6	Glycerol dehydrogenase	Martinelli and Kinghorn (1994)	ANIG, ANID	An01g06970	196413
r123	:	GL + O2 ⇒ GLYAL + H2O2	1.1.3.13	Alcohol oxidase		ANID	An15g02200; An18g05480	56311; 42956
r124	:	GLYAL + NADPH ⇒ GL + NADP	1.1.1.72	Glycerol dehydrogenase	Jennings (1984); Schuurink et al. (1990); Martinelli and Kinghorn (1994)	ANIG, ANID	An01g06970	196413

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r126	:	GL + O2 ⇒ GLYN + H2O2	1.1.3.13	Alcohol oxidase		ANID	An15g02200; An18g05480	56311; 42956
r127	:	GL + NADP ⇒ GLYN + NADPH	1.1.1.72	Glycerol dehydrogenase (NADP+)	Baliga et al. (1964); Schuurink et al. (1990)	ANEW	An01g06970	196413
r128	:	GL + ATP ⇒ GL3P + ADP	2.7.1.30	Glycerol kinase	Witteveen et al. (1990); Witteveen and Visser (1995)	ANIG, ANID	An04g04890	45434
r129	:	GL3P + FADm ⇒ T3P2 + FADH2m	1.1.99.5	Glycerol 3-phosphate dehydrogenase (FAD dependent) (FAD-dependent sn-glycerol-3-phosphate dehydrogenase)	Witteveen et al. (1990)	ANIG, ANID	An08g00210	55910
r130	:	GLYN + ATP ⇒ T3P2 + ADP	2.7.1.29	Glycerone kinase	Witteveen et al. (1990)	ANIG, ANID	An14g06500	56628
r131	:	T3P2 + NADH ⇒ GL3P + NAD	1.1.1.8	Glycerol 3-phosphate dehydrogenase (NAD+ dependent)	David et al. (2003)	ANIG, ANID	An15g07390	48886
r132	:	GL3P + H2O ⇒ GL + PI	3.1.3.21	Glycerol 3-phosphate phosphatase	David et al. (2003)	ANIG, ANID	An08g02530	176581
Glycerate metabolism								
r133	:	G + NADP ⇆ 3HPYR + NADPH	1.1.1.29	glycerate dehydrogenase	Behal and Hamilton (1962); Behal (1967)	ANEW	An08g06710	207936
L-lactate								
r183	:	LLAC + NAD ⇒ PYR + NADH	1.1.1.27	L-Lactate dehydrogenase	David et al. (2003)	ANIG, ANID	An04g08220	137087
C4 METABOLISM								
Tartrate metabolism								
r134	:	TAR + NAD ⇆ OXGLY + NADH	1.1.1.93	Tartrate dehydrogenase	David et al. (2003)	ANIG, ANID	An01g03030	171830
r135	:	TAR ⇆ OA + H2O	4.2.1.32	Tartrate dehydratase	Patil and Ramakrishnan (1966)	ANEW		
D-Erythrose/Erythritol metabolism								
r136	:	E + NADPH ⇒ EOL + NADP	1.1.1.72	Glycerol dehydrogenase	Schuurink et al. (1990)	ANIG, ANID	An01g06970	196413
r138	:	E + ATP ⇒ E4P + ADP		Erythrulose kinase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
r139	:	E4P + H2O ⇒ PI + E		Erythrose 4-phosphate phosphatase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
r140	:	EOL + NAD ⇒ E + NADH		Erythrose reductase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
r141	:	EOL + NAD ⇒ EU + NADH		Erythrose dehydrogenase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
r142	:	EU + ATP ⇒ EU1P + ADP		Erythrulose kinase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
r143	:	EU1P ⇒ T3P1 + FALD	4.1.2.2	Ketotetrose-phosphate aldolase	David et al. (2003), Hondmann (1994, A. nidulans)	ANIG		
C5 METABOLISM								
L-Arabinose/Arabitol metabolism					Witteveen et al. (1989)			
r144	:	LAOL + NADP ⇆ LARAB + NADPH	1.1.1.21	L-arabinose reductase	Witteveen et al. (1989); Martinelli and Kinghorn (1994); vanKuyk et al. (2001); de Groot et al. (2003); de Groot et al. (2005)	ANIG	An01g14880; An16g01720	46249; 53686

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r145	:	LAOL + NAD ⇆ LXUL + NADH	1.1.1.12	L-Arabitol dehydrogenase	Witteveen et al. (1989); Martinelli and Kinghorn (1994); vanKuyk et al. (2001); de Groot et al. (2003); de Groot et al. (2005)	ANIG, ANID	An01g10920	46405
r146	:	LXUL + NADPH ⇆ XOL + NADP	1.1.1.10	L-Xylulose reductase	Martinelli and Kinghorn (1994); vanKuyk et al. (2001); de Groot et al. (2003); Witteveen et al. (1989, 1994)	ANIG, ANID	An11g03260	47908
D-Xylose/D,L-Xylulose/Xylitol metabolism					Witteveen et al. (1994); de Groot et al. (2003)			
r147	:	XYL + NADPH ⇆ XOL + NADP	1.1.1.21	D-Xylose reductase (xyrA) (xylitol dehydrogenase)	Witteveen et al. (1989); Martinelli and Kinghorn (1994); Witteveen et al. (1994); vanKuyk et al. (2001); Hasper et al. (2002); de Groot et al. (2003); de Groot et al. (2005)	ANIG, ANID	An01g03740	51997
r148	:	XOL + NADP ⇒ XUL + NADPH	1.1.1.10	xylitol dehydrogenase		ANIG, ANID	An11g03260	47908
r149	:	XOL + NAD ⇒ XUL + NADH	1.1.1.9	D-Xylulose reductase (xylitol dehydrogenase)	Witteveen et al. (1989); Martinelli and Kinghorn (1994); Witteveen et al. (1994); de Groot et al. (2003); vanKuyk et al. (2001)	ANIG, ANID	An05g02260; An07g01320; An08g09380; An12g00030; An15g04610	212968; N/A; 37988; 203198; 48775
D-arabinose metabolism					Witteveen et al. (1989)			
r150	:	ARABLAC + NADPH ⇆ ARAB + NADP	1.1.1.117	D-Arabinose 1-dehydrogenase [NAD(P)+]	Witteveen et al. (1989)	ANID	An01g06970	196413
r151	:	ARAB + NADPH ⇆ AOL + NADP	1.1.1.21	Aldehyde reductase	Witteveen et al. (1989, 1994)	ANIG	An01g14880; An16g01720	46249; 53686
r152	:	AOL + NAD ⇒ XUL + NADH	1.1.1.11	D-arabitol dehydrogenase	Witteveen et al. (1989, 1994); vanKuyk et al. (2001)	ANIG, ANID	An04g09410	51398
r153	:	AOL + NADP ⇒ XUL + NADPH	1.1.1.11	D-arabitol dehydrogenase	Witteveen et al. (1989); vanKuyk et al. (2001)	ANIG, ANID	An04g09410	51398
Xylulose								
r154	:	ATP + XUL ⇒ ADP + XUL5P	2.7.1.17	Xylulose kinase	Witteveen et al. (1989, 1994); Martinelli and Kinghorn (1994); vanKuyk et al. (2001); de Groot et al. (2003)	ANIG, ANID	An07g03140	209771
r155	:	XUL5P + FALD ⇆ T3P1 + GLYN	2.2.1.3	Dihydroxyacetone synthase	Lusta et al. (1991, A. terrerus)	ANID	An14g03500	184680
Ribose								
r156	:	ATP + RIB ⇒ ADP + R5P	2.7.1.15	Ribokinase	David et al. (2003)	ANIG, ANID	An15g07500	40855
r157	:	R5P ⇆ R1P	5.4.2.2	Phosphoglucomutase	Khanna and Tewari (1963)	ANID	An02g07650	55590
r158	:	RIB + NADPH ⇆ RIBOL + NADP	1.1.1.21	D-Ribose reductase	Witteveen et al. (1989)	ANIG	An01g14880; An16g01720	46249; 53686
r159	:	RIBOL + NAD ⇒ RL + NADH	1.1.1.56	Ribitol dehydrogenase	Witteveen et al. (1989)	ANIG	An13g02310; An18g00010	192184; 42574
r160	:	RIBOL + NADP ⇒ RL + NADPH	1.1.1.56	Ribitol dehydrogenase	Witteveen et al. (1989)	ANIG	An13g02310; An18g00010	192184; 42574
Ribulose								
r161	:	ATP + RL ⇒ ADP + RL5P	2.7.1.47	Ribulokinase		ANID	An14g00160	53716
r162	:	RL + NADPH ⇒ AOL + NADP	No EC	ribulose reductase	Hondmann (1994, A.nidulans), Morozova et al. (2002, Inferred)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
C6 METABOLISM								
Gluconic acid/Gluconate metabolism								
r163	:	bDGLCe + O2e ⇆ GLCN15LACe + H2O2e	1.1.3.4	Glucose oxidase (goxC)	Muller (1977); Frederick et al. (1990); Martinelli and Kinghorn (1994); Witteveen et al. (1992); Kim et al. (2001); Leskovac et al. (2005)	ANIG, ANID	An12g03430; An12g03440; An01g14740; An07g00450	50376; 50376; 55227; 40254
r164	:	bDGLC + O2 ⇆ GLCN15LAC + H2O2	1.1.3.4	Glucose oxidase (god)	Muller (1977); Frederick et al. (1990); Martinelli and Kinghorn (1994); Witteveen et al. (1992); Kim et al. (2001); Leskovac et al. (2005); Bhatti et al. (2006)	ANID	An12g03430; An12g03440; An01g14740; An07g00450	50376; 50376; 55227; 40254
r165	:	GLCN15LACe + H2Oe ⇒ GLCNTe	3.1.1.17	Gluconolactonase (lactonase)	Witteveen et al. (1992, 1993); Ogawa et al. (2002)	ANIG, ANID	An12g01570	N/A
NE6	:	GLCN15LAC + H2O ⇒ GLCNT	No EC	Spontaneous reaction or catalyzed by glucose oxidase	Bhatti et al. (2006)	ANIG, ANID		
r166	:	D6PGC + H2O ⇒ GLCNT + PI	3.1.3.1	Alkaline phosphatase	Ramaswamy and Bheemeswar (1976); Muller (1977); Rokosu and Uadia (1980); Karaffa et al. (2001)	ANIG, ANID	An07g07520; An18g04040	209506; 42852
r167	:	D6PGC + H2O ⇒ GLCNT + PI	3.1.3.2	Acid phosphatase (aphA)	Muller (1977); Wyss et al. (1998)	ANIG, ANID	An14g02650; An08g09850; An09g00310; An12g10630; An13g01750; An14g01550; An16g01730; An16g09130; An18g04140	49304; 52587; 43568; 51468; 57215; 56545; 183355; 193642; 42861
r169	:	GLCNT + ATP ⇒ D6PGC + ADP	2.7.1.12	Gluconokinase	Lakshminarayana et al. (1969b); Muller (1986)	ANIG	An01g07300; An01g14850	127436; 170633
r168	:	D6PGC + NADP ⇆ D6PDGC + NADPH	1.1.1.43	6-phosphogluconate dehydrogenase	Lakshminarayana et al. (1969b,c); Muller (1986)	ANEW	An11g02040	199133
r170	:	GLCNT ⇆ KDDGC + H2O	4.2.1.39	Gluconate dehydratase	Elzainy et al. (1973); Kersters and de Ley (1975); Martinelli and Kinghorn (1994)	ANIG		
r171	:	KDDGC ⇆ PYR + GLYAL	4.1.2.14	2-keto-3-deoxygluconate aldolase	Elzainy et al. (1973); Allam et al. (1975); Martinelli and Kinghorn (1994)	ANIG		
Galactose/Galactitol metabolism								
r172	:	GALOL + NADP ⇆ GLAC + NADPH	1.1.1.21	Aldehyde reductase (Polyol dehydrogenase (NADP+))	Martinelli and Kinghorn (1994)	ANIG, ANID	An01g14880; An16g01720	46249; 53686
r173	:	ATP + GLAC ⇒ ADP + GAL1P	2.7.1.6	Galactokinase	Martinelli and Kinghorn (1994)	ANIG, ANID	An16g04160	56431
r174	:	UTP + GAL1P ⇆ PPI + UDPGAL	2.7.7.10	UTP-hexose-1-phosphate uridylyltransferase (UDP-galactose pyrophosphorylase)	Martinelli and Kinghorn (1994)	ANIG, ANID	An02g03590	174413

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r175	:	UDPGAL ⇆ UDPG	5.1.3.2	UDPglucose 4-epimerase	Martinelli and Kinghorn (1994)	ANIG, ANID	An01g12220; An01g11440; An02g08750; An12g04260; An12g10410; An14g03820	55278; 35645; 175089; 135865; 45989; 56583
r176	:	UTP + G1P ⇒ PPI + UDPG	2.7.7.9	UTP-glucose-1-phosphate uridylyltransferase (UDP glucose pyrophosphorylase)	Martinelli and Kinghorn (1994)	ANIG, ANID	An12g00820	212837
r177	:	G6P ⇆ G1P	5.4.2.2	Phosphoglucomutase	Khanna and Tewari (1963); Martinelli and Kinghorn (1994)	ANIG, ANID	An02g07650	55590
r178	:	UDPG + GAL1P ⇆ G1P + UDPGAL	2.7.7.12	UDP-glucose-hexose-1-phosphate uridylyltransferase		ANID	An02g03590	174413
Galactonic acid/Galactonate metabolism								
r179	:	GLAC + NAD ⇆ GALN14LAC + NADH	1.1.1.48	Galactose 1-dehydrogenase	David et al. (2003)	ANIG, ANID		
r180	:	GALN14LAC + H2O ⇆ GALNT	3.1.1.25	1,4-Lactonase (gamma-Lactonase)	David et al. (2003)	ANIG	An05g02030; An16g06620	212961; N/A
r181	:	GALNT ⇆ 2D3DGALT + H2O	4.2.1.6	Galactonate dehydratase	David et al. (2003), Elshafei et al. (1995, A. terreus)	ANIG, ANID	An04g02760	50500
r182	:	2D3DGALT ⇆ PYR + GLYAL	No EC	2-Dehydro-3-deoxy-D-galactonate aldolase	David et al. (2003), Elshafei et al. (1995, A. terreus)	ANIG		
Galacturonate degradation					Witteveen et al. (1990, Inferred)			
r1215	:	ATP + GALUNT ⇆ GALUNTP + ADP	2.7.1.44	Galacturonokinase		ANEW		
r1216	:	GALUNTP + UTP ⇆ UDPGALU + PPI	No EC	Galacturonate-1-phosphate uridylyl transferase		ANEW		
r1217	:	UDPGALU + 2 NADH ⇆ UDPGAL + 2 NAD + H2O	1.1.1.-	UDP-D-galactose dehydrogenase		ANEW		
Rhamnose metabolism					de Vries et al. (2002); Fries and Kallstromer (1965)			
r1218	:	RHA ⇆ RHAMN	5.3.1.14	L-Rhamnose isomerase	Fries and Kallstromer (1965, Inferred)	ANEW		
r1219	:	ATP + RHAMN ⇆ ADP + RHAMNP	2.7.1.5	L-Rhamnulose kinase	Fries and Kallstromer (1965, Inferred)	ANEW		
r1220	:	RHAMNP ⇆ T3P2 + LACAL	4.1.2.19	Rhamnulose phosphate aldolase	Fries and Kallstromer (1965, Inferred)	ANEW		
Mannose/Mannitol, Fructose and Sorbose/Sorbitol metabolism								
r184	:	ATP + MAN ⇒ ADP + MAN6P	2.7.1.1	Hexokinase (hxk) (mannokinase)	Martinelli and Kinghorn (1994); Panneman et al. (1998)	ANIG, ANID	An02g14380; An06g00380; An13g00510	55651; 134301; 50817
r185	:	MAN6P ⇆ F6P	5.3.1.8	Mannose-6-phosphate isomerase	Martinelli and Kinghorn (1994)	ANIG, ANID	An08g06350; An04g03200	55763; 44098
r186	:	ATP + FRU ⇒ ADP + F6P	2.7.1.1	Hexokinase (hxk)	Martinelli and Kinghorn (1994); Panneman et al. (1998); Karaffa et al. (2001)	ANIG, ANID	An02g14380; An06g00380; An13g00510	55651; 134301; 50817
r187	:	F6P + NADH ⇆ MNT1P + NAD	1.1.1.17	Mannitol-1-phosphate 5-dehydrogenase	Kiser and Niehaus Jr. (1981); Martinelli and Kinghorn (1994)	ANIG, ANID	An02g05830	55560

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r188	:	MNT1P + H2O ⇒ MNT + PI	3.1.3.22	Mannitol-1-phosphatase (Mannitol-1-phosphate phosphatase)	Hult et al. (1980)	ANIG, ANID		
r189	:	MNT + NADP ⇆ FRU + NADPH	1.1.1.138	Mannitol 2-dehydrogenase (NADP+)	Martinelli and Kinghorn (1994)	ANIG, ANID	An06g00750	177668
r190	:	MNT + ATP ⇒ MNT1P + ADP	3.1.3.22	Mannitol kinase	Martinelli and Kinghorn (1994)	ANEW		
r191	:	MAN1P ⇆ MAN6P	5.4.2.8	Phosphomannomutase		ANID	An07g06780; An18g06500	209558; 132771
r192	:	GTP + MAN1P ⇒ PPI + GDPMAN	2.7.7.13	Mannose-1-phosphate guanylyltransferase		ANID	An11g02380; An04g04990	55950; 204833
r193	:	ATP + F6P ⇒ ADP + F26P	2.7.1.105	6-Phosphofructo-2-kinase (Phosphofructokinase 2)	Kubicek-Pranz et al. (1990); Harmsen et al. (1992); Karaffa et al. (2001)	ANIG, ANID	An07g02100; An15g00200	128609; 209963
r194	:	F26P + H2O ⇒ F6P + PI	3.1.3.46	D-Fructose-2,6-bisphosphate 2-phosphohydrolase		ANID	An07g02100; An15g00200	128609; 209963
r195	:	IDOL + NAD ⇒ SOR + NADH	1.1.1.14	L-Iditol 2-dehydrogenase (NAD-dependent sorbitol dehydrogenase)	Desai et al. (1969c)	ANID	An09g03900; An12g00030; An16g01700; An16g01710	188914; 203198; 183939; 183900
r196	:	SOR + NADH ⇒ SOT + NAD	1.1.99.21	D-Sorbitol dehydrogenase (acceptor)	Desai et al. (1967)	ANIG, ANID	An01g03480; An01g10920; An03g05190; An14g03510	206203; 46405; 50731; 185262
r197	:	SOT + NAD ⇆ FRU + NADH	1.1.1.9	Sorbitol (glucitol) dehydrogenase (NAD+)	Desai et al. (1967, 1969b,c); Witteveen et al. (1994)	ANIG, ANID	An05g02260; An08g09380; An15g04610	212968; 37988; 48775
DISACCHARIDES METABOLISM								
Trehalose								
Biosynthesis								
r198	:	UDPG + G6P ⇒ UDP + TRE6P	2.4.1.15	Alpha,alpha-trehalose-phosphate synthase (UDP-forming) 1 (tpsA, tpsB)	Wolschek and Kubicek (1997); Karaffa et al. (2001)	ANIG, ANID	An07g08710; An08g10510; An14g02180	55704; 211004
Hydrolysis								
r199	:	TRE6P + H2O ⇒ TRE + PI	3.1.3.12	Trehalose-phosphatase	Arisan-Atac et al. (1996)	ANIG, ANID	An11g10990	119446
r200	:	TRE + H2O ⇒ 2 DGLC	3.2.1.28	Alpha,alpha-trehalase	David et al. (2003), d'Enfert and Fontaine (1997, A. nidulans)	ANIG, ANID	An01g01540	52061
Maltose								
r201	:	MLT + H2O ⇒ 2 GLC	3.2.1.20	Alpha-glucosidase (Maltase) (aglA)	Smirnov and Chubova (1965); Rudick et al. (1979); den Herder et al. (1992); Martinelli and Kinghorn (1994)	ANIG, ANID	An13g03710; An01g04880; An07g00350; An09g05880	50927; 55419; 40261; 128654
r202	:	MLTe + H2Oe ⇒ 2 GLCe	3.2.1.20	Alpha-glucosidase (Maltase) (aglA/aglU)	Smirnov and Chubova (1965); Rudick et al. (1979); den Herder et al. (1992); Martinelli and Kinghorn (1994)	ANIG, ANID	An04g06920	214233
Lactose								
r203	:	LACT + H2O ⇒ GLC + GLAC	3.2.1.23	Beta-galactosidase	Martinelli and Kinghorn (1994)	ANID	An01g10350; An06g00290	46429; 177434

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r204	:	LACTe + H2Oe ⇒ GLCe + GLACe	3.2.1.23	Beta-galactosidase (lacA)	Widmer and Leuba (1979); Sykes et al. (1983); Martinelli and Kinghorn (1994); Manzanares et al. (1998); de Vries et al. (1999)	ANIG, ANID	An01g12150; An07g04420; An14g05820	51764; 180727; 41910
Melibiose								
r205	:	MELIe + H2Oe ⇒ GLCe + GLACe	3.2.1.22	Alpha-galactosidase (melibiase) (aglA, aglC)	Manzanares et al. (1998); de Vries and Visser (2001); Wallis et al. (2001)	ANID	An09g00260; An09g00270; An01g01320; An02g11150; An06g00170; An11g06330; An14g01800	212736; 212736; 172232; 207264; 37736; 39180; 185285
Stachyose / Raffinose / Sucrose degradation								
r228	:	STACe + H2Oe ⇆ RAFFe + GLACe	3.2.1.22	alpha-galactosidase	Knap et al. (1994); Manzanares et al. (1998); de Vries and Visser (2001)	ANEW	An09g00260; An09g00270; An01g01320; An02g11150; An06g00170; An11g06330; An14g01800	212736; 212736; 172232; 207264; 37736; 39180; 185285
r229	:	RAFFe + H2Oe ⇆ SUCe + GLACe	3.2.1.22	alpha-galactosidase	Adya and Elbein (1977); Boddy et al. (1993); Knap et al. (1994); Manzanares et al. (1998); Wallis et al. (2001)	ANEW	An09g00260; An09g00270; An01g01320; An02g11150; An06g00170; An11g06330; An14g01800	212736; 212736; 172232; 207264; 37736; 39180; 185285
r230	:	SUCe + H2Oe ⇒ FRUe + GLCe	3.2.1.26	Invertase (suc1)	Schreferl-Kunar et al. (1989); Berges et al. (1993); Boddy et al. (1993); Martinelli and Kinghorn (1994); L'Hocine et al. (2000); Yanai et al. (2001)	ANIG	An08g11070; An15g00320	198063; N/A
METABOLISM OF AROMATICS								
Phenylalanine/phenylacetate degradation					Kishore et al. (1976)			
r386	:	PHPYR ⇒ PHAL + CO2	4.1.1.43	Phenylpyruvate decarboxylase	Kishore et al. (1976)	ANEW		
r387	:	PHAL + NAD + H2O ⇆ PHAC + NADH	1.2.1.39	Phenylacetaldehyde dehydrogenase	Kishore et al. (1976, Inferred)	ANEW	An02g04110	175251
r388	:	PHAC + O2 + NADPH ⇒ 2HPAC + H2O + NADP	No EC	Phenylacetate 2-hydroxylase	Kishore et al. (1976)	ANEW		
r389	:	2HPAC + O2 + NADPH ⇒ HOMOGEN + H2O + NADP	No EC	2-Phenylacetate 5-hydroxylase	Kishore et al. (1976, Inferred)	ANEW		
r390	:	HOMOGEN + O2 ⇆ MACAC	1.13.11.5	Homogentisate oxygenase	Kishore et al. (1976); Sugumaran and Vaidyanathan (1978)	ANID	An11g00430	178499
r391	:	MACAC ⇆ FUACAC	5.2.1.2	Maleylacetoacetate isomerase	Sugumaran et al. (1973)	ANID	An07g06280	180792
r392	:	FUACAC + H2O ⇒ FUM + ACTAC	3.7.1.2	Fumarylacetoacetase	Sugumaran et al. (1973)	ANID	An02g10000; An04g04150	37286; N/A
r393	:	PHAC + O2 + NADPH ⇒ 4HPAC + H2O + NADP	No EC	Phenylacetate hydroxylase	Kishore et al. (1976)	ANEW		
r394	:	4HPAC + NADPH + O2 ⇆ 4HMAND + H2O + NADP	No EC	4-hydroxyphenylacetic acid monoxygenase	Kishore et al. (1976, Inferred)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r395	:	4HMAND + NADP ⇒ 4HBFOR + NADPH	No EC	4-hydroxymandelate dehydrogenase	Kishore et al. (1976)	ANEW		
r396	:	4HMAND + NAD ⇒ 4HBFOR + NADH	No EC	4-hydroxymandelate dehydrogenase	Kishore et al. (1976)	ANEW		
r397	:	4HBFOR ⇒ 4HBAL + CO2	No EC	4-hydroxybenzoylformic acid decarboxylase	Kishore et al. (1976)	ANEW		
r398	:	4HBAL + NAD + H2O ⇆ 4HBA + NADH	No EC	4-hydroxybenzaldehyde dehydrogenase	Kishore et al. (1976)	ANEW		
r399	:	4HBA + NADPH + O2 ⇆ PCC + NADP + H2O	1.14.13.33	4-hydroxybenzoate 3-hydroxylase	Kishore et al. (1976); Shailubhai et al. (1982); Boschloo et al. (1990); Martinelli and Kinghorn (1994)	ANEW		
Coumarate degradation					Milstein et al. (1988)	ANEW		
r1192	:	COUM + H2O ⇆ AC + 4HBAL	No EC	Inferred reaction from Milstein et al. (1988)	Milstein et al. (1988, Inferred)	ANEW		
Dimethylterephthalate degradation					Ganji et al. (1995); Kanehisa et al. (2002)			
r1193	:	DMT + H2O ⇆ MTPHTH + METHOL		Dimethylterephthalate esterase	Ganji et al. (1995)	ANEW		
r1194	:	MTPHTH + H2O ⇆ TPHTH + METHOL		Dimethylterephthalate esterase	Ganji et al. (1995)	ANEW		
r1195	:	TPHTH + NADPH + O2 ⇆ DHCHDDC + NADP	1.14.12.15	1,4-dicarboxybenzoate 1,2-dioxygenase	Kanehisa et al. (2002); Ganji et al. (1995, Inferred)	ANEW		
r1196	:	DHCHDDC + NADP ⇆ PCC + CO2 + NADPH	1.3.1.61	cis-4,5-dihydroxycyclohexa-1(6),2-diene-1,4-dicarboxylate:NADP+oxidor (decarboxylating)	Kanehisa et al. (2002); Ganji et al. (1995, Inferred)	ANEW		
3-hydroxybenzoate degradation								
r1210	:	3HBA + O2 + NADPH ⇆ PCC + NADP + H2O	1.14.13.23	3-hydroxybenzoate 4-hydroxylase	Premkumar et al. (1969); Kumar et al. (1973); Sugumaran et al. (1973); Faber et al. (2001)	ANEW	An02g13270; An01g08690; An01g15110; An04g08410; An08g06250; An09g01850; An09g03500; An12g04510	37516; 172555; 171519; 51444; 175996; 43449; 212597; 42416
Ferulic acid degradation					Milstein et al. (1988, Inferred)			
r1268	:	FER + ATP + COA ⇒ AMP + PPI + FERCOA	6.2.1.12	Ferulate:CoA ligase (AMP-forming)	Milstein et al. (1988, Inferred)	ANEW	An04g04330; An08g06100; An09g01820; An12g02430; An14g05630	44006; 38230; 188806; 43775; 184942
r1269	:	FERCOA + H2O ⇆ FERHCOA	4.2.1.101	trans-feruloyl-CoA hydratase	Milstein et al. (1988, Inferred)	ANEW		
r1270	:	FERHCOA ⇆ VANIN + ACCOA	4.1.2.41	vanillin synthase	Milstein et al. (1988, Inferred)	ANEW		
r1271	:	VANIN + NAD + H2O ⇆ VAN + NADH	1.2.1.67	vanillin dehydrogenase	Milstein et al. (1988, Inferred)	ANEW		
Vanillate degradation					Milstein et al. (1988); Lesage-Meessen et al. (1996)			
r1200	:	VAN ⇒ GUA + CO2	No EC	vanillate decarboxylase	Milstein et al. (1988, Inferred)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1201	:	GUA + NADPH + O2 ⇆ CCL + NADP + H2O + FALD	2.1.1.6	S-adenosyl-L-methionine:catechol O-methyltransferase	Milstein et al. (1988, Inferred)	ANEW	An04g04700; An15g02990; An17g00200	190631; 40535; N/A
Benzonitrile degradation								
r958	:	BN + 2 H2O ⇆ BA + NH3	3.5.5.1	benzonitrilase	Snajdrova et al. (2004)	ANEW	An16g00550; An01g07510; An01g12090; An06g01960; An08g08940; An08g10150; An12g01260; An16g06210; An18g01740	41410; 35944; 170270; 175987; N/A; 52578; 141873; 40928; 211815
r959	:	BA + NADPH + O2 ⇒ 4HBA + NADP + H2O	1.14.13.12	benzoate 4-monooxygenase (benzoate-para-hydroxylase A, bphA)	Reddy and Vaidyanathan (1975); Boschloo et al. (1990); van Gorcom et al. (1990); Boschloo et al. (1991); Faber et al. (2001); Malonek et al. (2004)	ANEW	An02g13270; An01g08690; An01g15110; An04g08410; An08g06250; An09g01850; An09g03500; An12g04510	37516; 172555; 171519; 51444; 175996; 43449; 212597; 42416
Indole degradations					Subba Rao et al. (1971); Kamath and Vaidyanathan (1990)			
r1206	:	IND + O2 + NADPH ⇆ 3HIND + H2O + NADP	No EC	indole monooxygenase	Kamath and Vaidyanathan (1990)	ANEW		
r1207	:	3HIND + O2 ⇆ NFAN	No EC	3-hydroxyindoxyl dioxygenase	Kamath and Vaidyanathan (1990)	ANEW		
r1208	:	NFAN + H2O ⇆ FOR + AN	3.5.1.9	N-formylanthranilate deformylase	Kamath and Vaidyanathan (1990)	ANEW		
Tannic acid degradation					Ramirez-Coronel et al. (2003); Bhardwaj et al. (2003); van Diepeningen et al. (2004)			
r1222	:	TANAe + 10 H2Oe ⇒ 10 345THBe + GLCe	3.1.1.20	tannin acyl hydrolase (tannase)	Ramirez-Coronel et al. (2003); Bhardwaj et al. (2003); van Diepeningen et al. (2004)	ANEW	An01g02740; An01g11560; An01g14800; An02g00350; An03g05300; An04g04430; An08g08140; An08g09800; An09g00890; An10g00910; An10g00950; An11g01220; An11g03590; An12g10390; An13g03810; An17g00830	N/A; 35636; 35388; 172914; 44518; 191085; N/A; 175881; 189231; 50972; 50973; 178324; 38960; 51478; 131509; 45118
Tryptophan degradation								
r400	:	TRP + O2 ⇒ FKYN	1.13.11.11	Indoleamine 2,3-dioxygenases, Tryptophan 2,3-dioxygenase	Subba Rao et al. (1971)	ANID	An04g07210	45277

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r401	:	FKYN + H2O ⇒ FOR + KYN	3.5.1.49	Kynurenine formamidase (formamidase)	Subba Rao et al. (1971)	ANID	An07g05830	180458
r402	:	KYN + H2O ⇒ ALA + AN	3.7.1.3	Kynureninase	Subba Rao et al. (1971); Shetty and Gaertner (1975)	ANID	An04g07200; An16g04630	45278; 210508
r403	:	AN + NADPH + O2 ⇆ DHBA + NADP + NH3	1.14.13.35	anthranilate 3-monooxygenase (deaminating)	Sreeleela et al. (1969); Subba Rao et al. (1971); Subramanian and Vaidyanathan (1984); Kamath and Vaidyanathan (1990)	ANEW		
r404	:	DHBA ⇒ CCL + CO2	4.1.1.46	2,3-Dihydroxybenzoate carboxylyase (dhbD)	Rao et al. (1967); Subba Rao et al. (1971); Ramachandran et al. (1979); Kamath et al. (1987); Kamath and Vaidyanathan (1990); Santha et al. (1995)	ANEW	An07g02050; An02g05560	209864; 36964
3-Hydroxykynurenine degradation								
r406	:	HKYN + H2O ⇒ HAN + ALA	3.7.1.3	Kynureninase	Shetty and Gaertner (1975)	ANEW	An04g07200; An16g04630	45278; 210508
Tyrosine degradation								
r411	:	4HPP + O2 ⇒ HOMOGEN + CO2	1.13.11.27	4-hydroxyphenylpyruvate dioxygenase	Utkin (1950)	ANEW	An04g01280; An07g01900	190603; 124205
Salicylic acid degradation					Krupka et al. (1967); Shailubhai et al. (1982, 1983)	ANEW		
r968	:	SALI + NADPH + O2 ⇆ CCL + NADP + H2O + CO2	1.14.13.1	Salicylate hydroxylase	Krupka et al. (1967); Shailubhai et al. (1982, 1983)	ANEW	An01g07130; An02g01050; An03g00530; An03g01540; An03g02130; An03g05310; An03g06690; An04g07370; An05g01200; An07g00550; An07g05650; An07g06800; An09g00590; An09g01840; An09g04390; An11g02480; An11g03060; An11g03150; An11g05130	172298; 36659; 45799; 133101; 194221; 191298; 191475; 45265; N/A; 181136; 46219; N/A; 50241; 188800; 189090; 178872; 178362; 38917; 208837
Benzoylamine degradation								
r979	:	BAMN + H2O + O2 ⇆ BAL + H2O2 + NH3	1.4.3.6	Amine oxidase (AO-I and AO-II)	Schilling and Lerch (1995a); Frebort et al. (1999)	ANEW	An02g10920; An09g01550; An03g00730; An07g06400; An12g03290; An13g00710; An17g00010	37354; 54408; 45789; 120706; 57198; 204355
Mandelate degradation					Jamaluddin et al. (1970)	ANEW		
r974	:	DMAND + NAD ⇆ NADH + BFOR	DMAN	D-mandelate dehydrogenase	Jamaluddin et al. (1970); Ramanarayanan and Vaidyanathan (1973)	ANEW	An03g05150	50728

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r975	:	LMAND + NAD ⇆ NADH + BFOR	LMAN	L-mandelate dehydrogenase	Jamaluddin et al. (1970)	ANEW		
r976	:	BFOR ⇒ CO2 + BAL	4.1.1.7	benzoylformate decarboxylase	Jamaluddin et al. (1970)	ANEW	An02g05590	52239
r977	:	BAL + NAD + H2O ⇒ BA + NADH	1.2.1.6	NAD-benzaldehyde dehydrogenase	Raman and Shanmugasundaram (1962); Jamaluddin et al. (1970)	ANEW		
r978	:	BAL + NADP + H2O ⇒ BA + NADPH	1.2.1.7	NADP-benzaldehyde dehydrogenase	Jamaluddin et al. (1970); Kishore et al. (1976)	ANEW		
Resorcinol degradation					Shailubhai et al. (1982, 1983)	ANEW		
r971	:	RES + O2 + NADPH ⇆ BTOL + NADP + H2O	1.3.1.32	Resorcinol hydroxylase	Shailubhai et al. (1982, 1983)	ANEW		
r972	:	BTOL + O2 ⇆ 2MAC	1.13.11.37	hydroxyquinol 1,2-dioxygenase	Shailubhai et al. (1982, 1983)	ANEW	An01g12310	46358
Hydroxyquinol pathway								
r973	:	2MAC + NADPH ⇆ 3OA + NADP	1.3.1.32	maleylacetate reductase	Shailubhai et al. (1982, 1983)	ANEW	An03g05490; An07g09360	44532; 48257
Gentisate pathway					Kanehisa et al. (2002); Yogambal and Karegoudar (1997, Inferred)			
r980	:	HOMOGEN + O2 ⇒ GNTAL + CO2 + H2O	1.13.12.-	Homogentisate monooxidase		ANEW		
r981	:	GNTAL + H2O + O2 ⇒ GEN + H2O2	1.2.3.1			ANEW		
r982	:	GEN + O2 ⇆ 3MPYR	1.13.11.4	gentisate 1,2-dioxygenase	Yogambal and Karegoudar (1997); Kishore et al. (1976, Inferred)	ANEW	An02g12800; An11g10310; An18g01020	135462; 125331; 187293
r983	:	3MPYR ⇆ 3FPYR	5.2.1.4	maleylpyruvate isomerase	Yogambal and Karegoudar (1997); Kishore et al. (1976, Inferred)	ANEW		
r984	:	3FPYR + H2O ⇆ FUM + PYR	3.7.1.5	acylpyruvate hydrolase	Yogambal and Karegoudar (1997); Kishore et al. (1976, Inferred)	ANEW		
Catechol and protocatechuate pathways					Cook and Cain (1977); Martinelli and Kinghorn (1994); Mazur et al. (1994), Kuswandi and Roberts (1992, A. nidulans)	ANEW		
r960	:	CCL + O2 ⇆ MUCO	1.13.11.1	catechol 1,2-dioxygenase	Shailubhai et al. (1983); Sahasrabudhe et al. (1986); Milstein et al. (1988); Kamath and Vaidyanathan (1990)	ANEW		
r961	:	MUCO ⇆ MUCL	5.5.1.1	muconate cycloisomerase	Thatcher and Cain (1972)	ANEW	An01g14730	205361
r962	:	MUCL ⇆ OAEL	5.3.3.4	muconolactone delta-isomerase	Halsall et al. (1969)	ANEW		
r963	:	DHSK ⇆ PCC + H2O	4.2.1.10	5-dehydroshikimate dehydrase	Cain (1972b)	ANEW	An08g06800	207929
r964	:	PCC + O2 ⇆ 3CMUCO	1.13.11.3	protocatechuate 3,4-dioxygenase	Milstein et al. (1988); Martinelli and Kinghorn (1994)	ANEW		
r965	:	3CMUCO ⇆ 4CMUCL	5.5.1.2	3-Carboxy-cis,cis-muconate cycloisomerase	Halsall et al. (1969); Thatcher and Cain (1972); Cook and Cain (1977); Mazur et al. (1994)	ANEW	An14g01340	185353
r966	:	4CMUCL ⇒ OAEL + CO2	4.1.1.44	4-carboxymuconolactone decarboxylase	Thatcher and Cain (1972)	ANEW	An03g06020	191430
r967	:	OAEL + H2O ⇆ 3OA	3.1.1.24	3-oxoadipate enol-lactonase	Halsall et al. (1969)	ANEW	An13g01940; An07g07290	44810; 180211

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r969	:	3OAm + SUCCOAm ⇆ SUCCm + 3OACOAm	2.8.3.6	3-oxoadipate CoA-transferase	Halsall et al. (1969)	ANEW	An01g00200; An06g01370	172302; 55680
r970	:	3OACOAm + COAm ⇆ ACCOAm + SUCCOAm	2.3.1.16	3-ketoacyl-CoA thiolase	Halsall et al. (1969)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
METABOLISM OF AMINES								
Butylamine								
r1188	:	BUTN + H2O + O2 ⇆ BUTAL + H2O2 + NH3	1.4.3.6	Amine oxidase (maoN, AO-I, AO-II)	Frebort et al. (1996); Schilling and Lerch (1995a)	ANEW	An02g10920; An09g01550; An03g00730; An07g06400; An12g03290; An13g00710; An17g00010	37354; 54408; 45789; 120706; 57198; 204355
r1189	:	BUTAL + COA + NAD ⇆ C40COA + NADH	1.2.1.57	Butanal dehydrogenase	Frebort et al. (1996, Inferred)	ANEW		
Pentylamine								
r1202	:	PENN + H2O + O2 ⇆ PENAL + H2O2 + NH3	1.4.3.6	Amine oxidase (maoN, AO-I, AO-II)	Frebort et al. (1996); Schilling and Lerch (1995a)	ANEW	An02g10920; An09g01550; An03g00730; An07g06400; An12g03290; An13g00710; An17g00010	37354; 54408; 45789; 120706; 57198; 204355
r1203	:	PENAL + COA + NAD ⇆ C50COA + NADH	1.2.1.57	Butanal dehydrogenase	Schilling and Lerch (1995a, Inferred)	ANEW		
POLYSACCHARIDES METABOLISM								
CELL WALL COMPONENTS								
Glucan Biosynthesis								
r206	:	UDPG ⇒ UDP + 13GLUCAN	2.4.1.34	1,3-beta-Glucan synthase	David et al. (2003)	ANIG, ANID	An17g02120	54934
r207	:	UDPG ⇒ UDP + 14GLUCAN	2.4.1.18	1,4-alpha-Glucan branching enzyme	Stagg and Feather (1973)	ANEW	An14g04190	211162
r208	:	UDPG ⇒ UDP + PSNIG	2.4.1.-	1,3-alpha-Glucan (Pseudonigeran) synthase	Horisberger et al. (1972); Damveld et al. (2005)	ANEW	An01g06120; An02g03260; An04g09890; An09g03070; An12g02450; An14g04190; An15g07810	46621; 36809; 55204; 54378; 212915; 211162; 40878
r209	:	UDPG ⇒ UDP + NIG	2.4.1.-	1,3-alpha-1,4-alpha-Glucan (Nigeran) synthase	Bobbitt et al. (1977, Inferred)	ANEW	An01g06120; An02g03260; An04g09890; An09g03070; An12g02450; An14g04190; An15g07810	46621; 36809; 55204; 54378; 212915; 211162; 40878
Chitin Biosynthesis								

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	ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
	r210	:	GLN + F6P ⇒ GLU + GA6P	2.6.1.16	Glutamine-fructose-6-phosphate transaminase (isomerizing)	Ram et al. (2004)	ANIG, ANID	An03g05940; An18g06820	139271; N/A
	r211	:	ACCOA + GA6P ⇆ COA + NAGA6P	2.3.1.4	Glucosamine-phosphate N-acetyltransferase	David et al. (2003)	ANIG, ANID	An12g07840	49553
	r212	:	NAGA6P ⇆ NAGA1P	5.4.2.3	Phosphoacetylglucosamine mutase	David et al. (2003)	ANIG, ANID	An18g05160; An18g05170	212120; 212120
	r213	:	UTP + NAGA1P ⇆ PPI + UDPNAG	2.7.7.23	UDP-N-acetylglucosamine pyrophosphorylase	David et al. (2003)	ANIG, ANID	An12g00480	54451
	r214	:	UDPNAG ⇒ UDP + CHIT	2.4.1.16	Chitin synthase (chs1, chs2)	Gomez et al. (1977)	ANIG, ANID	An03g06360; An07g05570; An08g05290; An09g02290; An09g04010; An12g10380; An14g00660	44589; 53259; 38285; 50188; 56923; 45992; 49223
Hydrolysis									
	r215	:	CHIT + H2O ⇒ NAG	3.2.1.14	Chitinase (Endochitinase)	Gomez et al. (1977); Fukazawa et al. (2004)	ANID	An01g05360; An02g07020; An14g07420; An01g05160; An02g13580; An04g04670; An08g09030; An09g06400; An11g01160; An12g02920; An12g05330; An15g00840; An19g00100	170148; 197446; N/A; 196559; 129219; 190616; 38015; 119587; 127214; 189361; N/A; 40367; 122923
	r216	:	CHIT + H2O ⇒ NAG	3.2.1.52	N-Acetyl-beta-glucosaminidase	Gomez et al. (1977); Pera et al. (1997); Jones and Kosman (1980)	ANID	An01g01920; An09g02240	36363; 121359 and 54398
	r217	:	NAG + H2O ⇒ GLCN + AC	3.5.1.33	N-acetylglucosamine deacetylase		ANID	An11g00920; An18g04560	199058; 126860
	r218	:	ATP + GLCN ⇒ ADP + GA6P	2.7.1.1	Hexokinase (hxk)	Panneman et al. (1998)	ANID	An02g14380; An06g00380; An13g00510	55651; 134301; 50817
	r219	:	CHIT + H2O ⇒ CHITO + AC	3.5.1.41	Chitin deacetylase		ANID	An04g07110; An02g13530; An12g04480	45285; 173767; 186040
Galactosaminogalactan									
	r220	:	UDPNAG ⇆ UDPNAGAL	5.1.3.7	UDP-N-acetylglucosamine 4-epimerase	Bardalaye and Nordin (1976, Inferred)	ANEW		
	r221	:	0.754 UDPGAL + 0.181 UDPNAGAL + 0.065 UDPG ⇒ GAG + UDP	No EC	Lumped reaction for biosynthesis of galactosaminogalactan	Bardalaye and Nordin (1976, Inferred)	ANEW		
Galactoglucomannan									
	r222	:	0.435 UDPGAL + 0.435 GDPMAN + 0.13 UDPG ⇒ GGM + 0.565 UDP + 0.435 GDP	No EC	Lumped reaction for biosynthesis of galactoglucomannan	Bardalaye and Nordin (1977, Inferred)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
ENERGY METABOLISM									
r235	:	NADHm + Qm ⇒ QH2m + NADm	1.6.5.3	NADH-ubiquinone oxidoreductase (nad5, nuo51, nd4L)	Promper et al. (1993); Juhász et al. (2004)	ANIG, ANID	*	An02g05470; An02g05880; An02g09730; An02g11200; An04g00060; An04g00110; An04g05640; An06g01390; An07g04180; An08g04240; An08g04910; An08g10690; An09g06850; An11g06200; An11g08840; An11g09350; An11g09390; An12g04780; An12g07520; An14g00060	206795; 55562; 174046; 207272; 54674; 213396; 55011; 37834; 209689; 208150; 52695; 207707; 56863; 208884; 143222; 208985; 199481; 56704; 201966; 201294
r236	:	PPI + H2O ⇒ 2 PI	3.6.1.1	Inorganic diphosphatase	Pathak and Sreenivasan (1955); Rama and Shanmugasundaram (1985)	ANIG, ANID		An02g12010	207331
r237	:	PPIm + H2O ⇒ 2 PIm	3.6.1.1	Inorganic diphosphatase	David et al. (2003)	ANIG, ANID		An02g12010	207331
r238	:	QH2m + 0.5 O2m ⇒ Qm + H2Om	UBIOX	Ubiquinol oxidase (mitochondrial alternative oxidase (aox))	Kirimura et al. (1999, 2006)	ANIG		An11g04810	47967
r239	:	NADHm + Qm + 4 H+$_P$Om ⇒ NADm + QH2m + 4 H+$_P$O	1.6.5.3	Respiratory-chain NADH dehydrogenase (nad5, nuo51, nd4L)	Promper et al. (1993); Juhász et al. (2004)	ANIG, ANID	*	An02g05470; An02g05880; An02g09730; An02g11200; An04g00060; An04g00110; An04g05640; An06g01390; An07g04180; An08g04240; An08g04910; An08g10690; An09g06850; An11g06200; An11g08840; An11g09350; An11g09390; An12g04780; An12g07520; An14g00060	206795; 55562; 174046; 207272; 54674; 213396; 55011; 37834; 209689; 208150; 52695; 207707; 56863; 208884; 143222; 208985; 199481; 56704; 201966; 201294

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r240	:	NADH + Qm + 4 H+$_P$Om ⇒ NAD + QH2m + 4 H+$_P$O	1.6.5.3	Proton pumping Mitochondrial NADH dehydrogenase that catalyzes the oxidation of cytosolic NADH	Promper et al. (1993)	ANEW	*	An02g05470; An02g05880; An02g09730; An02g11200; An04g00060; An04g00110; An04g05640; An06g01390; An07g04180; An08g04240; An08g04910; An08g10690; An09g06850; An11g06200; An11g08840; An11g09350; An11g09390; An12g04780; An12g07520; An14g00060	206795; 55562; 174046; 207272; 54674; 213396; 55011; 37834; 209689; 208150; 52695; 207707; 56863; 208884; 143222; 208985; 199481; 56704; 201966; 201294
r241	:	NADH + Qm ⇒ QH2m + NAD	1.6.5.3	NADH-ubiquinone oxidoreductase (nad5, nuo51, nd4L)	Promper et al. (1993); Juhász et al. (2004)	ANIG, ANID	*	An02g05470; An02g05880; An02g09730; An02g11200; An04g00060; An04g00110; An04g05640; An06g01390; An07g04180; An08g04240; An08g04910; An08g10690; An09g06850; An11g06200; An11g08840; An11g09350; An11g09390; An12g04780; An12g07520; An14g00060	206795; 55562; 174046; 207272; 54674; 213396; 55011; 37834; 209689; 208150; 52695; 207707; 56863; 208884; 143222; 208985; 199481; 56704; 201966; 201294
r242	:	NADPH + 2 FERIm ⇒ NADP + 2 FEROm	1.6.2.4	NADPH-ferrihemoprotein reductase (cprA)	van den Brink et al. (1996)	ANID		An04g06960; An05g00510; An08g07840	54972; 49744; 198350
r243	:	QH2m + 2 FERIm + 4 H+$_P$Om ⇒ Qm + 2 FEROm + 4 H+$_P$O	1.10.2.2	Ubiquinol-cytochrome c reductase	David et al. (2003)	ANIG, ANID	*	An01g12210; An01g06180; An04g05220; An08g06550; An14g04080	205553; 205959; 57369; 177548; 211145

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r244	:	2 FEROm + 0.5 O2m + 4 H+$_P$Om ⇒ 2 FERIm + H2Om + 4 H+$_P$O	1.9.3.1	Cytochrome c oxidase subunit I (cox5)	Kirimura et al. (2000); Juhász et al. (2004)	ANIG, ANID	*	An02g01720; An02g09930; An04g01560; An07g07390; An08g01550; An09g03990; An11g10200; An14g04170	206489; 207204; 213247; 199998; 175806; N/A; 209100; 211156
r245	:	ADPm + PIm + 3.88 H+$_P$O ⇒ ATPm + H2Om + 3.88 H+$_P$Om	3.6.3.14	F1F0-ATPase complex	David et al. (2003), Blair et al. (1996, A. nidulans)	ANIG, ANID	*	An01g04630; An01g04930; An01g10880; An02g04520; An02g06240; An07g06560; An12g00640; An12g04950; An14g04180; An16g07290; An16g07410	36164; 206061; 196131; 206734; N/A; N/A; 138230; 128507; 211159; 214565; 204982
r246	:	ATPm + H2Om + 3.88 H+$_P$Om ⇒ ADPm + PIm + 3.88 H+$_P$O	3.6.3.6	Mitochondrial membrane ATPase 1	Jernejc and Legisa (2001)	ANID		An12g08760	201858
r257	:	ATP + H2O + 3.88 H+ ⇒ ADP + PI + 3.88 H+e	3.6.3.6	Plasma membrane ATPase 1		ANEW		An01g05670	171582
r247	:	ATP + H2O + H+ + Ke ⇒ ADP + PI + H+e + K	3.6.3.10	Potassium-transporting ATPase		ANID		An02g06350; An02g09470; An02g09480; An08g03090; An12g04500; An17g02310; An19g00350	55567; 207175; 207175; 38450; 54015; 214148; 138839
r248	:	ATP + H2O + H+ + Cae ⇒ ADP + PI + H+e + Ca	3.6.3.8	Calcium-transporting ATPase		ANID		An02g06350; An02g09470; An02g09480; An08g03090; An12g04500; An17g02310; An19g00350	55567; 207175; 207175; 38450; 54015; 214148; 138839
r249	:	2 FERIm + LLACm ⇒ PYRm + 2 FEROm	1.1.2.3	Lactic acid dehydrogenase		ANID		An04g02840; An04g08560; An11g03500; An12g06530; An14g02250	213113; 45912; 140694; 186062; 211015
r250	:	2 FERIm + LACm ⇒ PYRm + 2 FEROm	1.1.2.4	Mitochondrial enzyme D-lactate ferricytochrome c oxidoreductase		ANID		An02g10670; An12g06290	47113; 186792
r251	:	ADP + PI + ATPm + H2Om + H+$_P$O ⇒ ADPm + PIm + ATP + H2O + H+$_P$Om	MCF	ADP/ATP translocase	David et al. (2003)	ANIG, ANID		An18g04220	212044
r252	:	NADPH + O2 ⇒ NADP + H2O2	1.6.3.1	NADPH oxidase		ANID		An08g10000	52585
r253	:	NADPH + Qm ⇒ QH2m + NADP	1.6.99.1	NADPH dehydrogenase (quinone) (NADPH oxidase)	David et al. (2003)	ANIG, ANID		An11g08510	39329

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r254	:	FADH2m + Qm ⇒ FADm + QH2m	1.5.5.1	Electron-transferring-flavoprotein dehydrogenase		ANID	An16g03910	210584
Oxygen metabolism								
r255	:	2 H2O2 ⇒ 2 H2O + O2	1.11.1.6	Catalase (catR)	Horie et al. (1976); Gruft et al. (1978); Kikuchi-Torii et al. (1982); Witteveen et al. (1992); Fowler et al. (1993); Fiedurek (2000); Martinelli and Kinghorn (1994)	ANIG, ANID	An01g01820; An03g05660; An01g01550	206342; 213578; 55494
r256	:	2 H2O2e ⇒ 2 H2Oe + O2e	1.11.1.6	Catalase (catR)	Martinelli and Kinghorn (1994); Witteveen et al. (1992); Rogalski et al. (1998)	ANIG, ANID	An03g05660; An01g01550	213578; 55494
AMINO ACID METABOLISM								
Alanine, aspartate and asparagine biosynthesis					Kanehisa et al. (2002)			
r258	:	OA + GLU ⇆ ASP + AKG	2.6.1.1	Aspartate transaminase	Patil and Ramakrishnan (1966); Alvarez-Vasquez et al. (2000)	ANID	An03g00050; An03g01120; An04g05130; An09g02390; An12g07870; An16g05570	141281; 45764; 214397; 50187; 186098; 56390
r263	:	ASP + ATP + GLN + H2O ⇒ GLU + ASN + AMP + PPI	6.3.5.4	Asparagine synthase		ANID	An01g07910; An04g01340; An12g07660	131513; 57091; 186429
r259	:	PYR + GLU ⇆ AKG + ALA	2.6.1.2	Alanine transaminase	Patil and Ramakrishnan (1966)	ANID	An11g02620	208695
r261	:	PYR + NH3 + NADPH ⇒ ALA + H2O + NADP	1.4.1.1	Alanine dehydrogenase (NADPH)	Hoshino et al. (1962); Savov et al. (1986)	ANEW		
r262	:	PYR + NH3 + NADH ⇒ ALA + H2O + NAD	1.4.1.1	Alanine dehydrogenase (NADH)	Savov et al. (1986)	ANEW		
r259m	:	PYRm + GLUm ⇆ AKGm + ALAm	2.6.1.2	Alanine transaminase	Alvarez-Vasquez et al. (2000)	ANID	An11g02620	208695
r258m	:	OAm + GLUm ⇆ ASPm + AKGm	2.6.1.1	Aspartate transaminase	Patil and Ramakrishnan (1966); Alvarez-Vasquez et al. (2000)	ANID	An04g06380	214270
Aspartate degradation								
r265	:	ASP + H2O + O2 ⇒ OA + NH3 + H2O2	1.4.3.2	L-amino acid oxidase	Oganesyan et al. (1998)	ANEW	An08g10800	176790
Asparagine degradation								
r266	:	ASN + H2O ⇒ ASP + NH3	3.5.1.1	Asparaginase	Wriston, Jr. and Yelling (1973)	ANID	An01g14960; An18g03190	51685; 187609
Arginine metabolism					Kanehisa et al. (2002)			
r267	:	ORN + AKG ⇒ GLUGSAL + GLU	2.6.1.13	Ornithine transaminase		ANEW	An04g04130; An11g08870	54525; 48081
r271	:	SAM ⇆ DSAM + CO2	4.1.1.50	S-adenosylmethionine decarboxylase		ANID	An09g06050	54311

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r274	:	GBAD ⇒ GBAT + NH3	3.5.1.4	Amidase/acetamidase		ANID	An16g07500; An01g12500; An02g00190; An02g00340; An03g05880; An07g00100; An07g03960; An09g01020; An09g04990; An11g02980; An11g08900; An12g01020; An14g00670; An15g00290	194059; 35556; 36604; 121987; 191243; 181662; 40014; 121710; 188491; 38912; 48084; 54468; 210891; 181881
r275	:	ARG + H2O ⇒ ORN + UREA	3.5.3.1	Arginase (argA)	Kiesel (1922); Sukhenko and Podgainaya (1959)	ANID	An02g07250	55582
Urea cycle								
r268m	:	CITRm + ASPm + ATPm ⇆ AMPm + PPIm + ARGSUCCm	6.3.4.5	Argininosuccinate synthase		ANID	An12g01280; An15g02340	43683; 40489
r269m	:	ARGSUCCm ⇆ FUMm + ARGm	4.3.2.1	Argininosuccinate lyase		ANID	An01g06560	51912
r275m	:	ARGm + H2Om ⇒ ORNm + UREAm	3.5.3.1	Arginase	Kiesel (1922); Sukhenko and Podgainaya (1959)	ANID	An14g01190	41557
r282m	:	ORNm + CAPm ⇒ CITRm + PIm	2.1.3.3	Ornithine carbamoyltransferase (argB)	Buxton et al. (1987); Swart et al. (1992); Lenouvel et al. (2002)	ANID	An14g03400	N/A
Ornithine cycle								
r277	:	GLUm + ACCOAm ⇒ COAm + NAGLUm	2.3.1.1	Amino-acid N-acetyltransferase		ANID	An03g02930	194534
r278	:	NAGLUm + ATPm ⇒ ADPm + NAGLUPm	2.7.2.8	Acetylglutamate kinase		ANID	An03g01910	194591
r279	:	NAGLUPm + NADPHm ⇒ NADPm + PIm + NAGLUSm	1.2.1.38	N-Acetyl-gamma-glutamyl-phosphate reductase (EC 1.2.1.38) and acetylglutamate kinase (EC 2.7.2.8)		ANID	An12g07580	211485
r280	:	NAGLUSm + GLUm ⇒ AKGm + NAORNm	2.6.1.11	Acetylornithine aminotransferase		ANID	An15g02360	35307
r281	:	NAORNm + GLUm ⇒ ORNm + NAGLUm	2.3.1.35	Glutamate N-acetyltransferase		ANID	An03g04330	50689
Cysteine biosynthesis								
r283	:	SER + ACCOA ⇒ COA + ASER	2.3.1.30	Serine transacetylase/serine O-acetyltransferase	Stepien et al. (1975); Sieńko and Paszewski (1999, A. nidulans)	ANID	An09g02800	212646 and 54391
r284	:	ASER + H2S ⇒ AC + CYS	2.5.1.47	Cysteine synthase (cysB) (O-acetylserine sulfhydrylase)	Pieniazek et al. (1973); Stepien et al. (1975); Topczewski et al. (1997, A. nidulans)	ANID	An02g10750; An12g09880; An14g00960; An15g05170; An16g07520	207249; N/A; 184767; 181861; 193596
Cysteine degradation								
r285	:	2 CYS + O2 ⇒ CYST + H2O2	1.8.3.3	Sulfhydryl oxidase (Sox)	Vignaud et al. (2002)	ANEW	An09g05940; An16g02470	189206; 183599
r286	:	2 CYS + NAD ⇒ CYST + NADH	1.8.1.6	Cystine reductase	Kasatkina and Zheltova (1963)	ANEW		
Glutamate and glutamine metabolism								

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r289	:	GLU + H2O + NAD ⇒ AKG + NH3 + NADH	1.4.1.2	Glutamate dehydrogenase	Patil and Ramakrishnan (1966); Punekar et al. (1985); Savov et al. (1986)	ANID	An02g14590	37620
r290	:	AKG + NH3 + NADPH ⇒ GLU + H2O + NADP	1.4.1.4	Glutamate dehydrogenase (gdhA)	Punekar et al. (1985); Savov et al. (1986); Noor and Punekar (2005)	ANID	An04g00990	203758
r291	:	GLU + NH3 + ATP ⇒ GLN + ADP + PI	6.3.1.2	Glutamate-ammonia ligase	Kim (1981); Punekar et al. (1985); Savov et al. (1986)	ANID	An14g01460; An15g01850	49256; 48679
r292	:	GLN ⇒ GLU + NH3	3.5.1.2	Glutaminase A	Shi et al. (1996)	ANID	An02g06720; An11g07960	197415; 208953
r287	:	AKG + GLN + NADPH ⇒ NADP + 2 GLU	1.4.1.14	Glutamate synthase (NADPH)	Savov et al. (1986)	ANEW	An01g08800	196278
r288	:	AKG + GLN + NADH ⇒ NAD + 2 GLU	1.4.1.13	Glutamate synthase (NADH)	Savov et al. (1986)	ANEW	An07g09920	209263
r293	:	GLUGSALm + NADPm + 2 H2Om ⇒ NADPHm + GLUm	1.5.1.12	Delta-1-pyrroline-5-carboxylate dehydrogenase		ANID	An02g02290; An11g06140	52149; 208879
r294	:	P5Cm + NADm + 2 H2Om ⇒ NADHm + GLUm	1.5.1.12	Delta-1-pyrroline-5-carboxylate dehydrogenase		ANID	An02g02290; An11g06140	52149; 208879
Serine, glycine and threonine biosynthesis								
r295	:	3PG + NAD ⇒ NADH + PHP	1.1.1.95	Phosphoglycerate dehydrogenase	Pei et al. (2003, A. nidulans)	ANID	An11g01390; An12g01580; An17g02330	38797; 128882; 57311
r296	:	PHP + GLU ⇒ AKG + 3PSER	2.6.1.52	Phosphoserine transaminase		ANID	An02g00890	206447
r297	:	3PSER + H2O ⇒ PI + SER	3.1.3.3	Phosphoserine phosphatase		ANID	An11g09770	179814
r298	:	THF + SER ⇆ GLY + METTHF + H2O	2.1.2.1	Glycine hydroxymethyltransferase/serine hydroxymethyltransferase	Lewandowska et al. (1996, A. nidulans)	ANID	An05g00410; An16g02970	211700; 56462
r301	:	GLY + ACAL ⇒ THR	4.1.2.5	Threonine aldolase		ANID	An15g03260; An03g01360; An03g02300; An07g00680	40551; 194373; 45688; 56260
r311	:	THR + NAD + H2O ⇒ GLY + AC + NADH	1.1.1.103	Threonine dehydrogenase		ANID	An05g02000	189384
r306	:	HSER + ATP ⇒ ADP + PHSER	2.7.1.39	Homoserine kinase		ANID	An17g02090	214104
r307	:	PHSER + H2O ⇒ PI + THR	4.2.3.1	Threonine synthase		ANID	An16g02520	183233
r299	:	GLY + THF + NAD ⇒ METTHF + NADH + CO2 + NH3	2.1.2.10	Aminomethyltransferase (2.1.2.10, 1.4.4.2 and 1.8.1.4 lumped)		ANID	An14g01150; An08g03070	210951; 122951
Homoserine biosynthesis								
r302	:	ASP + ATP ⇒ ADP + BASP	2.7.2.4	Aspartate kinase		ANID	An17g02280	54942
r303	:	BASP + NADPH ⇒ NADP + PI + ASPSA	1.2.1.11	Aspartic beta semialdehyde dehydrogenase, aspartate semialdehyde dehydrogenase		ANID	An11g09510	209010
r304	:	ASPSA + NADH ⇒ NAD + HSER	1.1.1.3	Homoserine dehydrogenase I		ANID	An02g07430	52305
r300	:	ALA + GLX ⇆ PYR + GLY	2.6.1.44	Alanine-glyoxylate transaminase	Oganesyan et al. (2004)	ANID	An09g03830	50140

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r308a	:	GLYm + HPLYSm ⇆ HPSAMLYSm + CO2m	2.1.2.10	Aminomethyltransferase (2.1.2.10, 1.4.4.2 and 1.8.1.4 lumped)		ANEW	An14g01150; An08g03070	210951; 122951
r308b	:	HPSAMLYSm + THFm ⇆ NH3m + METTHFm + DHPLYSm	2.1.2.1	Glycine hydroxymethyltransferase/serine hydroxymethyltransferase		ANEW	An05g00410; An16g02970	211700; 56462
r308c	:	DHPLYSm + NADm ⇆ HPLYSm + NADHm	1.4.4.2	Glycine dehydrogenase (decarboxylating) / glycine decarboxylase complex (P-subunit), glycine synthase (P-subunit), glycine cleavage system (P-subunit)		ANEW	An14g01150	210951
Threonine and serine degradation								
r312	:	SER ⇒ PYR + NH3	4.3.1.17	L-Serine ammonia-lyase		ANID	An04g02220	213166
r313	:	THR ⇒ NH3 + OBUT	4.3.1.19	Threonine dehydratase	MacDonald et al. (1974, A. nidulans)	ANID	An04g02580	190860
r313m	:	THRm ⇒ NH3m + OBUTm	4.3.1.19	Threonine dehydratase		ANID	An04g02580	190860
Histidine biosynthesis								
r316	:	R5P + ATP ⇆ PRPP + AMP	2.7.6.1	Ribose-phosphate pyrophosphokinase	Foley et al. (1965); Nielsen et al. (2004, A. nidulans)	ANID	An02g09240; An04g05860; An07g02210	52363; 204746; 209842
r317	:	PRPP + ATP ⇒ PPI + PRBATP	2.4.2.17	ATP phosphoribosyltransferase	Busch et al. (2001, A. nidulans)	ANID	An13g01080	54800
r318	:	PRBATP + H2O ⇒ PPI + PRBAMP	3.6.1.31	phosphoribosyl-ATP diphosphatase	Berlyn (1967); Busch et al. (2001, A. nidulans)	ANID	An01g12570	205513
r319	:	PRBAMP + H2O ⇒ PRFP	3.5.4.19	phosphoribosyl-AMP cyclohydrolase	Berlyn (1967); Busch et al. (2001, A. nidulans)	ANID	An01g12570	205513
r320	:	PRFP ⇒ PRLP	5.3.1.16	1-(5-phosphoribosyl)-5-[(5-phosphoribosylamino)methyl 4-carboxamide isomerase	Busch et al. (2001, A. nidulans)	ANID	An17g01640	51056
r321	:	PRLP + GLN ⇒ GLU + AICAR + DIMGP	2.4.2.-	Glutamine amidotransferase:cyclase/imidazole glycerol phosphate synthase	Valerius et al. (2001, A. nidulans)	ANID	An02g14890	198031
r322	:	DIMGP ⇒ IMACP + H2O	4.2.1.19	Imidazoleglycerol-phosphate dehydratase	Berlyn (1967); Busch et al. (2001, A. nidulans)	ANID	An15g00610	200493
r323	:	IMACP + GLU ⇒ AKG + HISOLP	2.6.1.9	Histidinol-phosphate aminotransferase	Pain et al. (2004, A. fumigatus)	ANID	An01g11930	171507
r324	:	HISOLP + H2O ⇒ PI + HISOL	3.1.3.15	Histidinol phosphatase		ANID	An14g00840	56528
r325	:	HISOL + 2 NAD + H2O ⇒ HIS + 2 NADH	1.1.1.23	Histidinol dehydrogenase	Berlyn (1967); Creaser and Varela-Torres (1971, A. nidulans)	ANID	An14g07210	56640
Histidine degradation								
r326	:	HIS ⇒ HISN + CO2	4.1.1.22	histidine decarboxylase	Tanaka et al. (1977)	ANEW		
r327	:	ACCOA + HISN ⇆ COA + NAHISN	No EC	histamine N-acetyltransferase	Tanaka et al. (1977)	ANEW		
Valine and leucine biosynthesis								
r328	:	2 PYRm ⇒ CO2m + ACLACm	2.2.1.6	Acetolactate synthase		ANID	An01g09250; An03g00480; An16g01310; An16g04170	35805; 51385; 139646; 210558

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r329	:	ACLACm + NADPHm ⇒ NADPm + DHVALm	1.1.1.86	Ketol-acid reductoisomerase		ANID	An09g03940	212581
r330	:	DHVALm ⇒ OIVALm + H2Om	4.2.1.9	Dihydroxy acid dehydratase		ANID	An07g09870; An11g09270; An15g06700; An18g02550; An18g04160	181283; 179001; 53523; 42733; 54174
r331	:	OIVALm + GLUm ⇆ AKGm + VALm	2.6.1.42	Branched chain amino acid aminotransferase		ANEW	An12g02890; An02g06150; An04g00430; An09g01990	43811; 197362; 190990; 124698
r337	:	OIVALm + ACCOAm + H2Om ⇒ COAm + IPPMALm	2.3.3.13	Alpha-isopropylmalate synthase (2-isopropylmalate synthase)		ANID	An01g13160; An09g00170	205459; 203189
r338	:	IPPMALm + NADm ⇒ NADHm + OICAPm + CO2m	1.1.1.85	Beta-IPM (isopropylmalate) dehydrogenase (leu2A and leu2B)	Williams et al. (1996); Kohlhaw (2003)	ANID	An04g10130; An01g14130	205291; 205395
r339	:	OICAPm + GLUm ⇆ AKGm + LEUm	2.6.1.42	Branched chain amino acid aminotransferase		ANID	An12g02890; An02g06150; An04g00430; An09g01990	43811; 197362; 190990; 124698
r339m	:	OICAP + GLU ⇆ AKG + LEU	2.6.1.42	Branched chain amino acid aminotransferase		ANID	An12g02890; An02g06150; An04g00430; An09g01990	43811; 197362; 190990; 124698
Isoleucine biosynthesis								
r332	:	OBUTm + PYRm ⇒ ABUTm + CO2m	2.2.1.6	Acetolactate synthase		ANID	An01g09250; An03g00480; An16g01310; An16g04170	35805; 51385; 139646; 210558
r333	:	ABUTm + NADPHm ⇒ NADPm + DHMVAm	1.1.1.86	Ketol-acid reductoisomerase		ANID	An09g03940	212581
r334	:	DHMVAm ⇒ OMVALm + H2Om	4.2.1.9	Dihydroxy acid dehydratase		ANID	An07g09870; An11g09270; An15g06700; An18g02550; An18g04160	181283; 179001; 53523; 42733; 54174
r335	:	OMVALm + GLUm ⇆ AKGm + ILEm	2.6.1.42	Branched chain amino acid aminotransferase		ANID	An12g02890; An02g06150; An04g00430; An09g01990	43811; 197362; 190990; 124698
r335m	:	OMVAL + GLU ⇆ AKG + ILE	2.6.1.42	Branched chain amino acid aminotransferase		ANID	An12g02890; An02g06150; An04g00430; An09g01990	43811; 197362; 190990; 124698
Lysine biosynthesis					Garrad and Bhattacharjee (1992, Fungi)			
r341	:	ACCOAm + H2Om + AKGm ⇒ HCITm + COAm	2.3.3.14	Homocitrate synthase	Garrad and Bhattacharjee (1992, A. fumigatus)	ANID	An04g06210	54991
r351	:	HCITm ⇆ HACNm + H2Om	4.2.1.79	2-methylcitrate dehydratase	Weidner et al. (1997, A. nidulans)	ANID	An15g01780	53423

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r352	:	HACNm + H2Om ⇆ HICITm	4.2.1.36	Homoaconitate hydratase	Weidner et al. (1997); Zabriskie and Jackson (2000, A. nidulans)	ANID	An15g00350	56275
r353	:	HICITm + NADm ⇆ OXAm + CO2m + NADHm	1.1.1.87	Homoisocitrate dehydrogenase	Garrad and Bhattacharjee (1992, A. fumigatus), Zabriskie and Jackson (2000); Weidner et al. (1997, A. nidulans)	ANID		
NE3	:	OXAm ⇆ CO2m + AKAm	Non enzymatic step	Non enzymatic reaction		ANID		
r346	:	AKAm + GLUm ⇆ AMAm + AKGm	2.6.1.39	2-aminoadipate transaminase	Garrad and Bhattacharjee (1992, A. fumigatus), Weidner et al. (1997); Zabriskie and Jackson (2000, A. nidulans)	ANID		
r347	:	AMAm + NADPHm ⇒ AMASAm + NADPm + H2Om	1.2.1.31	L-aminoadipate-semialdehyde dehydrogenase	Garrad and Bhattacharjee (1992, A. fumigatus), Zabriskie and Jackson (2000, A. nidulans)	ANID	An04g05420; An11g04250; An12g10090; An11g05500	55018; 129526; 194895; 39114
r348	:	AMAm + NADHm ⇒ AMASAm + NADm + H2Om	1.2.1.31	L-aminoadipate-semialdehyde dehydrogenase	Garrad and Bhattacharjee (1992, A. fumigatus), Zabriskie and Jackson (2000, A. nidulans)	ANID	An04g05420; An11g04250; An12g10090; An11g05500	55018; 129526; 194895; 39114
r349	:	GLUm + AMASAm + NADPHm ⇆ SACPm + NADPm + H2Om	1.5.1.10	Saccharopine dehydrogenase (NADP+, L-glutamate forming)	Garrad and Bhattacharjee (1992, A. fumigatus), Zabriskie and Jackson (2000, A. nidulans)	ANID	An01g13590; An04g05260	35485; 214383
r350	:	SACPm + NADm + H2Om ⇆ LYSm + AKGm + NADHm	1.5.1.7	Saccharopine dehydrogenase (NAD+, L-lysine forming)	Garrad and Bhattacharjee (1992, A. fumigatus), Zabriskie and Jackson (2000, A. nidulans)	ANID	An02g07500	207003
Methionine metabolism								
r354	:	SAM + HCYS ⇒ SAH + MET	2.1.1.10	Homocysteine S-methyltransferase	Stepien et al. (1975, A. nidulans)	ANID	An15g07110	210376
r355	:	ACCOA + HSER ⇆ COA + OAHSER	2.3.1.31	homoserine O-acetyltransferase	Stepien et al. (1975); Sieńko and Paszewski (1999); Grynberg et al. (2001, A. nidulans)	ANID	An17g00630	213962
r356	:	OAHSER + CYS ⇆ LLCT + AC	2.5.1.48	Cystathionine gamma-synthase	Paszewski and Grabski (1975); Stepien et al. (1975); Sieńko and Paszewski (1999, A. nidulans)	ANEW	An12g01110	128744
r357	:	OAHSER + METH ⇆ MET + AC	2.5.1.49	O-acetylhomoserine (thiol)-lyase		ANID	An09g06710	54281
r358	:	OAHSER + H2S ⇒ AC + HCYS	2.5.1.47	Cysteine synthase (O-acetylhomoserine sulfhydrylase)	Pieniazek et al. (1974); Paszewski and Grabski (1975); Stepien et al. (1975); Sieńko and Paszewski (1999, A. nidulans)	ANID	An02g10750; An12g09880; An14g00960; An15g05170; An16g07520	207249; N/A; 184767; 181861; 193596
r359	:	HCYS + SER ⇒ LLCT + H2O	4.2.1.22	Cystathionine beta-synthase	Pieniazek et al. (1974); Paszewski and Grabski (1975); Stepien et al. (1975, A. nidulans)	ANEW	An05g00160	49760
r360	:	LLCT ⇒ CYS + NH3 + OBUT	4.4.1.1	Cystathionine gamma-lyase	Pieniazek et al. (1974); Stepien et al. (1975); Sieńko and Paszewski (1999, A. nidulans)	ANID	An04g04720; An16g08720	190884; 194072
r361	:	LLCT + H2O ⇒ HCYS + PYR + NH3	4.4.1.8	Cystathionine-b-lyase	Stepien et al. (1975); Sieńko and Paszewski (1999, A. nidulans)	ANID	An14g00930	201388

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r362	:	HCYS + MTHF ⇒ THF + MET	2.1.1.13	Methionine synthase	Balinska and Paszewski (1979); Paszewski and Grabski (1975, A. nidulans)	ANID		An04g01750	203669
r363	:	MET + ATP + H2O ⇒ PPI + PI + SAM	2.5.1.6	S-adenosylmethionine synthetase	Martinelli and Kinghorn (1994, A. nidulans)	ANID	*	An02g10660; An08g02700	175387; 208283
r364	:	SAM + CALH ⇒ SAH + DPTH	2.1.1.98	Diphthine synthase	Martinelli and Kinghorn (1994, A. nidulans), Pain et al. (2004, A. fumigatus)	ANID		An08g07220	47429
r365	:	SAH + H2O ⇒ HCYS + ADN	3.3.1.1	Adenosylhomocysteinase (S-adenosyl-l-homocysteine hydrolase)	David et al. (2003), Sieńko and Paszewski (1999, A. nidulans)	ANIG, ANID		An08g01960	208343
Phenylalanine, tyrosine and tryptophan biosynthesis (aromatic amino acids)									
r367	:	E4P + PEP + H2O ⇒ PI + 3DDAH7P	2.5.1.54	3-deoxy-7-phosphoheptulonate synthase	Hartmann et al. (2001, A. nidulans)	ANID		An01g06150	196476
r368	:	3DDAH7P ⇒ DQT + PI	4.2.3.4	Pentafunctional arom polypeptide (contains: 3-dehydroquinate synthase, 3-dehydroquinate dehydratase (3-dehydroquinase), shikimate 5-dehydrogenase, shikimate kinase, and EPSP synthase)	Hawkins (1987); Nichols et al. (2004, A. nidulans)	ANID		An08g06800; An08g06810	207929; 207929
r369	:	DQT ⇒ DHSK + H2O	4.2.1.10	Catabolic 3-dehydroquinase (3-dehydroquinate dehydratase)	Cain (1972a)	ANID		An08g06800; An08g06810	207929; 207929
r370	:	QT + NAD ⇆ DQT + NADH	1.1.1.24	Quinate 5-dehydrogenase	Cain (1972a)	ANID		An03g03710; An04g08100	44404; 51457
r371	:	DHSK + NADH ⇒ SME + NAD	1.1.1.24	Quinate 5-dehydrogenase	Cain (1972a)	ANEW		An03g03710; An04g08100	44404; 51457
r372	:	DHSK + NADPH ⇒ SME + NADP	1.1.1.25	dehydroshikimate dehydrogenase	Cain (1972a)	ANID		An08g06800; An08g06810	207929; 207929
r373	:	SME + ATP ⇒ ADP + SME3P	2.7.1.71	Shikimate kinase I, II	Hawkins (1987, A. nidulans)	ANID		An08g06800; An08g06810	207929; 207929
r374	:	SME3P + PEP ⇒ 3PSME + PI	2.5.1.19	3-phosphoshikimate-1-carboxyvinyltransferase	Hawkins (1987, A. nidulans)	ANID		An08g06800; An08g06810	207929; 207929
r375	:	3PSME ⇒ PI + CHOR	4.2.3.5	Chorismate synthase	Martinelli and Kinghorn (1994, A. nidulans)	ANID			
r376	:	CHOR ⇒ PHEN	5.4.99.5	Chorismate mutase	Yelton et al. (1983); Krappmann et al. (1999, A. nidulans)	ANID		An14g06010	41927
r377	:	PHEN ⇒ CO2 + H2O + PHPYR	4.2.1.51	Prephenate dehydratase		ANID		An17g02200	54937
r378	:	PHPYR + GLU ⇆ AKG + PHE	2.6.1.1	Phenylalanine:alpha-ketoglutarate aminotransferase	Alvarez-Vasquez et al. (2000)	ANID		An03g00050; An03g01120; An04g05130; An04g06380; An09g02390; An12g07870; An16g05570	141281; 45764; 214397; 214270; 50187; 186098; 56390
r379	:	PHEN + NADP ⇒ 4HPP + CO2 + NADPH	1.3.1.13	Prephenate dehydrogenase (NADP+)		ANID		An02g06120	46999

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r380	:	4HPP + GLU ⇆ AKG + TYR	2.6.1.1	Aspartate transaminase	Alvarez-Vasquez et al. (2000)	ANID	An03g00050; An03g01120; An04g05130; An04g06380; An09g02390; An12g07870; An16g05570	141281; 45764; 214397; 214270; 50187; 186098; 56390
r381	:	CHOR + GLN ⇒ GLU + PYR + AN	4.1.3.27	Anthranilate synthase (trpC)	Kos et al. (1985); Horng et al. (1989); Adams and Royer (1990)	ANID	An08g06080	52668
r382	:	AN + PRPP ⇒ PPI + NPRAN	2.4.2.18	Anthranilate phosphoribosyl transferase		ANID	An01g07260	51886
r383	:	NPRAN ⇒ CPAD5P	5.3.1.24	N-(5'-phosphoribosyl)-anthranilate isomerase (trpC)	Kos et al. (1985); Horng et al. (1989); Adams and Royer (1990)	ANID	An08g06080	52668
r384	:	CPAD5P ⇒ CO2 + IGP + H2O	4.1.1.48	Indoleglycerol phosphate synthase (trpC)	Kos et al. (1985); Horng et al. (1989); Adams and Royer (1990)	ANID	An08g06080	52668
r385	:	IGP + SER ⇒ T3P1 + TRP + H2O	4.2.1.20	Tryptophan synthetase		ANID	An02g02170; An12g03230; An16g02500	52146; 43841; 183278
Proline biosynthesis								
r412	:	GLU + NADH ⇒ NAD + GLUGSAL + 2 H2O	1.5.1.12	1-pyrroline-5-carboxylate dehydrogenase	Jones et al. (1981); Hull et al. (1989, A. nidulans)	ANEW	An02g02290; An07g05000; An11g06140	52149; 181275; 208879
NE4	:	GLUGSAL ⇆ P5C + H2O	Non enzymatic step	Non enzymatic reaction		ANID		
r413	:	P5C + NADPH ⇆ PRO + NADP	1.5.1.2	Pyrroline-5-carboxylate reductase	Jones et al. (1981); Hull et al. (1989, A. nidulans)	ANID	An07g05050; An01g01520; An04g02800	136532; 36398; 57044
r414	:	GLU + ATP ⇒ ADP + GLUP	2.7.2.11	Gamma-glutamyl kinase, glutamate kinase		ANID	An05g00120	124391
r415	:	PROm + NADm ⇒ P5Cm + NADHm	1.5.99.8	Proline dehydrogenase		ANID	An01g01530; An11g06160	132598; 179947
NE5	:	GLUGSALm ⇆ P5Cm	Non enzymatic step	Non enzymatic reaction		ANID		
Proline degradation								
r416	:	P5C + NAD + 2 H2O ⇒ GLU + NADH	1.5.1.12	1-pyrroline-5-carboxylate dehydrogenase	Jones et al. (1981); Hull et al. (1989, A. nidulans)	ANEW	An02g02290; An07g05000; An11g06140	52149; 181275; 208879
METABOLISM OF OTHER AMINO ACIDS						ANID		
Beta-alanine biosynthesis					Kanehisa et al. (2002); Jerebzoff and Jerebzoff-Quintin (1971)			
r417	:	ASP ⇒ CO2 + bALA	4.1.1.11	Aspartate alpha-decarboxylase		ANID		
Cyanoamino acid metabolism								

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r418	:	APROP ⇒ ALA + NH3	3.5.5.1	Nitrilase	Snajdrova et al. (2004)	ANID	An16g00550; An01g07510; An01g12090; An06g01960; An08g08940; An08g10150; An12g01260; An16g06210; An18g01740	41410; 35944; 170270; 175987; N/A; 52578; 141873; 40928; 211815
r419	:	ACYBUT ⇒ GLU + NH3	3.5.5.1	Nitrilase	Snajdrova et al. (2004)	ANID	An16g00550; An01g07510; An01g12090; An06g01960; An08g08940; An08g10150; An12g01260; An16g06210; An18g01740	41410; 35944; 170270; 175987; N/A; 52578; 141873; 40928; 211815
Glutathione biosynthesis								
r420	:	CYS + GLU + ATP ⇒ GC + PI + ADP	6.3.2.2	Gamma-glutamylcysteine synthetase		ANID	An08g01270	38585
r421	:	GLY + GC + ATP ⇒ RGT + PI + ADP	6.3.2.3	Glutathione synthetase	Murata et al. (1989)	ANID	An01g13620; An09g03030	170255; 50166
r422	:	OGT + O2 ⇒ RGT + H2O2	1.11.1.9	Glutathione peroxidase	Vignaud et al. (2002); Kuzniak et al. (2006)	ANID	An02g02750	206591
r423	:	NADPH + OGT ⇒ NADP + RGT	1.8.1.7	glutathione-disulfide reductase		ANID	An03g03660	213429
NUCLEOTIDE METABOLISM						ANID		
Purine Biosynthesis (ATP, dATP, IMP, XMP, GTP, dGTP)					Foley et al. (1965, A. nidulans)			
r424	:	PRPP + GLN + H2O ⇒ PPI + GLU + PRAM	2.4.2.14	Phosphoribosylpyrophospha amidotransferase/amidophosphoribosyltransferase	Foley et al. (1965, A. nidulans)	ANID	An15g01760	129349
r425	:	PRAM + ATP + GLY ⇆ ADP + PI + GAR	6.3.4.13	Glycinamide ribotide synthetase and aminoimidazole ribotide synthetase/phosphoribosylamine-glycine ligase	Foley et al. (1965, A. nidulans)	ANID	An15g00570	53390
r426	:	GAR + FTHF ⇒ THF + FGAR	2.1.2.2	Phosphoribosylglycinamide formyltransferase	Foley et al. (1965, A. nidulans)	ANID	An02g02700	36764
r427	:	FGAR + ATP + GLN + H2O ⇒ GLU + ADP + PI + FGAM	6.3.5.3	5'-phosphoribosylformylglycinamidine synthetase	Foley et al. (1965, A. nidulans)	ANID	An02g09960	37283
r428	:	FGAM + ATP ⇒ ADP + PI + AIR	6.3.3.1	Phosphoribosylformylglycinamide cyclo-ligase	Foley et al. (1965, A. nidulans)	ANID	An15g00570	53390
r429	:	AIR + CO2 ⇆ CAIR	4.1.1.21	Phosphoribosylaminoimidazole carboxylase (Ade2 homolog)	Jin et al. (2004, A. oryzae)	ANID	An01g08090	55358
r430	:	CAIR + ATP + ASP ⇒ ADP + PI + SAICAR	6.3.2.6	Phosphoribosyl amino imidazolesuccinocarbozamide synthetase (Ade1 homolog)	Jin et al. (2004, A. oryzae)	ANID	An11g10150	48145

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r431	:	SAICAR ⇆ FUM + AICAR	4.3.2.2	5'-phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole lyase	Jin et al. (2004, A. oryzae)	ANID		An02g04020	206692
r432	:	AICAR + FTHF ⇆ THF + PRFICA	2.1.2.3	5-aminoimidazole-4-carboxamide ribonucleotide (AICAR) transformylase / IMP cyclohydrolase	Jin et al. (2004, A. oryzae)	ANID		An04g02060	57068
r433	:	PRFICA ⇆ IMP + H2O	3.5.4.10	5-aminoimidazole-4-carboxamide ribonucleotide (AICAR) transformylase / IMP cyclohydrolase	Jin et al. (2004, A. oryzae)	ANID		An04g02060	57068
r434	:	IMP + GTP + ASP ⇒ GDP + PI + ASUC	6.3.4.4	Adenylosuccinate synthetase	Foley et al. (1965); Ribard et al. (2001, A. nidulans)	ANID		An01g13920	51711
r435	:	ASUC ⇒ FUM + AMP	4.3.2.2	5'-phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole lyase	Foley et al. (1965); Ribard et al. (2001, A. nidulans)	ANID		An02g04020	206692
r436	:	ATP + AMP ⇆ 2 ADP	2.7.4.3	Adenylate kinase	Perl (1982)	ANIG, ANID		An01g04710; An07g10100	46678; 56109
r437	:	ADP + RTHIO ⇒ DADP + OTHIO + H2O	1.17.4.1	Ribonucleotide reductase	Hockertz et al. (1987)	ANID	*	An04g01080; An14g06870	57102; 56635
r438	:	DAMP + ATP ⇆ DADP + ADP	2.7.4.11	Adenylate kinase, dAMP kinase		ANID		An01g04710	46678
r439	:	DADP + ATP ⇆ DATP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans)	ANID		An09g05870	212435
r440	:	IMP + NAD ⇒ NADH + XMP	1.1.1.205	Inosine-5'-monophosphate dehydrogenase		ANID		An07g08170	53197
r441	:	XMP + ATP + GLN + H2O ⇒ GLU + AMP + PPI + GMP	6.3.5.2	GMP synthase		ANID		An02g14520	37616
r442	:	GMP + ATP ⇆ GDP + ADP	2.7.4.8	Guanylate kinase		ANID		An01g07070; An08g00300	143052; 130364
r443	:	GDP + ATP ⇆ GTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans), David et al. (2003)	ANIG, ANID		An09g05870	212435
r444	:	GTP + AMP ⇆ ADP + GDP	2.7.4.3	Adenylate kinase	Perl (1982)	ANIG, ANID		An01g04710; An07g10100	46678; 56109
r445	:	GDP + RTHIO ⇒ DGDP + OTHIO + H2O	1.17.4.1	Ribonucleotide reductase	Hockertz et al. (1987)	ANID	*	An04g01080; An14g06870	57102; 56635
r446	:	DGDP + ATP ⇆ DGTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans)	ANID		An09g05870	212435
r447	:	DGDP + ADP ⇆ DGMP + ATP	2.7.4.8	Guanylate kinase		ANID		An01g07070; An08g00300	143052; 130364
r448	:	ITP + AMP ⇆ ADP + IDP	2.7.4.6	Adenylate kinase	Perl (1982)	ANIG, ANID		An09g05870	212435
r449	:	IDP + H2O ⇒ IMP + PI	3.6.1.6	Inosine diphosphatase		ANID			

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
Purine conversions								
r450	:	GMP + DATP ⇆ GDP + DADP	2.7.4.8	Guanylate kinase		ANID	An01g07070; An08g00300	143052; 130364
Purine degradation					Darlington et al. (1965); .Scazzocchio et al. (1982, A. nidulans), Kanehisa et al. (2002); Elzainy et al. (1989)			
r451	:	AMP + H2O ⇒ PI + ADN	3.1.3.5	5'-nucleotidase	Kuwahara and Fujii (1978); Elzainy et al. (1989); Elzainy and Ali (2000); Ali and Elzainy (2000)	ANID	An08g08080	128775
r452	:	AMP + H2O ⇆ AD + R5P	3.2.2.4	AMP nucleosidase	Kuwahara and Fujii (1978)	ANEW		
r453	:	ADN + H2O ⇒ AD + RIB	3.2.2.1	Purine nucleoside hydrolase	Kuwahara and Fujii (1978); Elzainy et al. (1978, 1989)	ANID	An08g03980	55818
r454	:	ADN + H2O ⇒ INS + NH3	3.5.4.4	Adenosine deaminase	Ribard et al. (2003, A. nidulans), Mitschell and McElroy (1946); Grosshans and Wolfenden (1993, A. oryzae), Abu-Shady et al. (1994, A. terricola)	ANID	An12g04800; An16g02890	49658; 183577
r455	:	AD + H2O ⇒ NH3 + HYXN	3.5.4.2	Adenine deaminase	.Scazzocchio et al. (1982); Ribard et al. (2001, A. nidulans)	ANID	An12g04800; An16g02890	49658; 183577
r456	:	DAMP + H2O ⇒ DA + PI	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID	An08g08080	128775
r457	:	DA + PI ⇆ AD + DR1P	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID	An11g06110	178461
r458	:	DA + H2O ⇒ DIN + NH3	3.5.4.4	Adenine deaminase/adenosine deaminase	Ribard et al. (2003, Inferred), Grosshans and Wolfenden (1993, A. oryzae)	ANID	An12g04800; An16g02890	49658; 183577
r459	:	DIN + PI ⇆ HYXN + DR1P	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID	An11g06110	178461
r460	:	IMP + H2O ⇒ PI + INS	3.1.3.5	5'-nucleotidase	Kuwahara and Fujii (1978)	ANID	An08g08080	128775
r461	:	IMP + H2O ⇒ HYXN + R5P	3.2.2.1	purine nucleosidase	Kuwahara and Fujii (1978)	ANEW	An08g03980	55818
r462	:	INS + PI ⇒ HYXN + R1P	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase	Kuwahara and Fujii (1978); Elzainy et al. (1978)	ANID	An11g06110	178461
r463	:	INS + H2O ⇒ HYXN + RIB	3.2.2.1	Purine nucleosidase/purine nucleoside hydrolase	Kuwahara and Fujii (1978); Elzainy et al. (1978)	ANEW	An08g03980	55818
r464	:	HYXN + NAD + H2O ⇆ XAN + NADH	1.17.1.4	Xanthine dehydrogenase	Darlington et al. (1965); .Scazzocchio et al. (1982, A. nidulans)	ANEW	An03g01530	214667
r465	:	GMP + H2O ⇒ PI + GSN	3.1.3.5	5'-nucleotidase	Elzainy et al. (1989); Ali and Elzainy (2000)	ANID	An08g08080	128775
r466	:	GSN + PI ⇆ GN + R5P	3.2.2.1	purine nucleosidase	Kuwahara and Fujii (1978)	ANEW	An08g03980	55818
r467	:	GSN + H2O ⇒ GN + RIB	3.2.2.1	Purine nucleosidase/purine nucleoside hydrolase	Kuwahara and Fujii (1978); Elzainy et al. (1978, 1989)	ANID	An08g03980	55818
r468	:	GN + H2O ⇆ XAN + NH3	3.5.4.3	Guanine aminohydrolase	Darlington et al. (1965, Inferred)	ANEW	An11g01070; An14g01140	38774; 184651

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r469	:	DGMP + H2O ⇒ DG + PI	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID		An08g08080	128775
r470	:	DG + PI ⇆ GN + DR1P	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID		An11g06110	178461
r471	:	XMP + H2O ⇒ PI + XTSINE	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID		An08g08080	128775
r472	:	PI + XTSINE ⇆ XAN + R1P	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID		An11g06110	178461
r473	:	XAN + NAD + H2O ⇆ URIC + NADH	1.17.1.4	Xanthine dehydrogenase (purine hydroxylase I)	Darlington et al. (1965); Arst and Cove (1969); .Scazzocchio et al. (1982, A. nidulans)	ANEW		An03g01530	214667
r474	:	URIC + O2 + H2O ⇆ HIUR + H2O2	1.7.3.3	Uricase	Ertan and Aksoz (2000)	ANEW		An02g06030; An03g02330	55563; 51359
r475	:	HIUR + H2O ⇒ ATN + CO2	3.5.2.17	Hydroxyisourate hydrolase + spontaneous conversion	Darlington et al. (1965, A. nidulans)	ANEW			
r476	:	ATN + H2O ⇆ ATT	3.5.2.5	Allantoinase	Darlington et al. (1965); Arst and Cove (1969); .Scazzocchio et al. (1982, A. nidulans)	ANID		An14g03370	N/A
r477	:	ATT + H2O ⇆ UGC + UREA	3.5.3.4	Allantoicase	Darlington et al. (1965); Arst and Cove (1969); .Scazzocchio et al. (1982, A. nidulans)	ANID		An02g08520	172988
r478	:	UGC + H2O ⇒ GLX + 2 NH3 + CO2	3.5.3.19	Ureidoglycolate hydrolase	Darlington et al. (1965, A. nidulans)	ANID		An16g08100	193909
Pyrimidine biosynthesis (UTP, CTP, dCTP, dUTP and dTTP)					Evans and Guy (2004); Kanehisa et al. (2002)				
r479	:	GLN + 2 ATP + CO2 + 2 H2O ⇒ GLU + CAP + 2 ADP + PI	6.3.5.5	Carbamoyl-phosphate synthetase, aspartate transcarbamylase, and glutamine amidotransferase	Palmer et al. (1975); Aleksenko et al. (1999, A. nidulans)	ANID	*	An16g04960; An16g04970; An17g00820	53574; 53574; 54890
r480	:	CAP + ASP ⇒ CAASP + PI	2.1.3.2	Aspartate-carbamoyltransferase	Palmer et al. (1975, A. nidulans)	ANID		An08g07420	55738
r481	:	CAASP ⇆ DOROA + H2O	3.5.2.3	Dihydroorotase		ANID		An01g10650; An08g07420	205639; 55738
r482	:	DOROA + O2 ⇒ H2O2 + OROA	1.3.3.1	Dihydroorotate dehydrogenase	Gustafson and Waldron (1992, A. nidulans)	ANID		An02g02910	36779
r483	:	OROA + PRPP ⇆ PPI + OMP	2.4.2.10	Orotate phosphoribosyltransferase 1		ANID		An04g08330	55173
r484	:	OMP ⇒ CO2 + UMP	4.1.1.23	Orotidine-5'-phosphate decarboxylase (pyrA)	Goosen et al. (1987)	ANID		An12g03570	56726
r485	:	ADP + UDP ⇆ ATP + UMP	2.7.4.14	Cytidylate kinase		ANID		An13g00440	50815
r486	:	UTP + AMP ⇆ UDP + ADP	2.7.4.3	Adenylate kinase	David et al. (2003)	ANIG		An01g04710; An07g10100	46678; 56109
r487	:	UDP + ATP ⇆ UTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans), David et al. (2003)	ANIG, ANID		An09g05870	212435

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r488	:	UTP + GLN + ATP + H2O ⇒ GLU + CTP + ADP + PI	6.3.4.2	CTP synthase		ANID		An03g01310	57431
r489	:	ATP + UTP + NH3 ⇒ ADP + PI + CTP	6.3.4.2	CTP synthase		ANID		An03g01310	57431
r490	:	CTP + ADP ⇆ CDP + ATP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans), David et al. (2003)	ANIG, ANID		An09g05870	212435
r491	:	CTP + AMP ⇆ CDP + ADP	2.7.4.3	Adenylate kinase	David et al. (2003)	ANIG		An01g04710; An07g10100	46678; 56109
r492	:	ADP + CDP ⇆ CMP + ATP	2.7.4.14	Cytidylate kinase		ANID		An13g00440	50815
r493	:	CDP + RTHIO ⇒ DCDP + OTHIO + H2O	1.17.4.1	Ribonucleotide reductase, small subunit (alt), beta chain	Hockertz et al. (1987)	ANID	*	An04g01080; An14g06870	57102; 56635
r494	:	UDP + RTHIO ⇒ OTHIO + DUDP + H2O	1.17.4.1	Ribonucleotide reductase, small subunit (alt), beta chain	Hockertz et al. (1987)	ANID	*	An04g01080; An14g06870	57102; 56635
r495	:	DUMP + METTHF ⇒ DHF + DTMP	2.1.1.45	Thymidylate synthase		ANID		An14g00570	49219
r496	:	DCDP + ATP ⇆ DCTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans)	ANID		An09g05870	212435
r497	:	DCMP + ATP ⇆ ADP + DCDP	2.7.4.14	Nucleoside-phosphate kinase/ATP:UMP-CMP phosphotransferase/-cytidylate kinase		ANID		An13g00440	50815
r498	:	DUDP + ATP ⇆ DUTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans)	ANID		An09g05870	212435
r499	:	DUMP + ATP ⇆ DUDP + ADP	2.7.4.9	Uridylate kinase		ANID		An09g05840	56895
r500	:	DTMP + ATP ⇆ ADP + DTDP	2.7.4.9	dTMP kinase/thymidylate kinase		ANID		An09g05840	56895
r501	:	DTDP + ATP ⇆ DTTP + ADP	2.7.4.6	Nucleoside-diphosphate kinase	Lin et al. (2003, A. nidulans)	ANID		An09g05870	212435
Pyrimidine conversions									
r502	:	URI + GTP ⇒ UMP + GDP	2.7.1.48	Uridine kinase		ANID		An11g09320	53035
r503	:	URI + ATP ⇒ ADP + UMP	2.7.1.48	Uridine kinase		ANID		An11g09320	53035
r504	:	CYTD + GTP ⇒ GDP + CMP	2.7.1.48	Uridine kinase		ANID		An11g09320	53035
r505	:	URA + PRPP ⇒ UMP + PPI	2.4.2.9	UPRTase, uracil phospho-ribosyltransferase (furA)		ANID		An12g09660; An12g09670; An15g06580; An17g02370	42030; 49490; 53518; 54952
r506	:	DUTP + H2O ⇒ PPI + DUMP	3.6.1.23	dUTP pyrophosphatase (dUTPase)		ANID		An01g05040	172313
r507	:	DOROA + Qm ⇒ QH2m + OROA	1.3.1.14	Dihydroorotate dehydro-genase	Gustafson and Waldron (1992); Aleksenko et al. (1999, A. nidulans)	ANID		An02g02910	36779
r508	:	OTHIO + NADPH ⇒ NADP + RTHIO	1.8.1.9	Thioredoxin reductase		ANID		An12g02850	50359
r509	:	OTHIOm + NADPHm ⇒ NADPm + RTHIOm	1.8.1.9	Thioredoxin reductase		ANID		An12g02850	50359

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
Pyrimidine degradation					Darlington et al. (1965, A. nidulans), Kanehisa et al. (2002); Elzainy et al. (1989)			
r510	:	UMP + H2O ⇒ PI + URI	3.1.3.5	5'-nucleotidase	Ali and Elzainy (2000)	ANID	An08g08080	128775
r511	:	URI + H2O ⇒ URA + RIB	3.2.2.3	Uridine hydrolase	Fukami (1961, A. nidulans)	ANEW	An18g04340	42881
r512	:	CMP + H2O ⇒ CYTD + PI	3.1.3.5	5'-nucleotidase	Elzainy et al. (1989); Ali and Elzainy (2000)	ANID	An08g08080	128775
r513	:	CYTD + H2O ⇒ URI + NH3	3.5.4.5	Cytidine deaminase	Elzainy et al. (1989); Ali (1998)	ANID	An03g06870	50782
r514	:	CMP + H2O ⇒ CYTS + R5P	3.2.2.10	CMP glycosylase		ANID		
r515	:	CYTS + H2O ⇒ URA + NH3	3.5.4.1	Cytosine deaminase	Fukami (1961, A. nidulans)	ANID	An01g04260	206127
r516	:	DCMP + H2O ⇒ DC + PI	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID	An08g08080	128775
r517	:	DC + H2O ⇒ NH3 + DU	3.5.4.5	Deoxycytidine deaminase	Fukami (1961, A. nidulans)	ANID	An03g06870	50782
r518	:	DUMP + H2O ⇒ DU + PI	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID	An08g08080	128775
r519	:	URA + DR1P ⇒ DU + PI	2.4.2.1	Purine-nucleoside phosphorylase		ANEW	An11g06110	178461
r520	:	DTMP + H2O ⇒ DT + PI	3.1.3.5	5'-nucleotidase	Rama and Shanmugasundaram (1985, A. nidulans)	ANID	An08g08080	128775
r521	:	THY + DR1P ⇒ DT + PI	2.4.2.1	Purine-nucleoside phosphorylase		ANEW	An11g06110	178461
Salvage pathways for nucleotides								
r522	:	HYXN + PRPP ⇒ PPI + IMP	2.4.2.8	Hypoxanthine phosphoribosyltransferase		ANID	An14g00280	210854
r523	:	GN + PRPP ⇒ PPI + GMP	2.4.2.8	Hypoxanthine phosphoribosyltransferase		ANID	An14g00280	210854
r524	:	AD + PRPP ⇒ PPI + AMP	2.4.2.7	Adenine phosphoribosyltransferase	Ribard et al. (2001, A. nidulans)	ANID	An12g00320	54445
r525	:	XAN + PRPP ⇒ XMP + PPI	2.4.2.22	Xanthine-guanine phosphoribosyltransferase		ANID	An14g00280	210854
r526	:	PRPP + H2O ⇒ PRCP + PI	No EC	Non Enz	Trembacz and Jezewska (1990)	ANEW		
r527	:	PRCP + H2O ⇒ R1P + PI	No EC	Non Enz	Trembacz and Jezewska (1990)	ANEW		
r528	:	AD + R1P ⇒ PI + ADN	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID		
r529	:	GN + R1P ⇒ PI + GSN	2.4.2.1	Purine nucleotide phosphorylase, xanthosine phosphorylase		ANID		
r531	:	ADN + ATP ⇒ AMP + ADP	2.7.1.20	Adenosine kinase	David et al. (2003)	ANIG, ANID	An17g01330	214022
r532	:	INS + ATP ⇒ IMP + ADP	2.7.1.73	Inosine kinase		ANID		
r533	:	GSN + ATP ⇒ GMP + ADP	2.7.1.73	Inosine kinase		ANID		
r534	:	ATP ⇒ cAMP + PPI	4.6.1.1	Adenylate cyclase	Wold and Suzuki (1974)	ANID	An11g01520	178015
r535	:	cAMP ⇒ AMP	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase	Wold and Suzuki (1974); Pall (1981)	ANID	An01g04450; An01g13010	36176; 195992
r536	:	cdAMP ⇒ DAMP	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase		ANID	An01g04450; An01g13010	36176; 195992

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r537	:	cIMP ⇒ IMP	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase		ANID	An01g04450; An01g13010	36176; 195992
r538	:	cGMP ⇒ GMP	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase, low affinity		ANID	An01g04450; An01g13010	36176; 195992
r539	:	cCMP ⇒ CMP	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase, low affinity		ANID	An01g04450; An01g13010	36176; 195992
r540	:	cAMPe ⇒ AMPe	3.1.4.17	3',5'-cyclic-nucleotide phosphodiesterase	Wold and Suzuki (1974)	ANEW	An01g04450; An01g13010	36176; 195992
r541	:	ATPm + AMPm ⇆ 2 ADPm	2.7.4.3	Adenylate kinase		ANIG, ANID	An01g04710; An07g10100	46678; 56109
r542	:	GTPm + AMPm ⇆ ADPm + GDPm	2.7.4.3	Adenylate kinase		ANIG, ANID	An01g04710; An07g10100	46678; 56109
r543	:	ITPm + AMPm ⇆ ADPm + IDPm	2.7.4.3	Adenylate kinase		ANID	An01g04710; An07g10100	46678; 56109
NAD and NADPH metabolism					Kuwahara and Fujii (1978); Kuwahara et al. (1982, 1983)			
Nicotinate and Nicotinamide biosynthesis					Kuwahara and Fujii (1978); Kuwahara et al. (1983)			
r544	:	ASP + O2 ⇒ IMASP + H2O2	1.4.3.16	L-aminoacid oxidase	Sarma et al. (1962, Inferred)	ANEW		
r1267	:	IMASP + T3P1 ⇆ QUIN + 2 H2O + PI	No Ec	quinolinate synthetase, NadA	Sarma et al. (1962, Inferred)	ANEW		
r545	:	QUIN + PRPP ⇒ NAMN + PPI + CO2	2.4.2.19	Nicotinate mononucleotide pyrophosphorylase	Sarma et al. (1962, Inferred)	ANEW	An11g10910	56085
r546	:	NICD + H2O ⇆ NICA + NH3	3.5.1.19	nicotinamidase	Sarma et al. (1964); Kuwahara et al. (1983)	ANEW	An07g08360	48305
r547	:	NICA + PRPP ⇒ NAMN + PPI	2.4.2.11	Nicotinate phosphoribosyltransferase	Sarma et al. (1962); Kuwahara et al. (1983, Inferred)	ANEW	An12g00760	50290
r548	:	ATP + NAMN ⇒ PPI + DMNAD	2.7.7.1	Nicotinamide-nucleotide adenylyltransferase	Kuwahara et al. (1983, Inferred)	ANEW	An11g06610	178093
r549	:	ATP + DMNAD + GLN + H2O ⇆ AMP + PPI + NAD + GLU	6.3.5.1	NAD synthetase	Kuwahara et al. (1983, Inferred)	ANEW	An09g05660	54326
r550	:	ATP + NAD ⇒ ADP + NADP	2.7.1.23	NAD kinase	Kuwahara et al. (1982, Inferred)	ANEW	An03g05090; An14g06430	191587; 53896
NADP and NAD degradation					Kuwahara and Fujii (1978); Kuwahara et al. (1983); Elzainy and Ali (2000)			
r551	:	NADP + H2O ⇒ NAD + PI	No EC	NADPH phosphatase	Kuwahara et al. (1982, Inferred)	ANEW		
r552	:	NAD + H2O ⇒ NAMR + ADP	No EC	acid phosphatase	Elzainy and Ali (2000)	ANEW		
r553	:	NAD + H2O ⇒ ADPR + NICD	3.2.2.5	NAD-glycohydrolase	Sarma et al. (1964),	ANEW		
r554	:	NAD + H2O ⇒ AMP + NMN	3.6.1.22	NAD pyrophosphatase	Kuwahara et al. (1983, Inferred)	ANEW	An09g05670	212451
r555	:	NMN + H2O ⇒ NAMR + PI	3.1.3.5	5'-nucleotidase	Kuwahara et al. (1983, Inferred)	ANEW	An08g08080	128775
r556	:	NAMR + H2O ⇒ NAR + NH3	No EC	nicotinate nucleotide amidase	Kuwahara et al. (1983)	ANEW		
r557	:	NMN + H2O ⇆ R5P + NICD	3.2.2.14	NMN nucleosidase	Kuwahara et al. (1983, Inferred)	ANEW		
r558	:	NAMN + H2O ⇒ NAR + PI	3.1.3.5	5'-nucleotidase	Kuwahara et al. (1982, 1983, Inferred)	ANEW	An08g08080	128775
3-Cyanopyridine degradation					Snajdrova et al. (2004)			

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r1213	:	3CPYRD + 2 H2O ⇒ NICA + NH3	3.5.5.1	benzonitrilase	Snajdrova et al. (2004)	ANEW		An16g00550; An01g07510; An01g12090; An06g01960; An08g08940; An08g10150; An12g01260; An16g06210; An18g01740	41410; 35944; 170270; 175987; N/A; 52578; 141873; 40928; 211815
LIPID METABOLISM									
FATTY ACIDS METABOLISM									
Formation of saturated cytosolic fatty acids (Even numbers)									
r559	:	CBCCP + ACCOA ⇆ BCCP + MALCOA	6.4.1.2	Acetyl-CoA carboxylase (ACC) / biotin carboxylase	Schwenk and Bennett (1969)	ANID		An12g04020	56715
r560	:	ATP + BCCP + CO2 + H2O ⇆ ADP + PI + CBCCP	6.3.4.14	Biotin carboxylase	Schwenk and Bennett (1969)	ANEW		An12g04020	56715
r561	:	MALCOA + ACP ⇆ MALACP + COA	2.3.1.39	Malonyl transferase		ANEW		An04g00040	190484
r562	:	ACCOA + ACP ⇆ ACACP + COA	2.3.1.38	[ACP]acetyltransferase		ANEW		An12g01990	43740
r563	:	ACACP + MALACP ⇒ AACACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r564	:	AACACP + NADPH ⇆ C4HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r565	:	C4HACP ⇆ C4DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r566	:	C4DACP + NADPH ⇆ C40ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r568	:	C40ACP + MALACP ⇒ C6OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r569	:	C6OACP + NADPH ⇆ C6HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r570	:	C6HACP ⇆ C6DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r571	:	C6DACP + NADPH ⇆ C60ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r573	:	C60ACP + MALACP ⇒ C8OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r574	:	C8OACP + NADPH ⇆ C8HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r575	:	C8HACP ⇆ C8DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r576	:	C8DACP + NADPH ⇆ C80ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r578	:	C80ACP + MALACP ⇒ C10OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r579	:	C10OACP + NADPH ⇆ C10HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r580	:	C10HACP ⇆ C10DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r581	:	C10DACP + NADPH ⇆ C100ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r583	:	C100ACP + MALACP ⇒ C12OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r584	:	C12OACP + NADPH ⇆ C12HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r585	:	C12HACP ⇆ C12DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r586	:	C12DACP + NADPH ⇆ C120ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r588	:	C120ACP + MALACP ⇒ C14OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r589	:	C14OACP + NADPH ⇆ C14HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW	An01g12400; An01g14000; An03g02840; An05g02050; An06g02000; An06g02610; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An16g07090; An18g00290	35566; 172477; 45652; 43929; 37709 and 47218; 137016; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 45606; 187979
r590	:	C14HACP ⇆ C14DACP + H2O	4.2.1.61	Long chain beta-hydroxypalmitoyl thioester dehydratase		ANEW	An12g01990	43740
r591	:	C14DACP + NADPH ⇆ C140ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW	An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r598	:	C140ACP + MALACP ⇒ C16OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW	An02g14220; An14g01760	55650; 41604
r599	:	C16OACP + NADPH ⇆ C16HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW	An01g12400; An01g14000; An03g02840; An05g02050; An06g02000; An06g02610; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An16g07090; An18g00290	35566; 172477; 45652; 43929; 37709 and 47218; 137016; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 45606; 187979
r600	:	C16HACP ⇆ C16DACP + H2O	4.2.1.61	Long chain beta-hydroxypalmitoyl thioester dehydratase		ANEW	An12g01990	43740
r601	:	C16DACP + NADPH ⇆ C160ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW	An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r608	:	C160ACP + MALACP ⇒ C18OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW	An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r609	:	C18OACP + NADPH ⇆ C18HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW	An01g12400; An01g14000; An03g02840; An05g02050; An06g02000; An06g02610; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An16g07090; An18g00290	35566; 172477; 45652; 43929; 37709 and 47218; 137016; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 45606; 187979
r610	:	C18HACP ⇆ C18DACP + H2O	4.2.1.61	Long chain beta-hydroxypalmitoyl thioester dehydratase		ANEW	An12g01990	43740
r611	:	C18DACP + NADPH ⇆ C180ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW	An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r618	:	C180ACP + MALACP ⇒ C20OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW	An02g14220; An14g01760	55650; 41604
r619	:	C20OACP + NADPH ⇆ C20HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW	An01g12400; An01g14000; An03g02840; An05g02050; An06g02000; An06g02610; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An16g07090; An18g00290	35566; 172477; 45652; 43929; 37709 and 47218; 137016; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 45606; 187979
r620	:	C20HACP ⇆ C20DACP + H2O	4.2.1.61	Long chain beta-hydroxypalmitoyl thioester dehydratase		ANEW	An12g01990	43740
r621	:	C20DACP + NADPH ⇆ C200ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW	An07g03290; An16g05340; An04g02300	209754; 56395; 190311
Formation of saturated cytosolic fatty acids (Odd numbers)								
r1224	:	PROPCOA + ACP ⇆ PROPACP + COA	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r1225	:	PROPACP + MALACP ⇒ C5OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r1226	:	C5OACP + NADPH ⇆ C5HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1227	:	C5HACP ⇆ C5DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1228	:	C5DACP + NADPH ⇆ C50ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1230	:	C50ACP + MALACP ⇒ C7OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r1231	:	C7OACP + NADPH ⇆ C7HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1232	:	C7HACP ⇆ C7DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1233	:	C7DACP + NADPH ⇆ C70ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1235	:	C70ACP + MALACP ⇒ C9OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r1236	:	C9OACP + NADPH ⇆ C9HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1237	:	C9HACP ⇆ C9DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1238	:	C9DACP + NADPH ⇆ C90ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1240	:	C90ACP + MALACP ⇒ C11OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r1241	:	C11OACP + NADPH ⇆ C11HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1242	:	C11HACP ⇆ C11DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1243	:	C11DACP + NADPH ⇆ C110ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1245	:	C110ACP + MALACP ⇒ C13OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r1246	:	C13OACP + NADPH ⇆ C13HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1247	:	C13HACP ⇆ C13DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1248	:	C13DACP + NADPH ⇆ C130ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1250	:	C130ACP + MALACP ⇒ C15OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r1251	:	C15OACP + NADPH ⇆ C15HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1252	:	C15HACP ⇆ C15DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1253	:	C15DACP + NADPH ⇆ C150ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1255	:	C150ACP + MALACP ⇒ C17OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r1256	:	C17OACP + NADPH ⇆ C17HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1257	:	C17HACP ⇆ C17DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1258	:	C17DACP + NADPH ⇆ C170ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
r1260	:	C170ACP + MALACP ⇒ C19OACP + CO2 + ACP	2.3.1.41	3-oxoacyl-[acyl-carrier-protein] synthase		ANEW		An02g14220; An14g01760	55650; 41604
r1261	:	C19OACP + NADPH ⇆ C19HACP + NADP	1.1.1.100	3-oxoacyl-[acyl-carrier-protein] reductase		ANEW		An01g12400; An03g02840; An05g02050; An06g02000; An08g01930; An11g00760; An12g02320; An12g05100; An13g01130; An14g01270; An14g06740; An18g00290	35566; 45652; 43929; 37709 and 47218; 177736; 124830; 189865; 49639; 44744; 124614; 185180; 187979
r1262	:	C19HACP ⇆ C19DACP + H2O	2.3.1.85	Fatty-acid synthase		ANEW	*	An08g10930; An09g02010; An12g01980	47227; 188253; 189622
r1263	:	C19DACP + NADPH ⇆ C190ACP + NADP	1.3.1.9	Enoyl-ACP reductase		ANEW		An07g03290; An16g05340; An04g02300	209754; 56395; 190311
Formation of unsaturated cytosolic fatty acids					Chattopadhyay et al. (1985b,a)				
r623	:	C190ACP + NADH + O2 ⇆ C191ACP + NAD + 2 H2O	1.14.19.1	C190-CoA 9-desaturase	Chattopadhyay et al. (1985b)	ANEW		An07g01960; An12g09940	209875; 195065
r624	:	C191ACP + NADH + O2 ⇆ C192ACP + NAD + 2 H2O	1.14.19.3	C190-CoA 12-desaturase	Chattopadhyay et al. (1985a)	ANEW		An07g06770; An16g06350	209561; 48908
r625	:	C180ACP + NADH + O2 ⇆ C181ACP + NAD + 2 H2O	1.14.19.1	stearoyl-CoA 9-desaturase	Chattopadhyay et al. (1985b)	ANEW		An07g01960; An12g09940	209875; 195065
r626	:	C181ACP + NADH + O2 ⇆ C182ACP + NAD + 2 H2O	1.14.19.3	stearoyl-CoA 12-desaturase	Chattopadhyay et al. (1985a)	ANEW		An07g06770; An16g06350	209561; 48908

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r627	:	C182ACP + NADH + O2 ⇆ C183ACP + NAD + 2 H2O	No EC	stearoyl-CoA 15-desaturase	Chattopadhyay et al. (1985a)	ANEW		
r988	:	C170ACP + NADH + O2 ⇆ C171ACP + NAD + 2 H2O	No EC	C170-CoA 9-desaturase	Levery et al. (2000, Inferred)	ANEW		
r628	:	C160ACP + NADH + O2 ⇆ C161ACP + NAD + 2 H2O	1.14.19.1	C160-CoA 9-desaturase	Chattopadhyay et al. (1985b, Inferred)	ANEW	An07g01960; An12g09940	209875; 195065
r629	:	C161ACP + NADH + O2 ⇆ C162ACP + NAD + 2 H2O	1.14.19.3	C160-CoA 12-desaturase	Chattopadhyay et al. (1985a, Inferred)	ANEW	An07g06770; An16g06350	209561; 48908
r630	:	C140ACP + NADH + O2 ⇆ C141ACP + NAD + 2 H2O	1.14.19.1	C160-CoA 9-desaturase	Chattopadhyay et al. (1985a, Inferred)	ANEW	An07g01960; An12g09940	209875; 195065
Removal of ACPs								
r936	:	C40ACP + H2O ⇒ C40 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r937	:	C60ACP + H2O ⇒ C60 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r938	:	C80ACP + H2O ⇒ C80 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r939	:	C100ACP + H2O ⇒ C100 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r940	:	C120ACP + H2O ⇒ C120 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r941	:	C140ACP + H2O ⇒ C140 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r942	:	C141ACP + H2O ⇒ C141 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r943	:	C150ACP + H2O ⇒ C150 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r944	:	C160ACP + H2O ⇒ C160 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r945	:	C161ACP + H2O ⇒ C161 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r946	:	C162ACP + H2O ⇒ C162 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r947	:	C170ACP + H2O ⇒ C170 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r987	:	C171ACP + H2O ⇒ C171 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r948	:	C180ACP + H2O ⇒ C180 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r949	:	C181ACP + H2O ⇒ C181 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r950	:	C182ACP + H2O ⇒ C182 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r951	:	C183ACP + H2O ⇒ C183 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r952	:	C190ACP + H2O ⇒ C190 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r953	:	C191ACP + H2O ⇒ C191 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r954	:	C192ACP + H2O ⇒ C192 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
r955	:	C200ACP + H2O ⇒ C200 + ACP	3.1.2.14	Acyl-ACP-hydrolase		ANEW		
Transfer of ACP-Acyls to COA for transport and biosynthesis								
r631	:	C40ACP + COA ⇆ C40COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r617	:	C40ACP + COA ⇆ C40COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW		
r632	:	C60ACP + COA ⇆ C60COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r633	:	C80ACP + COA ⇆ C80COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r634	:	C100ACP + COA ⇆ C100COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r635	:	C120ACP + COA ⇆ C120COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r636	:	C140ACP + COA ⇆ C140COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r637	:	C141ACP + COA ⇆ C141COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r638	:	C150ACP + COA ⇆ C150COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r639	:	C160ACP + COA ⇆ C160COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r640	:	C161ACP + COA ⇆ C161COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r641	:	C162ACP + COA ⇆ C162COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r642	:	C170ACP + COA ⇆ C170COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r985	:	C171ACP + COA ⇆ C171COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r643	:	C180ACP + COA ⇆ C180COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r644	:	C181ACP + COA ⇆ C181COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r645	:	C182ACP + COA ⇆ C182COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r646	:	C183ACP + COA ⇆ C183COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r647	:	C190ACP + COA ⇆ C190COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r648	:	C191ACP + COA ⇆ C191COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r649	:	C192ACP + COA ⇆ C192COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
r650	:	C200ACP + COA ⇆ C200COA + ACP	2.3.1.38	[ACP]acetyltransferase		ANEW	An12g01990	43740
Transfer of Acyls to COA for transport and biosynthesis								
r651	:	C40 + COA + ATP ⇒ C40COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800	187366
r652	:	C60 + COA + ATP ⇒ C60COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800	187366
r653	:	C80 + COA + ATP ⇒ C80COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800	187366
r654	:	C100 + COA + ATP ⇒ C100COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800	187366
r655	:	C120 + COA + ATP ⇒ C120COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800; An09g06740	187366; 188673
r656	:	C140 + COA + ATP ⇒ C140COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800; An09g06740	187366; 188673
r657	:	C141 + COA + ATP ⇒ C141COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800; An09g06740	187366; 188673
r658	:	C150 + COA + ATP ⇒ C150COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An18g03800; An09g06740	187366; 188673
r659	:	C160 + COA + ATP ⇒ C160COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r660	:	C161 + COA + ATP ⇒ C161COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r661	:	C162 + COA + ATP ⇒ C162COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r662	:	C170 + COA + ATP ⇒ C170COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r986	:	C171 + COA + ATP ⇒ C171COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r663	:	C180 + COA + ATP ⇒ C180COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r664	:	C181 + COA + ATP ⇒ C181COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r665	:	C182 + COA + ATP ⇒ C182COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r666	:	C183 + COA + ATP ⇒ C183COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r667	:	C190 + COA + ATP ⇒ C190COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r668	:	C191 + COA + ATP ⇒ C191COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r669	:	C192 + COA + ATP ⇒ C192COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
r670	:	C200 + COA + ATP ⇒ C200COA + PPI + AMP	6.2.1.3	Acyl-CoA synthetase	Baltazar et al. (1999)	ANEW	An09g06740	188673
Fatty acids conversions					Kanehisa et al. (2002)			
r671	:	2 ACCOA ⇆ COA + AACCOA	2.3.1.9	Acetyl-CoA C-acetyltransferase, acetoacetyl-CoA thiolase		ANID	An16g09190	214441

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r672	:	ACTAC + ATP + COA ⇆ ADP + AACCOA + PI	6.4.1.2, 6.3.4.14	Acetyl-CoA carboxylase (ACC) / biotin carboxylase	Inferred for ACTAC connection	ANEW		
Fa ac de da ti					Baltazar et al. (1999)			
Carnitine shuttle								
r678	:	C120COA + CAR ⇆ COA + C120CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r679	:	C140COA + CAR ⇆ COA + C140CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r680	:	C141COA + CAR ⇆ COA + C141CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r681	:	C150COA + CAR ⇆ COA + C150CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r682	:	C160COA + CAR ⇆ COA + C160CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r683	:	C161COA + CAR ⇆ COA + C161CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r684	:	C162COA + CAR ⇆ COA + C162CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r685	:	C170COA + CAR ⇆ COA + C170CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r1211	:	C171COA + CAR ⇆ COA + C171CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r686	:	C180COA + CAR ⇆ COA + C180CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r687	:	C181COA + CAR ⇆ COA + C181CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r688	:	C182COA + CAR ⇆ COA + C182CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r689	:	C183COA + CAR ⇆ COA + C183CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r690	:	C190COA + CAR ⇆ COA + C190CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r691	:	C191COA + CAR ⇆ COA + C191CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r692	:	C192COA + CAR ⇆ COA + C192CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r693	:	C200COA + CAR ⇆ COA + C200CAR	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r699	:	CARm + C120CAR ⇒ CAR + C120CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r700	:	CARm + C140CAR ⇒ CAR + C140CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r701	:	CARm + C141CAR ⇒ CAR + C141CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r702	:	CARm + C150CAR ⇒ CAR + C150CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r703	:	CARm + C160CAR ⇒ CAR + C160CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r704	:	CARm + C161CAR ⇒ CAR + C161CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r705	:	CARm + C162CAR ⇒ CAR + C162CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r706	:	CARm + C170CAR ⇒ CAR + C170CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r989	:	CARm + C171CAR ⇒ CAR + C171CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r707	:	CARm + C180CAR ⇒ CAR + C180CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r708	:	CARm + C181CAR ⇒ CAR + C181CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r709	:	CARm + C182CAR ⇒ CAR + C182CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r710	:	CARm + C183CAR ⇒ CAR + C183CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r711	:	CARm + C190CAR ⇒ CAR + C190CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r712	:	CARm + C191CAR ⇒ CAR + C191CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r713	:	CARm + C192CAR ⇒ CAR + C192CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r714	:	CARm + C200CAR ⇒ CAR + C200CARm		Carnitine transport reaction	Jernejc and Legisa (1996)	ANEW		
r720	:	C120CARm + COAm ⇆ CARm + C120COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r721	:	C140CARm + COAm ⇆ CARm + C140COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r722	:	C141CARm + COAm ⇆ CARm + C141COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r723	:	C150CARm + COAm ⇆ CARm + C150COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r724	:	C160CARm + COAm ⇆ CARm + C160COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r725	:	C161CARm + COAm ⇆ CARm + C161COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r726	:	C162CARm + COAm ⇆ CARm + C162COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r727	:	C170CARm + COAm ⇆ CARm + C170COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r990	:	C171CARm + COAm ⇆ CARm + C171COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r728	:	C180CARm + COAm ⇆ CARm + C180COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r729	:	C181CARm + COAm ⇆ CARm + C181COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r730	:	C182CARm + COAm ⇆ CARm + C182COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r731	:	C183CARm + COAm ⇆ CARm + C183COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r732	:	C190CARm + COAm ⇆ CARm + C190COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r733	:	C191CARm + COAm ⇆ CARm + C191COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r734	:	C192CARm + COAm ⇆ CARm + C192COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
r735	:	C200CARm + COAm ⇆ CARm + C200COAm	2.3.1.7	Carnitine O-acetyltransferase	Jernejc and Legisa (1996); Baltazar et al. (1999)	ANEW	An08g04990; An18g01590	198577; 120926
Oxidation of fatty acids (even numbers)								
r736	:	C200COAm + FADm ⇒ C20DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r737	:	C200COAm + FADm ⇒ C20DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r738	:	C20DCOAm + H2Om ⇆ C20HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r739	:	C20HCOAm + NADm ⇆ C20OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r740	:	C20OCOAm + COAm ⇒ ACCOAm + C180COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r746	:	C180COAm + FADm ⇒ C18DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r747	:	C180COAm + FADm ⇒ C18DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r748	:	C18DCOAm + H2Om ⇆ C18HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r749	:	C18HCOAm + NADm ⇆ C18OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r750	:	C18OCOAm + COAm ⇒ ACCOAm + C160COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r756	:	C160COAm + FADm ⇒ C16DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r757	:	C160COAm + FADm ⇒ C16DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r758	:	C16DCOAm + H2Om ⇆ C16HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r759	:	C16HCOAm + NADm ⇆ C16OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r760	:	C16OCOAm + COAm ⇒ ACCOAm + C140COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r766	:	C140COAm + FADm ⇒ C14DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r767	:	C140COAm + FADm ⇒ C14DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r768	:	C14DCOAm + H2Om ⇆ C14HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r769	:	C14HCOAm + NADm ⇆ C14OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r770	:	C14OCOAm + COAm ⇒ ACCOAm + C120COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r771	:	C120COAm + FADm ⇒ C12DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r772	:	C120COAm + FADm ⇒ C12DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r773	:	C12DCOAm + H2Om ⇆ C12HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r774	:	C12HCOAm + NADm ⇆ C12OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r775	:	C12OCOAm + COAm ⇒ ACCOAm + C100COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r776	:	C100COAm + FADm ⇒ C10DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r777	:	C100COAm + FADm ⇒ C10DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r778	:	C10DCOAm + H2Om ⇆ C10HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r779	:	C10HCOAm + NADm ⇆ C10OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r780	:	C10OCOAm + COAm ⇒ ACCOAm + C80COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r781	:	C80COAm + FADm ⇒ C8DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r782	:	C80COAm + FADm ⇒ C8DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r783	:	C8DCOAm + H2Om ⇆ C8HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r784	:	C8HCOAm + NADm ⇆ C8OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r785	:	C8OCOAm + COAm ⇒ ACCOAm + C60COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r786	:	C60COAm + FADm ⇒ C6DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r787	:	C6DCOAm + H2Om ⇆ C6HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r788	:	C6HCOAm + NADm ⇆ C6OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r789	:	C6OCOAm + COAm ⇒ ACCOAm + C40COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r790	:	C40COAm + FADm ⇒ C4DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Kazimirova and Novotel'nov (1956, Inferred)	ANEW	An17g01150	128861
r791	:	C4DCOAm + H2Om ⇆ C4HCOAm	4.2.1.17	Enoyl-CoA hydratase	Kazimirova and Novotel'nov (1956, Inferred)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r792	:	C4HCOAm + NADm ⇆ AACCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Kazimirova and Novotel'nov (1956, Inferred)	ANEW	An14g00990; An12g03260	201398; 43844
r793	:	AACCOAm + COAm ⇒ 2 ACCOAm	2.3.1.9	Acetyl-CoA C-acetyltransferase, acetoacetyl-CoA thiolase		ANEW	An13g01920	44808
Oxidation of fatty acids (odd chains)								
r741	:	C190COAm + FADm ⇒ C19DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r742	:	C190COAm + FADm ⇒ C19DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r743	:	C19DCOAm + H2Om ⇆ C19HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r744	:	C19HCOAm + NADm ⇆ C19OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r745	:	C19OCOAm + COAm ⇒ ACCOAm + C170COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r751	:	C170COAm + FADm ⇒ C17DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r752	:	C170COAm + FADm ⇒ C17DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r753	:	C17DCOAm + H2Om ⇆ C17HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r754	:	C17HCOAm + NADm ⇆ C17OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r755	:	C17OCOAm + COAm ⇒ ACCOAm + C150COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r761	:	C150COAm + FADm ⇒ C15DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r762	:	C150COAm + FADm ⇒ C15DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r763	:	C15DCOAm + H2Om ⇆ C15HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r764	:	C15HCOAm + NADm ⇆ C15OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r765	:	C15OCOAm + COAm ⇒ ACCOAm + C130COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r593	:	C130COAm + FADm ⇒ C13DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914
r594	:	C130COAm + FADm ⇒ C13DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r595	:	C13DCOAm + H2Om ⇆ C13HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r596	:	C13HCOAm + NADm ⇆ C13OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r597	:	C13OCOAm + COAm ⇒ ACCOAm + C110COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r603	:	C110COAm + FADm ⇒ C11DCOAm + FADH2m	1.3.99.13	Long-chain-acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An04g03290; An13g03940	57034; 191914

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r604	:	C110COAm + FADm ⇒ C11DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r605	:	C11DCOAm + H2Om ⇆ C11HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r606	:	C11HCOAm + NADm ⇆ C11OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r607	:	C11OCOAm + COAm ⇒ ACCOAm + C90COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r613	:	C90COAm + FADm ⇒ C9DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r614	:	C9DCOAm + H2Om ⇆ C9HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r615	:	C9HCOAm + NADm ⇆ C9OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r616	:	C9OCOAm + COAm ⇒ ACCOAm + C70COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r673	:	C70COAm + FADm ⇒ C7DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r674	:	C7DCOAm + H2Om ⇆ C7HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r675	:	C7HCOAm + NADm ⇆ C7OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r676	:	C7OCOAm + COAm ⇒ ACCOAm + C50COAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823
r694	:	C50COAm + FADm ⇒ C5DCOAm + FADH2m	1.3.99.3	Acyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An17g01150	128861
r695	:	C5DCOAm + H2Om ⇆ C5HCOAm	4.2.1.17	Enoyl-CoA hydratase	Baltazar et al. (1999)	ANEW	An14g00990; An02g02820; An02g05840; An02g07320	201398; 36773; N/A; 197480
r696	:	C5HCOAm + NADm ⇆ C5OCOAm + NADHm	1.1.1.35	3-hydroxyacyl-CoA dehydrogenase	Baltazar et al. (1999)	ANEW	An14g00990; An12g03260	201398; 43844
r697	:	C5OCOAm + COAm ⇒ ACCOAm + PROPCOAm	2.3.1.16	3-ketoacyl-CoA thiolase	Baltazar et al. (1999)	ANEW	An02g03320; An04g05720; An08g05400; An13g00590	46947; 55007; 38275; 50823

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
PHOSPHOLIPID BIOSYNTHESIS					Chopra and Khuller (1984); Kanehisa et al. (2002)			
Phosphatidylserine								
r794	:	GL3P + 0.022 C120ACP + 0.031 C140ACP + 0.022 C141ACP + 0.214 C160ACP + 0.045 C161ACP + 0.016 C162ACP + 0.045 C170ACP + 0.08 C180ACP + 0.2 C181ACP + 0.183 C182ACP + 0.081 C183ACP + 0.061 C200ACP ⇒ PSAGL3P + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r795	:	T3P2 + 0.022 C120ACP + 0.031 C140ACP + 0.022 C141ACP + 0.214 C160ACP + 0.045 C161ACP + 0.016 C162ACP + 0.045 C170ACP + 0.08 C180ACP + 0.2 C181ACP + 0.183 C182ACP + 0.081 C183ACP + 0.061 C200ACP ⇒ PSAT3P2 + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r796	:	PSAT3P2 + NADPH ⇒ PSAGL3P + NADP	1.1.1.101	Acyldihydroxyacetonephosphl reductase/ acylglycerone-phosphate reductase	Chopra and Khuller (1984, Inferred)	ANID	An16g06470	184098
r797	:	PSAGL3P + 0.022 C120ACP + 0.031 C140ACP + 0.022 C141ACP + 0.214 C160ACP + 0.045 C161ACP + 0.016 C162ACP + 0.045 C170ACP + 0.08 C180ACP + 0.2 C181ACP + 0.183 C182ACP + 0.081 C183ACP + 0.061 C200ACP ⇒ PSPA + ACP	2.3.1.51	1-acylglycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An13g00040	126602
r798	:	PSPA + CTP ⇆ PSCDPDG + PPI	2.7.7.41	Cdp-diacylglycerol synthetase (phosphatidate cytidylyltransferase)	Chopra and Khuller (1984, Inferred)	ANID	An07g09570	181254
r799	:	PSCDPDG + SER ⇆ CMP + PS	2.7.8.8	Phosphatidylserine synthase	Chopra and Khuller (1984, Inferred)	ANID	An17g01120	51030
Phosphatidylethanolamine								
r800	:	GL3P + 0.03 C120ACP + 0.015 C140ACP + 0.011 C141ACP + 0.001 C150ACP + 0.24 C160ACP + 0.046 C161ACP + 0.039 C162ACP + 0.041 C170ACP + 0.093 C180ACP + 0.135 C181ACP + 0.282 C182ACP + 0.065 C183ACP + 0.002 C200ACP ⇒ PEAGL3P + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r801	:	T3P2 + 0.03 C120ACP + 0.015 C140ACP + 0.011 C141ACP + 0.001 C150ACP + 0.24 C160ACP + 0.046 C161ACP + 0.039 C162ACP + 0.041 C170ACP + 0.093 C180ACP + 0.135 C181ACP + 0.282 C182ACP + 0.065 C183ACP + 0.002 C200ACP ⇒ PEAT3P2 + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r802	:	PEAT3P2 + NADPH ⇒ PEAGL3P + NADP	1.1.1.101	Acyldihydroxyacetonephosphl reductase/ acylglycerone-phosphate reductase	Chopra and Khuller (1984, Inferred)	ANID	An16g06470	184098

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r803	:	PEAGL3P + 0.03 C120ACP + 0.015 C140ACP + 0.011 C141ACP + 0.001 C150ACP + 0.24 C160ACP + 0.046 C161ACP + 0.039 C162ACP + 0.041 C170ACP + 0.093 C180ACP + 0.135 C181ACP + 0.282 C182ACP + 0.065 C183ACP + 0.002 C200ACP ⇒ PEPA + ACP	2.3.1.51	1-acylglycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An13g00040	126602
r804	:	PEPA + CTP ⇆ PECDPDG + PPI	2.7.7.41	Cdp-diacylglycerol synthetase (phosphatidate cytidylyltransferase)	Chopra and Khuller (1984, Inferred)	ANID	An07g09570	181254
r805	:	PECDPDG + SER ⇆ CMP + PEPS	2.7.8.8	Phosphatidylserine synthase	Chopra and Khuller (1984, Inferred)	ANID	An17g01120	51030
r806	:	PEPS ⇒ PE + CO2	4.1.1.65	Phosphatidylserine decarboxylase	Chopra and Khuller (1984, Inferred)	ANID	An03g02830; An01g14110; An04g10280; An09g04710; An12g00910; An14g01880	194479; 35440; N/A; 202968; 50299; 41614
Phosphatidylcholine								
r807	:	GL3P + 0.01 C120ACP + 0.044 C140ACP + 0.077 C141ACP + 0.224 C160ACP + 0.039 C161ACP + 0.018 C162ACP + 0.048 C170ACP + 0.068 C180ACP + 0.131 C181ACP + 0.308 C182ACP + 0.021 C183ACP + 0.012 C200ACP ⇒ PCAGL3P + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r808	:	T3P2 + 0.01 C120ACP + 0.044 C140ACP + 0.077 C141ACP + 0.224 C160ACP + 0.039 C161ACP + 0.018 C162ACP + 0.048 C170ACP + 0.068 C180ACP + 0.131 C181ACP + 0.308 C182ACP + 0.021 C183ACP + 0.012 C200ACP ⇒ PCAT3P2 + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
r809	:	PCAT3P2 + NADPH ⇒ PCAGL3P + NADP	1.1.1.101	Acyldihydroxyacetonephospł reductase/ acylglycerone-phosphate reductase	Chopra and Khuller (1984, Inferred)	ANID	An16g06470	184098
r810	:	PCAGL3P + 0.01 C120ACP + 0.044 C140ACP + 0.077 C141ACP + 0.224 C160ACP + 0.039 C161ACP + 0.018 C162ACP + 0.048 C170ACP + 0.068 C180ACP + 0.131 C181ACP + 0.308 C182ACP + 0.021 C183ACP + 0.012 C200ACP ⇒ PCPA + ACP	2.3.1.51	1-acylglycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An13g00040	126602
r811	:	PCPA + CTP ⇆ PCCDPDG + PPI	2.7.7.41	Cdp-diacylglycerol synthetase (phosphatidate cytidylyltransferase)	Chopra and Khuller (1984, Inferred)	ANID	An07g09570	181254
r812	:	PCCDPDG + SER ⇆ CMP + PCPS	2.7.8.8	Phosphatidylserine synthase	Chopra and Khuller (1984, Inferred)	ANID	An17g01120	51030

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	ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
	r813	:	PCPS ⇒ PCPE + CO2	4.1.1.65	Phosphatidylserine decarboxylase	Chopra and Khuller (1984, Inferred)	ANID	An03g02830; An01g14110; An04g10280; An09g04710; An12g00910; An14g01880	194479; 35440; N/A; 202968; 50299; 41614
	r814	:	PCPE + SAM ⇒ SAH + PCPMME	2.1.1.17	Phosphatidylethanolamine N-methyltransferase		ANID	An15g06310	53511
	r815	:	PCPMME + SAM ⇒ SAH + PCPDME	2.1.1.71	Methylene-fatty-acyl-phospholipid synthase		ANID	An08g00560	208474
	r816	:	PCPDME + SAM ⇒ PC + SAH	2.1.1.71	Methylene-fatty-acyl-phospholipid synthase		ANID	An08g00560	208474
Cardiolipin									
	r817	:	GL3P + 0.024 C120ACP + 0.032 C140ACP + 0.017 C141ACP + 0.232 C160ACP + 0.027 C161ACP + 0.009 C162ACP + 0.017 C170ACP + 0.081 C180ACP + 0.124 C181ACP + 0.326 C182ACP + 0.111 C183ACP ⇒ CLAGL3P + ACP	2.3.1.15	Glycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An18g01960	188006
	r818	:	CLAGL3P + 0.024 C120ACP + 0.032 C140ACP + 0.017 C141ACP + 0.232 C160ACP + 0.027 C161ACP + 0.009 C162ACP + 0.017 C170ACP + 0.081 C180ACP + 0.124 C181ACP + 0.326 C182ACP + 0.111 C183ACP ⇒ CLPA + ACP	2.3.1.51	1-acylglycerol-3-phosphate acyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An13g00040	126602
	r819	:	CLPA + CTP ⇆ CLCDPDG + PPI	2.7.7.41	Cdp-diacylglycerol synthetase (phosphatidate cytidylyltransferase)	Chopra and Khuller (1984, Inferred)	ANID	An07g09570	181254
	r820	:	CLCDPDG + GL3P ⇒ CMP + CLPIGP	2.7.8.5	CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An17g01120	51030
	r821	:	CLPIGP + H2O ⇒ PG + PI	3.1.3.27	Phosphatidylglycerophospha	Chopra and Khuller (1984, Inferred)	ANID		
	r822	:	CLCDPDG + PG ⇒ CMP + CL	CRD1	Cardiolipin synthase/CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase	Chopra and Khuller (1984, Inferred)	ANID	An15g01020	126969
PHOSPHOLIPID DEGRADATION						Chopra and Khuller (1984); Kanehisa et al. (2002)	ANIG, ANID		
	r823	:	PC ⇒ LPC + 0.01 C120 + 0.044 C140 + 0.077 C141 + 0.224 C160 + 0.039 C161 + 0.018 C162 + 0.048 C170 + 0.068 C180 + 0.131 C181 + 0.308 C182 + 0.021 C183 + 0.012 C200	3.1.1.4	Phospholipase A2/lecithinase a/phosphatidase/phosphatidolipase/phospholipase A	Mustranta et al. (1995)	ANID	An02g04040; An04g03360; An08g08490; An08g12250; An12g06690	52198; 44084; 176070; N/A; N/A
				3.1.1.32	Phospholipase B	Memon et al. (1983)		An15g05710	56347

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r824	:	PE ⇒ LPE + 0.03 C120 + 0.015 C140 + 0.011 C141 + 0.001 C150 + 0.24 C160 + 0.046 C161 + 0.039 C162 + 0.041 C170 + 0.093 C180 + 0.135 C181 + 0.282 C182 + 0.065 C183 + 0.002 C200	3.1.1.4	Phospholipase a2/lecithinase A/phosphatidase/phosphatidolipase/phospholipase a		ANID	An02g04040; An04g03360; An08g08490; An08g12250; An12g06690	52198; 44084; 176070; N/A; N/A
			3.1.1.32	Phospholipase B	Memon et al. (1983)		An15g05710	56347
GLYCOSPHINGOLIPID METABOLISM					Kanehisa et al. (2002)			
Biosynthesis of precursors								
r825	:	G6P ⇆ MI1P	5.5.1.4	Myo-inositol-1-phosphate synthase		ANID	An10g00530	54854
r826	:	MI1P ⇒ MYOI + PI	3.1.3.25	Myo-inositol-1(or 4)-monophosphatase	Neuwald et al. (1991, A. nidulans)	ANID	An03g03700	54687
r827	:	0.25 CLCDPDG + 0.25 PCCDPDG + 0.25 PECDPDG + 0.25 PSCDPDG ⇒ CDPDG	No EC	Artificial reaction for TGDMIPC		ANEW		
r828	:	CDPDG + MYOI ⇒ CMP + PINS	2.7.8.11	Phosphatidylinositol synthase	Chopra and Khuller (1984, Inferred)	ANID	An01g14140	55234
r829	:	ATP + PINS ⇒ ADP + PINSP	2.7.1.137	1-phosphatidylinositol 3-kinase/phosphoinositide 3-kinase	Ibrahim-Granet et al. (2003, A. fumigatus)	ANID	An07g04820; An16g04720	39962; 53581
r830	:	C160COA + SER ⇒ COA + C18DHSPH + CO2	2.3.1.50	Serine C-palmitoyltransferase	Mandala et al. (1994, A. fumigatus)	ANID	An08g04100; An18g03820	208165; 202464
r831	:	C18DHSPH + NADPH ⇒ C18SPH + NADP	1.1.1.102	3-dehydrosphinganine reductase		ANID	An01g06830	51907
r832	:	C18SPH + O2 + NADPH ⇒ C18PSPH + NADP + H2O	SUR2	Sphingosine hydroxylase/ syringomycin response protein 2		ANID	An01g10030	51801
r833	:	C180COA + SER ⇒ COA + C20DHSPH + CO2	2.3.1.50	Serine C-palmitoyltransferase	Mandala et al. (1994, A. fumigatus)	ANEW	An08g04100; An18g03820	208165; 202464
r834	:	C20DHSPH + NADPH ⇒ C20SPH + NADP	1.1.1.102	3-dehydrosphinganine reductase		ANEW	An01g06830	51907
r835	:	C20SPH + O2 + NADPH ⇒ C20PSPH + NADP + H2O	SUR2	Sphingosine hydroxylase/ syringomycin response protein 2		ANEW	An01g10030	51801
r836	:	C171COA + SER ⇒ COA + C191DHSPH + CO2	2.3.1.50	Serine C-palmitoyltransferase	Mandala et al. (1994, A. fumigatus)	ANEW	An08g04100; An18g03820	208165; 202464
r837	:	C191DHSPH + NADPH ⇒ C191SPH + NADP	1.1.1.102	3-dehydrosphinganine reductase		ANEW	An01g06830	51907
Biosynthesis of Cerebrin 1					Wagner and Fiegert (1969); Kanehisa et al. (2002)			
r838	:	C18PSPH + C180COA ⇒ CERB1A + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW	An11g00990	52868
r839	:	C18PSPH + C181COA ⇒ CERB1B + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW	An11g00990	52868
r840	:	C20PSPH + C180COA ⇒ CERB1C + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW	An11g00990	52868
r841	:	C20PSPH + C181COA ⇒ CERB1D + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW	An11g00990	52868

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r842	:	0.25 CERB1A + 0.25 CERB1B + 0.25 CERB1C + 0.25 CERB1D ⇒ CERB1	NO EC	Artificial reaction		ANEW			
Biosynthesis of Cerebrin 2					Wagner and Fiegert (1969); Kanehisa et al. (2002)				
r843	:	C18SPH + C180COA ⇒ CERB2A + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW		An11g00990	52868
r844	:	C18SPH + C181COA ⇒ CERB2B + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW		An11g00990	52868
r845	:	C20SPH + C180COA ⇒ CERB2C + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW		An11g00990	52868
r846	:	C20SPH + C181COA ⇒ CERB2D + COA	2.3.1.24	Ceramide synthase	Wagner and Fiegert (1969, Inferred)	ANEW		An11g00990	52868
r847	:	0.25 CERB2A + 0.25 CERB2B + 0.25 CERB2C + 0.25 CERB2D ⇒ CERB2	NO EC	Artificial reaction		ANEW			
Biosynthesis of Galactocerebroside					Wagner and Fiegert (1969); Kanehisa et al. (2002)				
r848	:	UDPGAL + CERB2A ⇒ UDP + GALCERA	2.4.1.45	2-hydroxyacylsphingosine 1-beta-galactosyltransferase	Wagner and Fiegert (1969, Inferred)	ANEW		An04g08370	45922
r849	:	UDPGAL + CERB2B ⇒ UDP + GALCERB	2.4.1.45	2-hydroxyacylsphingosine 1-beta-galactosyltransferase	Wagner and Fiegert (1969, Inferred)	ANEW		An04g08370	45922
r850	:	0.5 GALCERA + 0.5 GALCERB ⇒ GALCER	NO EC	Artifical reaction		ANEW			
Biosynthesis of Glucocerebroside 1					Levery et al. (2000); Kanehisa et al. (2002)	ANEW			
r851	:	C191SPH + C180COA ⇒ CEREB1 + COA	2.3.1.24	Ceramide synthase	Levery et al. (2000, Inferred)	ANEW		An11g00990	52868
r852	:	UDPG + CEREB1 ⇒ UDP + GLUCER1	2.4.1.80	2-hydroxyacylsphingosine 1-beta-glucosyltransferase	Levery et al. (2000, Inferred)	ANEW		An07g03380	209752
Biosynthesis of Glucocerebroside 2					Levery et al. (2000); Kanehisa et al. (2002)	ANEW			
r853	:	C191SPH + C181COA ⇒ CEREB2 + COA	2.3.1.24	Ceramide synthase	Levery et al. (2000, Inferred)	ANEW		An11g00990	52868
r854	:	UDPG + CEREB2 ⇒ UDP + GLUCER2	2.4.1.80	2-hydroxyacylsphingosine 1-beta-glucosyltransferase	Levery et al. (2000, Inferred)	ANEW		An07g03380	209752
Biosynthesis of ceramide-P-inositol and trigalactosyldimannosylinositolphosphorylceramide (GPSL G)					Byrne and Brennan (1976); Kanehisa et al. (2002)	ANEW			
r855	:	CERB2 + PINS ⇒ IPC + H2O	2.-.-.-	IPC synthase, mannosyl diphosphorylinositol ceramide synthase	Zhong et al. (2000)	ANID			
r856	:	IPC + GDPMAN ⇒ MIPC + GDP	SUR1	MIPC synthase	Byrne and Brennan (1976, Inferred)	ANID	*	An05g02310; An09g00100; An15g00630	189424; 43578; 210021
r857	:	MIPC + GDPMAN ⇒ DMIPC + GDP	SUR1	MIPC synthase	Byrne and Brennan (1976, Inferred)	ANID	*	An05g02310; An09g00100; An15g00630	189424; 43578; 210021
r858	:	UDPGAL + DMIPC ⇒ GDMIPC + UDP	2.4.1.-	Galactosyltransferase	Byrne and Brennan (1976, Inferred)	ANEW		An01g09810	170454
r859	:	UDPGAL + GDMIPC ⇒ DGDMIPC + UDP	2.4.1.-	Galactosyltransferase	Byrne and Brennan (1976, Inferred)	ANEW		An01g09810	170454

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r860	:	UDPGAL + DGDMIPC ⇒ TGDMIPC + UDP	2.4.1.-	Galactosyltransferase	Byrne and Brennan (1976, Inferred)	ANEW	An01g09810	170454
BIOSYNTHESIS OF LANOSTEROL					Servouse and Karst (1986); Kanehisa et al. (2002); Nemec and Jernejc (2002)	ANIG, ANID		
r861	:	ACCOA + AACCOA + H2O ⇆ H3MCOA + COA	2.3.3.10	3-hydroxy-3-methylglutaryl coenzyme A synthase		ANID	An02g06320; An07g04260	55566; 56215
r862	:	H3MCOA + 2 NADPH ⇆ MVL + COA + 2 NADP	1.1.1.34	3-hydroxy-3-methylglutaryl-coenzyme A (HMG-CoA) reductase isozyme	Evans and Gealt (1988, A. nidulans)	ANID	An04g00610; An07g08280; An09g03240; An13g04000	213343; 209439; 188317; 44946
r863	:	ATP + MVL ⇒ ADP + PMVL	2.7.1.36	Mevalonate kinase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An04g02190	213169
r864	:	ATP + PMVL ⇒ ADP + PPMVL	2.7.4.2	Phosphomevalonate kinase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An14g04010	211137
r865	:	ATP + PPMVL ⇒ ADP + PI + IPPP + CO2	4.1.1.33	Diphosphomevalonate decarboxylase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An04g01540	203692
r866	:	IPPP ⇆ DMPP	5.3.3.2	Isopentenyl diphosphate:dimethylallyl diphosphate isomerase (IPP isomerase)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An08g07570	52621
r867	:	DMPP + IPPP ⇒ GPP + PPI	2.5.1.1	Prenyltransferase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An11g02500	38877
r868	:	GPP + IPPP ⇒ FPP + PPI	2.5.1.10	Farnesyl diphosphate synthetase (FPP synthetase)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An16g01670; An04g04640	125382; 134931
r869	:	2 FPP + NADPH ⇒ NADP + SQL + 2 PPI	2.5.1.21	Squalene synthase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An02g11000	130900
r870	:	SQL + O2 + NADPH ⇒ S23E + NADP + H2O	1.14.99.7	Squalene monooxygenase	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An03g03770	213441
r871	:	S23E ⇒ LNST	5.4.99.7	2,3-oxidosqualene-lanosterol cyclase	Nemec and Jernejc (2002, Inferred), Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae) Servouse and Karst (1986); Kanehisa et al. (2002); Cherry et al. (1998)	ANID	An07g06150; An09g01330	181224; 189003
BIOSYNTHESIS OF ZYMOSTEROL AND ERGOSTEROL								
r872	:	LNST + 3 NADPH + 3 O2 ⇒ DCTOL + FOR + 3 NADP + 4 H2O	ERG11	Cytochrome p450 lanosterol 14A-demethylase (ERG11)	van den Brink et al. (1996)	ANID	An11g00270; An11g02230	38711; 55947
r873	:	DCTOL + NADPH ⇒ DCDOL + NADP	ERG24	C-14 sterol reductase (ERG24)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An01g07000	51895
r874	:	DCDOL + 3 O2 + 3 NADPH ⇒ DCDA + 3 NADP + 4 H2O	ERG25	C-4 sterol methyl oxidase (ERG25)	Chopra and Khuller (1984, Inferred), Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An03g06410	44595
r875	:	DCDA ⇒ CDOL + CO2	ERG26	C-4 sterol decarboxylase (ERG26)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An15g03090	200652
r876	:	CDOL + 3 O2 + 3 NADPH ⇒ CDA + 3 NADP + 4 H2O	ERG25	C-4 sterol methyl oxidase (ERG25)	Chopra and Khuller (1984, Inferred), Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An03g06410	44595
r877	:	CDA ⇒ ZYMST + CO2	ERG25	C-4 sterol decarboxylase (ERG26)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An15g03090	200652

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r879	:	ZYMST + SAM ⇒ FEST + SAH	2.1.1.41	S-adenosyl-methionine delta-24-sterol-C-methyltransferase (ERG6)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An04g04210; An14g01590	213016; 56548
r880	:	FEST ⇆ EPST	ERG2	C-8 sterol isomerase (ERG1)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANID	An01g03350	206219
r881	:	EPST + O2 + NADPH ⇒ NADP + ERGOD + 2 H2O	ERG3	C-5 sterol desaturase (ERG3)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An15g00150; An16g02930	200430; 53645
r882	:	ERGOD + O2 + NADPH ⇒ NADP + ERGOT + 2 H2O	ERG5	C-22 sterol desaturase (ERG5)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An01g02810; An11g03230	206266; 55967
r883	:	ERGOT + NADPH ⇒ ERGOST + NADP	ERG4	C-24 sterol reductase (ERG4)	Ferreira et al. (2005, A. nidulans, A. fumigatus, A. oryzae)	ANEW	An14g05780	49423
METABOLISM OF ERGOSTEROL ESTERS								
r884	:	0.074 C160ACP + 0.222 C181ACP + 0.704 C182ACP + GL3P ⇒ ACP + SEMAGP	2.3.1.15	Glycerol-3-phosphate O-acyltransferase		ANEW	An18g01960	188006
r885	:	0.074 C160ACP + 0.222 C181ACP + 0.704 C182ACP + SEMAGP ⇒ ACP + SEDAGP	2.3.1.51	1-acylglycerol-3-phosphate O-acyltransferase		ANEW	An13g00040	126602
r886	:	SEDAGP + H2O ⇒ SEDAG + PI	3.1.3.4	phosphatidate phosphatase		ANEW		
r887	:	SEDAG + ERGOST ⇒ SEMAG + ERGOSE	2.3.1.73	sterol O-acyltransferase		ANEW	An18g04660	54192
r888	:	ERGOSE + H2O ⇒ ERGOST + 0.074 C160 + 0.222 C181 + 0.704 C182	3.1.1.13	sterol esterase		ANEW		
r889	:	SEMAG + H2O ⇒ 0.074 C160 + 0.222 C181 + 0.704 C182 + GL	3.1.1.23	Acylglycerol lipase		ANEW		
METABOLISM OF COMPLEX LIPIDS					David et al. (2003)	ANIG, ANID		
Glycerolipid biosynthesis					Kanehisa et al. (2002)	ANIG, ANID		
r890	:	0.024 C120ACP + 0.013 C140ACP + 0.012 C141ACP + 0.002 C150ACP + 0.154 C160ACP + 0.02 C161ACP + 0.008 C162ACP + 0.002 C170ACP + 0.026 C180ACP + 0.374 C181ACP + 0.327 C182ACP + 0.032 C183ACP + 0.006 C200ACP + GL3P ⇒ ACP + MAGLYP	2.3.1.15	Glycerol-3-phosphate O-acyltransferase		ANEW	An18g01960	188006
r956	:	MAGLYP + H2O ⇒ MAGLY + PI	3.1.3.4	phosphatidate phosphatase		ANEW		
r891	:	0.024 C120ACP + 0.013 C140ACP + 0.012 C141ACP + 0.002 C150ACP + 0.154 C160ACP + 0.02 C161ACP + 0.008 C162ACP + 0.002 C170ACP + 0.026 C180ACP + 0.374 C181ACP + 0.327 C182ACP + 0.032 C183ACP + 0.006 C200ACP + MAGLYP ⇒ ACP + DAGLYP	2.3.1.51	Glycerol-3-phosphate O-acyltransferase		ANEW	An13g00040	126602
r892	:	DAGLYP + H2O ⇒ DAGLY + PI	3.1.3.4	phosphatidate phosphatase		ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r893	:	0.024 C120ACP + 0.013 C140ACP + 0.012 C141ACP + 0.002 C150ACP + 0.154 C160ACP + 0.02 C161ACP + 0.008 C162ACP + 0.002 C170ACP + 0.026 C180ACP + 0.374 C181ACP + 0.327 C182ACP + 0.032 C183ACP + 0.006 C200ACP + DAGLY ⇒ TAGLY + ACP	2.3.1.20	1-acylglycerol-3-phosphate acyltransferase	Tomoda et al. (1999)	ANID	An12g03600; An15g03770	186422; 181869
Glycerolipid degradation								
r894	:	TAGLY + H2O ⇒ DAGLY + 0.024 C120 + 0.013 C140 + 0.012 C141 + 0.002 C150 + 0.154 C160 + 0.02 C161 + 0.008 C162 + 0.002 C170 + 0.026 C180 + 0.374 C181 + 0.327 C182 + 0.032 C183 + 0.006 C200	3.1.1.3	Triacylglycerol lipase	Hannan (1959)	ANID	An13g01880; An03g06560; An03g06630; An06g00350; An07g00440; An07g04200; An09g02180; An09g02270; An09g03760; An09g05120; An12g06560; An13g00480; An14g00860; An16g08870	50877; N/A; 191506; 177254; 53361; 39997; 212664; 189135; 43311; 50087; 185927; 191767; 185301; 193610
r895	:	DAGLY + H2O ⇒ MAGLY + 0.024 C120 + 0.013 C140 + 0.012 C141 + 0.002 C150 + 0.154 C160 + 0.02 C161 + 0.008 C162 + 0.002 C170 + 0.026 C180 + 0.374 C181 + 0.327 C182 + 0.032 C183 + 0.006 C200	3.1.1.3	Triacylglycerol lipase	Hannan (1959)	ANID	An13g01880; An03g06560; An03g06630; An06g00350; An07g00440; An07g04200; An09g02180; An09g02270; An09g03760; An09g05120; An12g06560; An13g00480; An14g00860; An16g08870	50877; N/A; 191506; 177254; 53361; 39997; 212664; 189135; 43311; 50087; 185927; 191767; 185301; 193610
Glycolipids metabolism					David et al. (2003)	ANIG, ANID		
Mono- and di-galactosyldiglyceride biosynthesis								
r896	:	DAGLY + UDPGAL ⇆ UDP + MGDG	2.4.1.46	UDPgalactose:1,2-diacylglycerol 3-beta-D-galactosyltransferase		ANID		
r897	:	MGDG + UDPGAL ⇆ UDP + DGDG	2.4.1.184	Galactolipid galactosyltransferase		ANID		
Monoglucosyloxyoctadecenoic acid								
r898	:	C181COA + UDPG + H2O ⇆ MGC181 + UDP + COA	2.4.1.-	lipid galactosyltransferase		ANEW		
SECONDARY METABOLISM								
Ochratoxin A biosynthesis								

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1010	:	4 ACCOA + 1 MALCOA + 1 PHE ⇒ 5 COA + OTA	No EC	Artificial reaction, chlor left out	Abarca et al. (1994); Varga et al. (2003); O'Callaghan et al. (2003); Samson et al. (2004); Blumenthal (2004)	ANEW	An10g00140	44965
PROTEIN PRODUCTION								
Glucoamylase production								
r1266	:	0.951 ALA + 0.307 ARG + 0.366 ASN + 0.644 ASP + 0.146 CYS + 0.249 GLN + 0.38 GLU + 0.687 GLY + 0.059 HIS + 0.351 ILE + 0.702 LEU + 0.190 LYS + 0.044 MET + 0.322 PHE + 0.322 PRO + 1.272 SER + 1.082 THR + 0.278 TRP + 0.395 TYR + 0.614 VAL + 40.39 ATP ⇒ 40.39 ADP + 40.49 PI + GAMYLe	No EC	Artifical protein synthesis reaction		ANEW		
Alphaamylase production								
r1265	:	0.622 ALA + 0.226 ARG + 0.452 ASN + 0.773 ASP + 0.170 CYS + 0.283 GLN + 0.320 GLU + 0.754 GLY + 0.132 HIS + 0.509 ILE + 0.716 LEU + 0.189 LYS + 0.151 MET + 0.264 PHE + 0.358 PRO + 1.018 SER + 0.716 THR + 0.207 TRP + 0.660 TYR + 0.603 VAL + 39.37 ATP ⇒ 39.37 ADP + 39.37 PI + AAMYLe	No EC	Artifical protein synthesis reaction		ANEW		
Sulfur metabolism								
r899	:	H2SO3 + 3 NADPH ⇆ H2S + 3 NADP + 3 H2O	1.8.1.2	Sulfite reductase	Sieńko and Paszewski (1999, A. nidulans)	ANID	An11g06670	208898
r900	:	SLF + ATP ⇒ PPI + APS	2.7.7.4	ATP sulfurylase	Buxton et al. (1989)	ANID	An11g09790	209058
r901	:	APS + ATP ⇒ ADP + PAPS	2.7.1.25	Adenylylsulfate kinase	Borges-Walmsley et al. (1995); Clarke et al. (1997); Sieńko and Paszewski (1999, A. nidulans)	ANID	An08g02990	208264
r902	:	PAPS + RTHIO ⇒ OTHIO + H2SO3 + PAP	1.8.4.8	PAPS reductase	Borges-Walmsley et al. (1995); Sieńko and Paszewski (1999, A. nidulans)	ANID	An11g09780	56053
r903	:	CHOSLF + H2O ⇆ CHO + SLF	3.1.6.6	Choline sulphatase	Scott and Spencer (1968, A. nidulans)	ANEW	An08g08950	55721
r904	:	PAPS + CHO ⇆ PAP + CHOSLF	2.8.2.6	choline sulfotransferase	Hussey and Spencer (1966, A. nidulans)	ANEW		
r905	:	PAP + H2O ⇒ AMP + PI	3.1.3.7	3' - 5' bisphosphate nucleotidase		ANID	An11g06820	208912
r112	:	H2SO3 ⇆ S + O2 + H2O	1.13.11.18	Sulfur dioxygenase	Tepper et al. (1966, Inferred)	ANEW		
Nitrogen metabolism								
r906	:	HNO3 + NADPH ⇒ HNO2 + NADP + H2O	1.7.1.3	Nitrate reductase (niaD)	Unkles et al. (1992)	ANID	An08g05610	208048
r907	:	HNO2 + 3 NADPH ⇒ NH4OH + 3 NADP + H2O	1.7.1.4	Nitrite reductase	Unkles et al. (1992)	ANID	An08g05640	198539
r908	:	NH4OH ⇆ NH3 + H2O	Non enzymatic step	Non enzymatic reaction		ANEW		
r909	:	UREA + ATP + H2O + CO2 ⇆ ADP + PI + UREAC	6.3.4.6	Urea carboxylase		ANID	An01g13810	172796
r910	:	UREAC ⇒ 2 NH3 + 2 CO2	3.5.1.54	Allophanate hydrolase		ANID		

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
r911	:	ACNL ⇒ INAC + NH3	3.5.5.1	Nitrilase	Snajdrova et al. (2004)	ANID		An16g00550; An01g07510; An01g12090; An06g01960; An08g08940; An08g10150; An12g01260; An16g06210; An18g01740	41410; 35944; 170270; 175987; N/A; 52578; 141873; 40928; 211815
r912	:	UREA + H2O ⇒ CO2 + 2 NH3	3.5.1.5	urease	Ivanov (1925); Smith et al. (1993)	ANEW		An01g03550; An15g00940	52004; 200521
BIOMASS REACTIONS									
POLYMERIZATION REACTIONS (PROTEINS, DNA, RNA)									
Protein formation									
PROTEIN	:	1.033 ALA + 0.413 ARG + 0.209 ASN + 0.628 ASP + 0.079 CYS + 0.899 GLU + 0.300 GLN + 0.862 GLY + 0.205 HIS + 0.396 ILE + 0.704 LEU + 0.651 LYS + 0.105 MET + 0.312 PHE + 0.441 PRO + 0.628 SER + 0.503 THR + 0.126 TRP + 0.205 TYR + 0.536 VAL + 39.729 ATP + 30.489 H2O ⇒ 39.729 ADP + 39.729 PI + Protein	Artificial	Artificial reaction		ANEW			
RNA formation									
RNA	:	0.773 AMP + 0.931 GMP + 0.773 CMP + 0.616 UMP + 7.423 ATP + 4.330 H2O ⇒ 7.424 ADP + 7.424 PI + RNA	2.7.7.6	DNA-directed RNA polymerase		ANEW	*	An01g02200; An01g04380; An01g05740; An01g07250; An01g11950; An01g12710; An02g01800; An02g05460; An02g11470; An08g07050; An09g04100; An11g01770; An11g09370; An12g00720; An12g00780; An12g03900; An13g00280; An15g00700; An15g05780; An15g05790; An16g07430	196819; 36183; 171679; 143936; 205564; 205506; 52135; 206792; 128750; 176941; 128642; 55936; 39394; 54460; 190142; 211641; 57188; 40356; 48809; 48810; 55082
DNA formation									

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ID		Reaction	EC no	Enzyme	Source	Model		CBS	ATCC
DNA	:	0.794 DAMP + 0.826 DCMP + 0.794 DTMP + 0.826 DGMP + 11.019 ATP + 7.778 H2O ⇒ 11.019 ADP + 11.019 PI + DNA	2.7.7.7	DNA-directed DNA polymerase		ANEW	*	An02g02510; An02g14830; An04g02280; An08g02440; An11g00720; An11g09550; An14g06200; An14g06560; An15g07150; An16g03060	206569; 173303; 213157; 176678; 179102; 179788; 184522; 185612; 210383; 53636
Cell wall composition									
Cellwall	:	0.043 GAG + 0.254 NIG + 0.337 PSNIG + 0.381 GGM + 0.389 14GLUCAN + 2.726 13GLUCAN + 1.623 CHIT ⇒ CELLWALL	Artificial	Artificial reaction		ANEW			
Lipids:									
Lipidsassemb	:	0.010083 TAGLY + 0.001009 DAGLY + 0.008912 MAGLY + 0.000223 C140 + 0.001480 C160 + 0.000245 C180 + 0.001678 C181 + 0.001664 C182 + 0.000047 C183 + 0.034062 ERGOST + 0.010038 ERGOSE + 0.030053 MGDG + 0.012374 MGC181 + 0.007859 DGDG + 0.000005 TGDMIPC + 0.000030 CERB1 + 0.000031 CERB2 + 0.000025 GALCER + 0.000024 GLUCER1 + 0.000024 GLUCER2 + 0.001746 CL + 0.015312 PC + 0.000359 PS + 0.034807 PE ⇒ LIPIDS	Artificial	Artificial reaction		ANEW			
Small molecules pool:									
Pool	:	0.00039 ICIT + 0.013 CIT + 0.00091 SUCC + 0.00007 FUM + 0.00065 MAL + 0.0017 NAD + 0.00018 NADH + 0.00014 NADP + 0.00008 NADPH + 0.04 TRE + 0.18 MNT + 0.46 GL + 0.3 EOL + 0.01 AOL ⇒ POOL	Artificial	Artificial reaction		ANEW			
Biomass formation									
GROWTH	:	0.263 Protein + 0.00244 DNA + 0.01814 RNA + LIPIDS + POOL + 0.38 CELLWALL + 61 ATP + 61 H2O ⇒ 61 ADP + 61 PI + BIOMASS	Artificial	Artificial reaction		ANEW			
Maintenance requirements (non-growth associated)									
m_ATP	:	ATP + H2O ⇒ ADP + PI	Artificial	Artificial reaction		ANIG, ANID			
TRANSPORT PROCESSES									
Non-carrier-mediated (free diffusion)									
Across the cytoplasmastic membrane									
Others:									
r1092	:	CO2e ⇆ CO2			David et al. (2003)	ANIG, ANID			

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1093	:	H2Oe ⇆ H2O			David et al. (2003)	ANIG, ANID		
r1094	:	O2e ⇒ O2			David et al. (2003)	ANIG, ANID		
r1091	:	H2O2e ⇆ H2O2			Pel et al. (2007)	ANEW		
Alcohols:								
r1071	:	ETHe ⇆ ETH			David et al. (2003)	ANIG, ANID		
r1141	:	METHOLe ⇆ METHOL			David et al. (2003)	ANIG, ANID		
Acids:								
r1069	:	ACe ⇆ AC			David et al. (2003)	ANIG, ANID		
r1142	:	FORe ⇆ FOR			Hauge (1957, Inferred)	ANID		
r1066	:	LACe ⇆ LAC			Netik et al. (1997)	ANIG, ANID		
r1065	:	LLACe ⇆ LLAC			Netik et al. (1997)	ANIG, ANID		
Across the mitochondrial membrane								
Others:								
r1150	:	H2O ⇆ H2Om			David et al. (2003)	ANIG, ANID		
r1153	:	O2 ⇆ O2m			David et al. (2003)	ANIG, ANID		
r1152	:	CO2 ⇆ CO2m			David et al. (2003)	ANIG, ANID		
r1151	:	NH3 ⇆ NH3m			David et al. (2003)	ANIG, ANID		
Alcohols:								
r1149	:	ETH ⇆ ETHm				ANID		
Aldehydes:								
r1148	:	ACAL ⇆ ACALm				ANID		
Acids:								
r1147	:	AC ⇆ ACm			David et al. (2003)	ANIG, ANID		
Fatty acids:								
r1014	:	C40e ⇆ C40			Chattopadhyay et al. (1985b)	ANEW		
r1015	:	C60e ⇆ C60			Chattopadhyay et al. (1985b)	ANEW		
r1016	:	C80e ⇆ C80			Chattopadhyay et al. (1985b)	ANEW		
r1017	:	C100e ⇆ C100			Chattopadhyay et al. (1985b)	ANEW		
r1018	:	C120e ⇆ C120			Chattopadhyay et al. (1985b)	ANEW		
r1019	:	C140e ⇆ C140			Chattopadhyay et al. (1985b)	ANEW		
r1020	:	C141e ⇆ C141			Chattopadhyay et al. (1985b)	ANEW		
r1021	:	C150e ⇆ C150			Chattopadhyay et al. (1985b)	ANEW		
r1022	:	C160e ⇆ C160			Chattopadhyay et al. (1985b)	ANEW		
r1023	:	C161e ⇆ C161			Chattopadhyay et al. (1985b)	ANEW		
r1024	:	C162e ⇆ C162			Chattopadhyay et al. (1985b)	ANEW		
r1025	:	C170e ⇆ C170			Chattopadhyay et al. (1985b)	ANEW		
r1026	:	C171e ⇆ C171			Chattopadhyay et al. (1985b)	ANEW		
r1027	:	C180e ⇆ C180			Chattopadhyay et al. (1985b)	ANEW		
r1028	:	C181e ⇆ C181			Chattopadhyay et al. (1985b)	ANEW		
r1029	:	C182e ⇆ C182			Chattopadhyay et al. (1985b)	ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1030	:	C183e ⇆ C183			Chattopadhyay et al. (1985b)	ANEW		
r1031	:	C190e ⇆ C190			Chattopadhyay et al. (1985b)	ANEW		
r1032	:	C191e ⇆ C191			Chattopadhyay et al. (1985b)	ANEW		
r1033	:	C192e ⇆ C192			Chattopadhyay et al. (1985b)	ANEW		
r1034	:	C200e ⇆ C200			Chattopadhyay et al. (1985b)	ANEW		
Carrier-mediated								
Across the cytoplasmatic membrane								
Nucleotide related								
r1124	:	ATPe ⇆ ATP		ATP permease	Chowdhury et al. (1997)	ANEW		
r1123	:	AMPe ⇆ AMP		AMP permease	Inferred	ANEW		
r1125	:	ATNe ⇆ ATN		Allantoin permease	Arst and Cove (1969); Martinelli and Kinghorn (1994, A. nidulans)	ANEW		
r1119	:	HYXNe ⇆ HYXN		Hypoxanthine permease	Arst and Cove (1969); Martinelli and Kinghorn (1994, A. nidulans)	ANEW		
r1120	:	URAe ⇆ URAe		Uracil permease	Experimental	ANEW		
r1121	:	URIe ⇆ URIe		Uridine permease	Experimental	ANEW		
r1180	:	ADe ⇆ AD		adenine permease	Martinelli and Kinghorn (1994, A. nidulans)	ANEW		
r1129	:	QUINe ⇆ QUIN		Quinolinate permease		ANEW		
r1126	:	NICAe ⇆ NICA		Nicotinate permease		ANEW		
r1127	:	NICDe ⇆ NICD		Nicotinamide permease		ANEW		
r1122	:	XANe ⇆ XAN		Xanthine permease	Taha and Sharabash (1956, Inferred), Martinelli and Kinghorn (1994, A. nidulans)	ANEW		
r1128	:	KYNe ⇆ KYN		L-Kynurenine permease		ANEW		
r1214	:	3CPYRDe ⇆ 3CPYRD			Snajdrova et al. (2004, Inferred)	ANEW		
Aromatics and catabolic products								
r1182	:	ANe ⇆ AN		Anthranilate transporter	Kamath et al. (1987, Inferred)	ANEW		
r1074	:	PHACe ⇆ PHAC		Phenylacetate transporter	Sugumaran et al. (1973, Inferred)	ANEW		
r1076	:	DMANDe ⇆ DMAND		Mandelate-transporter	Jamaluddin et al. (1970, Inferred)	ANEW		
r1075	:	LMANDe ⇆ LMAND		Mandelate-transporter	Jamaluddin et al. (1970, Inferred)	ANEW		
r1073	:	PHALe ⇆ PHAL				ANEW		
r1078	:	BAe ⇆ BA		benzoate transporter	Martinelli and Kinghorn (1994, Inferred)	ANEW		
r1077	:	BNe ⇆ BN				ANEW		
r1084	:	DHSKe ⇆ DHSK				ANEW		
r1082	:	SALIe ⇆ SALI		salicylate transporter	Krupka et al. (1967); Martinelli and Kinghorn (1994, Inferred)	ANEW		
r1072	:	PHPYRe ⇆ PHPYR				ANEW		
r1079	:	BAMNe ⇆ BAMN				ANEW		
r1083	:	RESe ⇆ RES				ANEW		
r1272	:	COUMe ⇆ COUM			Milstein et al. (1988, Inferred)	ANEW		
r1197	:	DMTe ⇆ DMT			Ganji et al. (1995, Inferred)	ANEW		
r1198	:	TPHTHe ⇆ TPHTH			Ganji et al. (1995, Inferred)	ANEW		
r1199	:	PCCe ⇆ PCC			Ganji et al. (1995, Inferred)	ANEW		
r1204	:	FERe ⇆ FER				ANEW		
r1205	:	VANe ⇆ VAN				ANEW		
r1209	:	INDe ⇆ IND			Kamath and Vaidyanathan (1990, Inferred)	ANEW		
r1212	:	3HBAe ⇆ 3HBA				ANEW		
Alkylamines								
r1190	:	BUTN ⇆ BUTNe				ANEW		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1223	:	PENN ⇆ PENNe				ANEW		
Others								
r1095	:	PIe ⇆ PI			Seshadri et al. (2004, Inferred)	ANIG, ANID		
r1087	:	NH3e ⇆ NH3			David et al. (2003)	ANEW		
r1086	:	HNO3e ⇆ HNO3			Seshadri et al. (2004, Inferred)	ANEW		
r1088	:	H2SO3e ⇒ H2SO3				ANID		
r1089	:	CHOSLFe ⇆ CHOSLF		Choline sulphate permease	Scott and Spencer (1968, A. nidulans)	ANEW		
r1090	:	SLFe ⇆ SLF		Sulphate permease	Marzluf (1993); Borges-Walmsley et al. (1995, A. nidulans)	ANIG		
r1118	:	DTBe ⇆ DTB			Parry and Naidu (1980, Inferred)	ANEW		
r1085	:	UREAe ⇆ UREA			Ivanov (1925)	ANEW		
r1012	:	OTA ⇒ OTAe		Ochratoxin A exporter		ANEW		
r1273	:	GLYNe ⇆ GLYN			Witteveen et al. (1990, Inferred)	ANEW		
CARBOHYDRATES								
Dissacharides								
r1143	:	TREe ⇆ TRE				ANID		
r1144	:	LACTe ⇒ LACT				ANIG, ANID		
r1145	:	MLTe ⇒ MLT			Pendl et al. (2004)	ANIG, ANID		
Monosacharides								
Hexoses								
r1037	:	GLACe ⇒ GLAC			vanKuyk et al. (2004)	ANIG, ANID		
r1047	:	GLCe ⇒ GLC			Karaffa et al. (2001)	ANIG, ANID		
r1048	:	DGLCe ⇆ DGLC				ANIG		
r1046	:	bDGLCe ⇒ bDGLC			David et al. (2003)	ANIG, ANID		
r1044	:	FRUe ⇒ FRU			Karaffa et al. (2001); vanKuyk et al. (2004)	ANIG, ANID		
r1041	:	MANe ⇒ MAN			vanKuyk et al. (2004)	ANIG, ANID		
r1039	:	IDOLe ⇆ IDOL				ANIG, ANID		
r1040	:	SORe ⇆ SOR			Seshadri et al. (2004, Inferred)	ANIG, ANID		
r1221	:	RHAe ⇆ RHA			Fries and Kallstromer (1965, Inferred)	ANEW		
Pentoses								
r1052	:	ARABe ⇒ ARAB			David et al. (2003)	ANIG, ANID		
r1059	:	LARABe ⇒ LARAB			de Groot et al. (2003)	ANIG, ANID		
r1049	:	RIBe ⇒ RIB			David et al. (2003)	ANIG, ANID		
r1051	:	RLe ⇒ RL				ANID		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1054	:	XYLe ⇒ XYL			Martinelli and Kinghorn (1994); Prathumpai et al. (2003); de Groot et al. (2003); vanKuyk et al. (2004)	ANIG, ANID		
r1055	:	XULe ⇒ XUL				ANID		
r1056	:	LXULe ⇒ LXUL				ANID		
Tetroses								
r1062	:	Ee ⇒ E			Schuurink et al. (1990)	ANID		
r1060	:	EUe ⇒ EU				ANID		
ALCOHOLS (polyols)								
r1064	:	GLe ⇆ GL			Martinelli and Kinghorn (1994)	ANIG, ANID		
r1061	:	EOLe ⇆ EOL			David et al. (2003)	ANIG, ANID		
r1053	:	AOLe ⇆ AOL			Martinelli and Kinghorn (1994)	ANIG, ANID		
r1058	:	LAOLe ⇆ LAOL			Martinelli and Kinghorn (1994)	ANIG, ANID		
r1050	:	RIBOLe ⇆ RIBOL			David et al. (2003)	ANIG, ANID		
r1057	:	XOLe ⇆ XOL			Prathumpai et al. (2003)	ANIG, ANID		
r1038	:	GALOLe ⇆ GALOL				ANID		
r1043	:	MNTe ⇆ MNT			Martinelli and Kinghorn (1994)	ANIG, ANID		
r1042	:	SOTe ⇆ SOT			Martinelli and Kinghorn (1994)	ANIG, ANID		
ACIDS								
TCA cycle related organic acids								
r1139	:	MALe ⇆ MAL			Netik et al. (1997); Alvarez-Vasquez et al. (2000)	ANIG, ANID		
r1138	:	AKGe ⇆ AKG			Netik et al. (1997)	ANIG, ANID		
r1137	:	ACOe ⇆ ACO				ANID		
r1134	:	CITe ⇆ CIT			Burgstaller (2006); Netik et al. (1997)	ANIG, ANID		
r1136	:	FUMe ⇆ FUM			David et al. (2003)	ANIG, ANID		
r1135	:	ICITe ⇆ ICIT			Netik et al. (1997)	ANID		
r1140	:	OXALe ⇆ OXAL			David et al. (2003)	ANIG, ANID		
r1132	:	OAe ⇆ OA				ANID		
r1131	:	PYRe ⇆ PYR			Netik et al. (1997); Alvarez-Vasquez et al. (2000)	ANIG, ANID		
r1130	:	SUCCe ⇆ SUCC			Netik et al. (1997)	ANIG, ANID		
Other acids								
r1036	:	GALNTe ⇆ GALNT				ANID		
r1035	:	GALUNTe ⇒ GALUNT			Martinelli and Kinghorn (1994)	ANIG, ANID		
r1045	:	GLCNTe ⇆ GLCNT			Muller (1986, Inferred)	ANIG, ANID		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1179	:	GLCUNTe ⇆ GLCUNT			David et al. (2003)	ANIG, ANID		
r1178	:	KOJAe ⇆ KOJA				ANID		
r1063	:	TARe ⇆ TAR			Patil and Ramakrishnan (1966)	ANIG, ANID		
r1067	:	PROPe ⇆ PROP			Sealy-Lewis and Fairhurst (1998, Inferred)	ANIG, ANID		
r1096	:	QTe ⇆ QT			Cain (1972a, Inferred)	ANEW		
r1097	:	SMEe ⇆ SME			Cain (1972a, Inferred)	ANEW		
r1185	:	GABAe ⇆ GABA			Kumar and Punekar (1998, Inferred)	ANEW	An16g02000	210724
AMINO ACIDS								
r1098	:	GLYe ⇒ GLY				ANID		
r1099	:	ALAe ⇒ ALA			Oganesyan et al. (1998, Inferred)	ANID		
r1100	:	bALAe ⇒ bALA			Sarma et al. (1961, Inferred)	ANID		
r1101	:	ARGe ⇒ ARG				ANID		
r1102	:	ASNe ⇒ ASN				ANID		
r1103	:	ASPe ⇒ ASP			Sarma et al. (1961, Inferred)	ANID		
r1104	:	CYSe ⇒ CYS				ANID		
r1105	:	GLUe ⇒ GLU				ANID		
r1106	:	GLNe ⇒ GLN			Ram et al. (2004, Inferred)	ANID		
r1107	:	HISe ⇒ HIS				ANID		
r1108	:	ILEe ⇒ ILE				ANID		
r1109	:	LEUe ⇒ LEU				ANID		
r1110	:	LYSe ⇒ LYS				ANID		
r1111	:	METe ⇒ MET				ANID		
r1112	:	PHEe ⇒ PHE				ANID		
r1113	:	PROe ⇒ PRO			Jones et al. (1981, A. nidulans)	ANID		
r1114	:	SERe ⇒ SER				ANID		
r1115	:	THRe ⇒ THR				ANID		
r1080	:	TRPe ⇒ TRP			Sarma et al. (1961, Inferred)	ANID		
r1116	:	TYRe ⇒ TYR				ANID		
r1117	:	VALe ⇒ VAL				ANID		
r1184	:	CITRe ⇆ CITR			Lenouvel et al. (2002, Inferred)	ANEW		
r1187	:	ORNe ⇆ ORN			Lenouvel et al. (2002, Inferred)	ANEW		
ALDEHYDES								
r1068	:	PROPALe ⇒ PROPAL			Kazimirova and Novotel'nov (1956, Inferred)	ANEW		
r1070	:	ACALe ⇆ ACAL			Rippel and Wiangke (1941, Inferred)	ANEW		
Across the mitochondrial membrane								
OTHERS								
r1154	:	PIm ⇆ PI		Phosphate carrier		ANIG, ANID		
r1181	:	UREA ⇆ UREAm				ANEW		
ACIDS								
r1146	:	PYR ⇒ PYRm			Karaffa et al. (2001); Karaffa and Kubicek (2003)	ANIG, ANID		
r1169	:	CITm + MAL ⇒ CIT + MALm			Karaffa et al. (2001); Karaffa and Kubicek (2003); Pel et al. (2007)	ANIG, ANID	An11g11230; An18g00070	136079; 42578
r1170	:	ACOm + MAL ⇒ ACO + MALm				ANID		

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ID		Reaction	EC no	Enzyme	Source	Model	CBS	ATCC
r1171	:	ICITm + MAL ⇒ ICIT + MALm			David et al. (2003)	ANIG, ANID		
r1172	:	AKG ⇆ AKGm				ANID		
r1173	:	OA ⇆ OAm			Karaffa et al. (2001); Pel et al. (2007)	ANID	An14g06860	41991
r1174	:	SUCC ⇆ SUCCm			David et al. (2003)	ANIG, ANID		
r1175	:	FUM ⇆ FUMm				ANID		
r1176	:	ICIT ⇆ ICITm				ANIG, ANID		
r1168	:	FOR ⇆ FORm			Cossins and Chen (1997, Inferred)	ANEW		
r1166	:	THF ⇆ THFm			Cossins and Chen (1997, Inferred)	ANEW		
r1167	:	METTHF ⇆ METTHFm			Cossins and Chen (1997, Inferred)	ANEW		
r1177	:	CAP ⇆ CAPm				ANEW		
r1155	:	3OA ⇆ 3OAm				ANEW		
r1186	:	GABA ⇆ GABAm			Kumar and Punekar (1998, Inferred)	ANEW		
r1133	:	GLX ⇆ GLXm				ANEW		
r1191	:	PROPm ⇆ PROP				ANEW		
AMINO ACIDS								
r1158	:	THRm ⇆ THR				ANEW		
r1159	:	ARGm ⇆ ARG				ANEW		
r1160	:	ASPm ⇆ ASP				ANEW		
r1161	:	LEUm ⇆ LEU				ANEW		
r1162	:	ILEm ⇆ ILE				ANEW		
r1163	:	ORNm ⇆ ORN				ANEW		
r1164	:	VALm ⇆ VAL				ANEW		
r1165	:	LYSm ⇆ LYS				ANEW		
r1183	:	CITR ⇆ CITRm			Lenouvel et al. (2002, Inferred)	ANEW		
Shuttles								
Malate-Aspartate shuttle								
r1157	:	ASPm + GLU ⇆ ASP + GLUm			David et al. (2003)	ANIG, ANID		
r1156	:	MAL + AKGm ⇆ MALm + AKG				ANID		

Suppl. Table II: List of the abbreviations for metabolite-names used in the reaction list of A. niger iMA871 (Suppl. Table I) and their full name. An "m" denotes that the metabolite is found in the mitochondrion, whereas an "e" is used to mark an extracellular metabolite.

Abbreviation	**Full name**
13GLUCAN	1,3-beta-D-Glucan
13GLUCANe	1,3-beta-D-Glucan (extracellular)
13PDG	1,3-Bisphospho-D-glycerate
14GLUCAN	1,4-alphaglucan
2D3DGALT	2-Dehydro-3-deoxy-D-galactonate
2HPAC	2-hydroxyphenylacetic acid
2MAC	2-maleyl acetate
2MACOm	2-methyl aconitate
2MCITm	2-methyl citrate
2MICITm	2-methyl isocitrate
2PG	2-Phospho-D-glycerate
345THBe	Gallic acid
3CMUCO	3-Carboxymuconate
3CPYRD	3-cyanopyridine
3CPYRDe	3-cyanopyridine (extracellular)
3DDAH7P	2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate
3FPYR	3-fumarylpyruvate
3HBA	3-hydroxybenzoate; m-hydroxybenzoate
3HBAe	3-hydroxybenzoate; m-hydroxybenzoate (extracellular)
3HIND	3-hydroxyindoxyle
3HPYR	3-hydroxypyruvate
3MPYR	3-maleylpyruvate
3OA	3-oxoadipate
3OACOAm	3-oxoadipyl-CoA
3OAm	3-oxoadipate
3PG	3-Phospho-D-glycerate
3PSER	3-Phosphoserine
3PSME	5-O-(1-Carboxyvinyl)-3-phosphoshikimate
4CMUCL	4-Carboxymuconolactone
4HBA	4-hydroxybenzoic acid
4HBAL	4-hydroxybenzaldehyde
4HBFOR	4-hydroxybenzoylformic acid
4HMAND	4-hydroxymandelate

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Abbreviation	Full name
4HPAC	4-hydroxyphenylacetic acid
4HPP	3-(4-Hydroxyphenyl)pyruvate
4PPNCYS	(R)-4'-Phosphopantothenoyl-L-cysteine
4PPNTE	Pantetheine 4'-phosphate
4PPNTO	D-4'-Phosphopantothenate
AACACP	Acetoacetyl [acyl-carrier protein]
AACCOA	Acetoacetyl coenzyme A
AACCOAm	Acetoacetyl coenzyme A (mitochondrial)
AAMYLe	Alpha-amylase (secreted to the medium)
ABUTm	2-Aceto-2-hydroxy butyrate (mitochondrial)
AC	Acetate
ACACP	Acyl-[acyl-carrier protein]
ACAL	Acetaldehyde
ACALe	Acetaldehyde, extracellular
ACALm	Acetaldehyde (mitochondrial)
ACCOA	Acetyl coenzyme A
ACCOAm	Acetyl coenzyme A (mitochondrial)
ACe	Acetate (extracellular)
ACLACm	2-Acetolactate (mitochondrial)
ACm	Acetate (mitochondrial)
ACNL	3-Indoleacetonitrile
ACO	cis-Aconitate
ACOe	cis-Aconitate (extracellular)
ACOm	cis-Aconitate (mitochondrial)
ACP	Acyl-carrier protein
ACTAC	Acetoacetate
ACTP	Acetyl phosphate
ACYBUT	gamma-Amino-gamma-cyanobutanoate
AD	Adenine
ADCHOR	4-Amino-4-deoxychorismate
ADe	Adenine (extracellular)
ADHLIPOm	S-Acetyldihydrolipoamide (mitochondrial)
ADN	Adenosine
ADP	ADP
ADPm	ADP (mitochondrial)
ADPR	ADP-Ribose
AHHMD	2-Amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)pteridine

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Abbreviation	Full name
AHHMP	2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine
AHTD	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)-dihydropteridine triphosphate
AICAR	AICAR
AIR	Aminoimidazole ribotide
AKAm	2-Oxoadipate (mitochondrial)
AKG	2-Oxoglutarate
AKGe	2-Oxoglutarate (extracellular)
AKGE1m	Alpha-ketoglutarate bound to alpha-ketoglutarate dehydrogenase
AKGE2m	Alpha-ketoglutarate bound to dihydrolipoyl transsuccinylase
AKGm	2-Oxoglutarate (mitochondrial)
AKP	2-Dehydropantoate
ALA	L-Alanine
ALAe	L-Alanine (extracellular)
ALAm	L-Alanine (mitochondrial)
AMAm	2-aminoadipate (mitochondrial)
AMASAm	2-aminoadipate-semialdehyde (mitochondrial)
AMP	AMP
AMPe	AMP, extracellular
AMPm	AMP (mitochondrial)
AMYLPe	Amylopectin (extracellular)
AMYLSe	Amylose (extracellular)
AN	Anthranilate
ANe	Anthranilate (extracellular)
AOL	D-Arabitol
AOLe	D-Arabitol (extracellular)
AONA	8-Amino-7-oxononanoate
APROP	alpha-Aminopropiononitrile
APS	Adenylylsulfate
ARAB	D-Arabinose
ARABe	D-Arabinose (extracellular)
ARABINe	Arabinan (extracellular)
ARABLAC	D-Arabinono-1,4-lactone
ARG	L-Arginine
ARGe	L-Arginine (extracellular)
ARGm	L-Arginine (mitchondrial)

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Abbreviation	Full name
ARGSUCCm	Argininosuccinate (mitchondrial)
ASER	O-Acetyl-L-serine
ASN	L-Asparagine
ASNe	L-Asparagine (extracellular)
ASP	L-Aspartate
ASPe	L-Aspartate (extracellular)
ASPm	L-Aspartate (mitochondrial)
ASPSA	L-Aspartate 4-semialdehyde
ASUC	N6-(1,2-Dicarboxyethyl)-AMP
ATN	Allantoin
ATNe	Allantoin (extracellular)
ATP	ATP
ATPe	ATP (extracellular)
ATPm	ATP (mitochondrial)
ATT	Allantoate
BA	Benzoic acid
BAe	Benzoic acid (extracellular)
BAL	Benzaldehyde
bALA	beta-Alanine
bALAe	beta-Alanine (extracellular)
BAMN	Benzoylamine
BAMNe	Benzoylamine (extracellular)
BASP	4-Phospho-L-aspartate
BCCP	Biotin-carboxyl-carrier protein
bDG6P	beta-D-Glucose 6-phosphate
bDGLC	beta-D-Glucose
bDGLCe	beta-D-Glucose (extracellular)
BFOR	Benzoylformate
bFRU	beta-D-fructose
bGLAC	beta-D-galactose
bLARAB	beta-L-arabinose
BN	Benzonitrile
BNe	Benzonitrile (extracellular)
BT	Biotin
BTe	Biotin (extracellular)
BTOL	benzene-1,2,4-triol
BUTAL	Butanal
BUTN	n-butylamine
BUTNe	n-butylamine (extracellular)

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Abbreviation	Full name
C100	Decanoate
C100ACP	Decanoyl-[acyl-carrier protein]
C100COA	Decanoyl-CoA
C100COAm	Decanoyl-CoA (mitochondrial)
C100e	Decanoate (extracellular)
C10DACP	Dec-2-enoyl-[acyl-carrier protein]
C10DCOAm	Dec-2-enoyl-CoA (mitochondrial)
C10HACP	3-hydroxydecanoyl-[acyl-carrier protein]
C10HCOAm	3-hydroxydecanoyl-CoA (mitochondrial)
C10OACP	3-oxodecanoyl-[acyl-carrier protein]
C10OCOAm	3-oxodecanoyl-CoA (mitochondrial)
C110ACP	Undecanoyl-[acyl-carrier protein]
C110COAm	Undecanoyl-CoA (mitochondrial)
C11DACP	Undec-2-enoyl-[acyl-carrier protein]
C11DCOAm	Undec-2-enoyl-CoA (mitochondrial)
C11HACP	3-hydroxyundecanoyl-[acyl-carrier protein]
C11HCOAm	3-hydroxyundecanoyl-CoA (mitochondrial)
C11OACP	3-oxoundecanoyl-[acyl-carrier protein]
C11OCOAm	3-oxoundecanoyl-CoA (mitochondrial)
C120	Dodecanoate
C120ACP	Dodecanoyl-[acyl-carrier protein]
C120CAR	Dodecanoyl-carnitine
C120CARm	Dodecanoyl-carnitine (mitochondrial)
C120COA	Dodecanoyl-CoA
C120COAm	Dodecanoyl-CoA (mitochondrial)
C120e	Dodecanoate (extracellular)
C12DACP	Dodec-2-enoyl-[acyl-carrier protein]
C12DCOAm	Dodec-2-enoyl-CoA (mitochondrial)
C12HACP	3-hydroxydodecanoyl-[acyl-carrier protein]
C12HCOAm	3-hydroxydodecanoyl-CoA (mitochondrial)
C12OACP	3-oxododecanoyl-[acyl-carrier protein]
C12OCOAm	3-oxododecanoyl-CoA (mitochondrial)
C130ACP	Tridecanoyl-[acyl-carrier protein]
C130COAm	Tridecanoyl-CoA (mitochondrial)
C13DACP	Tridec-2-enoyl-[acyl-carrier protein]
C13DCOAm	Tridec-2-enoyl-CoA (mitochondrial)
C13HACP	3-hydroxytridecanoyl-[acyl-carrier protein]
C13HCOAm	3-hydroxytridecanoyl-CoA (mitochondrial)
C13OACP	3-oxotridecanoyl-[acyl-carrier protein]

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Abbreviation	Full name
C13OCOAm	3-oxotridecanoyl-CoA (mitochondrial)
C140	Tetradecanoate
C140ACP	Tetradecanoyl-[acyl-carrier protein]
C140CAR	Tetradecanoyl-carnitine
C140CARm	Tetradecanoyl-carnitine (mitochondrial)
C140COA	Tetradecanoyl-CoA
C140COAm	Tetradecanoyl-CoA (mitochondrial)
C140e	Tetradecanoate (extracellular)
C141	Tetradecenoate
C141ACP	Tetradecenoyl-[acyl-carrier protein]
C141CAR	Tetradecenoyl-carnitine
C141CARm	Tetradecenoyl-carnitine (mitochondrial)
C141COA	Tetradecenoyl-CoA
C141COAm	Tetradecenoyl-CoA (mitochondrial)
C141e	Tetradecenoate (extracellular)
C14DACP	Tetradec-2-enoyl-[acyl-carrier protein]
C14DCOAm	Tetradec-2-enoyl-CoA (mitochondrial)
C14HACP	3-hydroxytetradecanoyl-[acyl-carrier protein]
C14HCOAm	3-hydroxytetradecanoyl-CoA (mitochondrial)
C14OACP	3-oxotetradecanoyl-[acyl-carrier protein]
C14OCOAm	3-oxotetradecanoyl-CoA (mitochondrial)
C150	Pentadecanoate
C150ACP	Pentadecanoyl-[acyl-carrier protein]
C150CAR	Pentadecanoyl-carnitine
C150CARm	Pentadecanoyl-carnitine (mitochondrial)
C150COA	Pentadecanoyl-CoA
C150COAm	Pentadecanoyl-CoA (mitochondrial)
C150e	Pentadecanoate (extracellular)
C15DACP	Pentadec-2-enoyl-[acyl-carrier protein]
C15DCOAm	Pentadec-2-enoyl-CoA (mitochondrial)
C15HACP	3-hydroxypentadecanoyl-[acyl-carrier protein]
C15HCOAm	3-hydroxypentadecanoyl-CoA (mitochondrial)
C15OACP	3-oxopentadecanoyl-[acyl-carrier protein]
C15OCOAm	3-oxopentadecanoyl-CoA (mitochondrial)
C160	Hexadecanoate
C160ACP	Hexadecanoyl-[acyl-carrier protein]
C160CAR	Hexadecanoyl-carnitine
C160CARm	Hexadecanoyl-carnitine (mitochondrial)
C160COA	Hexadecanoyl-CoA

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Abbreviation	Full name
C160COAm	Hexadecanoyl-CoA (mitochondrial)
C160e	Hexadecanoate (extracellular)
C161	Hexadecenoate
C161ACP	Hexadecenoyl-[acyl-carrier protein]
C161CAR	Hexadecenoyl-carnitine
C161CARm	Hexadecenoyl-carnitine (mitochondrial)
C161COA	Hexadecenoyl-CoA
C161COAm	Hexadecenoyl-CoA (mitochondrial)
C161e	Hexadecenoate (extracellular)
C162	Hexadecadienoate
C162ACP	Hexadecadienoyl-[acyl-carrier protein]
C162CAR	Hexadecadienoyl-carnitine
C162CARm	Hexadecadienoyl-carnitine (mitochondrial)
C162COA	Hexadecadienoyl-CoA
C162COAm	Hexadecadienoyl-CoA (mitochondrial)
C162e	Hexadecadienoate (extracellular)
C16DACP	Hexadec-2-enoyl-[acyl-carrier protein]
C16DCOAm	Hexadec-2-enoyl-CoA (mitochondrial)
C16HACP	3-hydroxyhexadecanoyl-[acyl-carrier protein]
C16HCOAm	3-hydroxyhexadecanoyl-CoA (mitochondrial)
C16OACP	3-oxohexadecanoyl-[acyl-carrier protein]
C16OCOAm	3-oxohexadecanoyl-CoA (mitochondrial)
C170	Heptadecanoate
C170ACP	Heptadecanoyl-[acyl-carrier protein]
C170CAR	Heptadecanoyl-carnitine
C170CARm	Heptadecanoyl-carnitine (mitochondrial)
C170COA	Heptadecanoyl-CoA
C170COAm	Heptadecanoyl-CoA (mitochondrial)
C170e	Heptadecanoate (extracellular)
C171	Heptadecenoate
C171ACP	Heptadecenoyl-[acyl-carrier protein]
C171CAR	Heptadecenoyl-carnitine
C171CARm	Heptadecenoyl-carnitine (mitochondrial)
C171COA	Heptadecenoyl-CoA
C171COAm	Heptadecenoyl-CoA (mitochondrial)
C171e	Heptadecenoate (extracellular)
C17DACP	Heptadec-2-enoyl-[acyl-carrier protein]
C17DCOAm	Heptadec-2-enoyl-CoA (mitochondrial)
C17HACP	3-hydroxyheptadecanoyl-[acyl-carrier protein]

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Abbreviation	Full name
C17HCOAm	3-hydroxyheptadecanoyl-CoA (mitochondrial)
C17OACP	3-oxoheptadecanoyl-[acyl-carrier protein]
C17OCOAm	3-oxoheptadecanoyl-CoA (mitochondrial)
C180	Octadecanoate
C180ACP	Octadecanoyl-[acyl-carrier protein]
C180CAR	Octadecanoyl-carnitine
C180CARm	Octadecanoyl-carnitine (mitochondrial)
C180COA	Octadecanoyl-CoA
C180COAm	Octadecanoyl-CoA (mitochondrial)
C180e	Octadecanoate (extracellular)
C181	Octadecenoate
C181ACP	Octadecenoyl-[acyl-carrier protein]
C181CAR	Octadecenoyl-carnitine
C181CARm	Octadecenoyl-carnitine (mitochondrial)
C181COA	Octadecenoyl-CoA
C181COAm	Octadecenoyl-CoA (mitochondrial)
C181e	Octadecenoate (extracellular)
C182	Octadecadienoate
C182ACP	Octadecadienoyl-[acyl-carrier protein]
C182CAR	Octadecadienoyl-carnitine
C182CARm	Octadecadienoyl-carnitine (mitochondrial)
C182COA	Octadecadienoyl-CoA
C182COAm	Octadecadienoyl-CoA (mitochondrial)
C182e	Octadecadienoate (extracellular)
C183	Octadecatrienoate
C183ACP	Octadecatrienoyl-[acyl-carrier protein]
C183CAR	Octadecatrienoyl-carnitine
C183CARm	Octadecatrienoyl-carnitine (mitochondrial)
C183COA	Octadecatrienoyl-CoA
C183COAm	Octadecatrienoyl-CoA (mitochondrial)
C183e	Octadecatrienoate (extracellular)
C18DACP	Octadec-2-enoyl-[acyl-carrier protein]
C18DCOAm	Octadec-2-enoyl-CoA (mitochondrial)
C18DHSPH	3-dehydrosphinganine(C18)
C18HACP	3-hydroxyoctadecanoyl-[acyl-carrier protein]
C18HCOAm	3-hydroxyoctadecanoyl-CoA (mitochondrial)
C18OACP	3-oxooctadecanoyl-[acyl-carrier protein]
C18OCOAm	3-oxooctadecanoyl-CoA (mitochondrial)
C18PSPH	Phytosphingosine(C18)

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Abbreviation	Full name
C18SPH	Sphinganine(C18)
C190	Nonadecanoate
C190ACP	Nonadecanoyl-[acyl-carrier protein]
C190CAR	Nonadecanoyl-carnitine
C190CARm	Nonadecanoyl-carnitine (mitochondrial)
C190COA	Nonadecanoyl-CoA
C190COAm	Nonadecanoyl-CoA (mitochondrial)
C190e	Nonadecanoate (extracellular)
C191	Nonadecenoate
C191ACP	Nonadecenoyl-[acyl-carrier protein]
C191CAR	Nonadecenoyl-carnitine
C191CARm	Nonadecenoyl-carnitine (mitochondrial)
C191COA	Nonadecenoyl-CoA
C191COAm	Nonadecenoyl-CoA (mitochondrial)
C191DHSPH	3-dehydrosphinganine(C19:1)
C191e	Nonadecenoate (extracellular)
C191SPH	Sphinganine(C19:1)
C192	Nonadecadienoate
C192ACP	Nonadecadienoyl-[acyl-carrier protein]
C192CAR	Nonadecadienoyl-carnitine
C192CARm	Nonadecadienoyl-carnitine (mitochondrial)
C192COA	Nonadecadienoyl-CoA
C192COAm	Nonadecadienoyl-CoA (mitochondrial)
C192e	Nonadecadienoate (extracellular)
C19DACP	Nonadec-2-enoyl-[acyl-carrier protein]
C19DCOAm	Nonadec-2-enoyl-CoA (mitochondrial)
C19HACP	3-hydroxynonadecanoyl-[acyl-carrier protein]
C19HCOAm	3-hydroxynonadecanoyl-CoA (mitochondrial)
C19OACP	3-oxononadecanoyl-[acyl-carrier protein]
C19OCOAm	3-oxononadecanoyl-CoA (mitochondrial)
C200	Eicosanoate
C200ACP	Eicosanoyl-[acyl-carrier protein]
C200CAR	Eicosanoyl-carnitine
C200CARm	Eicosanoyl-carnitine (mitochondrial)
C200COA	Eicosanoyl-CoA
C200COAm	Eicosanoyl-CoA (mitochondrial)
C200e	Eicosanoate (extracellular)
C20DACP	Eicos-2-enoyl-[acyl-carrier protein]
C20DCOAm	Eicos-2-enoyl-CoA (mitochondrial)

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Abbreviation	Full name
C20DHSPH	3-dehydrosphinganine(C20)
C20HACP	3-hydroxyeicosanoyl-[acyl-carrier protein]
C20HCOAm	3-hydroxyeicosanoyl-CoA (mitochondrial)
C20OACP	3-oxoeicosanoyl-[acyl-carrier protein]
C20OCOAm	3-oxoeicosanoyl-CoA (mitochondrial)
C20PSPH	Phytosphingosine(C20)
C20SPH	Sphinganine(C20)
C40	Butanoate
C40ACP	Butanoyl-[acyl-carrier protein]
C40COA	Butanoyl-CoA
C40COAm	Butanoyl-CoA (mitochondrial)
C40e	Butanoate (extracellular)
C4DACP	But-2-enoyl-[acyl-carrier protein]
C4DCOAm	But-2-enoyl-CoA (mitochondrial)
C4HACP	3-hydroxybutanoyl-[acyl-carrier protein]
C4HCOAm	3-hydroxybutanoyl-CoA (mitochondrial)
C50ACP	Pentanoyl-[acyl-carrier protein]
C50COA	Pentanoyl-CoA
C50COAm	Pentanoyl-CoA (mitochondrial)
C5DACP	Pent-2-enoyl-[acyl-carrier protein]
C5DCOAm	Pent-2-enoyl-CoA (mitochondrial)
C5HACP	3-hydroxypentanoyl-[acyl-carrier protein]
C5HCOAm	3-hydroxypentanoyl-CoA (mitochondrial)
C5OACP	3-oxopentanoyl-[acyl-carrier protein]
C5OCOAm	3-oxopentanoyl-CoA (mitochondrial)
C60	Hexanoate
C60ACP	Hexanoyl-[acyl-carrier protein]
C60COA	Hexanoyl-CoA
C60COAm	Hexanoyl-CoA (mitochondrial)
C60e	Hexanoate (extracellular)
C6DACP	Hex-2-enoyl-[acyl-carrier protein]
C6DCOAm	Hex-2-enoyl-CoA (mitochondrial)
C6HACP	3-hydroxyhexanoyl-[acyl-carrier protein]
C6HCOAm	3-hydroxyhexanoyl-CoA (mitochondrial)
C6OACP	3-oxohexanoyl-[acyl-carrier protein]
C6OCOAm	3-oxohexanoyl-CoA (mitochondrial)
C70ACP	Heptanoyl-[acyl-carrier protein]
C70COAm	Heptanoyl-CoA (mitochondrial)
C7DACP	Hept-2-enoyl-[acyl-carrier protein]

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Abbreviation	Full name
C7DCOAm	Hept-2-enoyl-CoA (mitochondrial)
C7HACP	3-hydroxyheptanoyl-[acyl-carrier protein]
C7HCOAm	3-hydroxyheptanoyl-CoA (mitochondrial)
C7OACP	3-oxoheptanoyl-[acyl-carrier protein]
C7OCOAm	3-oxoheptanoyl-CoA (mitochondrial)
C80	Octanoate
C80ACP	Octanoyl-[acyl-carrier protein]
C80COA	Octanoyl-CoA
C80COAm	Octanoyl-CoA (mitochondrial)
C80e	Octanoate (extracellular)
C8DACP	Oct-2-enoyl-[acyl-carrier protein]
C8DCOAm	Oct-2-enoyl-CoA (mitochondrial)
C8HACP	3-hydroxyoctanoyl-[acyl-carrier protein]
C8HCOAm	3-hydroxyoctanoyl-CoA (mitochondrial)
C8OACP	3-oxooctanoyl-[acyl-carrier protein]
C8OCOAm	3-oxooctanoyl-CoA (mitochondrial)
C90ACP	Nonanoyl-[acyl-carrier protein]
C90COAm	Nonanoyl-CoA (mitochondrial)
C9DACP	Non-2-enoyl-[acyl-carrier protein]
C9DCOAm	Non-2-enoyl-CoA (mitochondrial)
C9HACP	3-hydroxynonanoyl-[acyl-carrier protein]
C9HCOAm	3-hydroxynonanoyl-CoA (mitochondrial)
C9OACP	3-oxononanoyl-[acyl-carrier protein]
C9OCOAm	3-oxononanoyl-CoA (mitochondrial)
CAASP	N-Carbamoyl-L-aspartate
CAIR	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate
CALH	2-(3-Carboxy-3-aminopropyl)-L-histidine
cAMP	3',5'-Cyclic AMP
cAMPe	3',5'-Cyclic AMP (extracellular)
CAP	Carbamoyl phosphate
CAPm	Carbamoyl phosphate (Mitochondrial)
CAR	Carnitine
CARm	Carnitine (mitochondrial)
CBCCP	Carboxybiotin-carboxyl-carrier protein
CCL	Catechol
cCMP	3',5'-Cyclic CMP
CDA	Cholesta-8,24-dien-3-ol-4-carboxylate
cdAMP	3',5'-Cyclic dAMP

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Abbreviation	Full name
CDOL	4-methylcholesta-8,24-diene-3-ol
CDP	CDP
CDPDG	CDPdiacylglycerol
CELLOBe	Cellobiose (extracellular)
CELLOTe	Cellotriose (extracellular)
CELLUe	Cellulose (extracellular)
CELLWALL	Cellwall (1 g dry cellwall)
CERB1	Cerebrin 1
CERB1A	Cerebrin 1(comp. A)
CERB1B	Cerebrin 1(comp. B)
CERB1C	Cerebrin 1(comp. C)
CERB1D	Cerebrin 1(comp. D)
CERB2	Cerebrin 2
CERB2A	Cerebrin 2(comp. A)
CERB2B	Cerebrin 2(comp. B)
CERB2C	Cerebrin 2(comp. C)
CERB2D	Cerebrin 2(comp. D)
CEREB1	Cerebroside 1
CEREB2	Cerebroside 2
cGMP	3',5'-Cyclic GMP
CHCOA	6-Carboxyhexanoyl-CoA
CHIT	Chitin
CHITO	Chitosan
CHO	Choline
CHOR	Chorismate
CHOSLF	Choline sulphate
CHOSLFe	Choline sulphate (extracellular)
cIMP	3',5'-Cyclic IMP
CIT	Citrate
CITe	Citrate (extracellular)
CITm	Citrate (mitochondrial)
CITR	L-Citrulline
CITRe	L-Citrulline (extracellular)
CITRm	L-Citrulline (mitochondrial)
CL	Cardiolipin
CLAGL3P	1-acyl-sn-glycerol-3-phosphate used for cardiolipin
CLCDPDG	Cdp-diacylglycerol used for cardiolipin
CLPA	Phosphatidate used for cardiolipin

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Abbreviation	Full name
CLPIGP	3(3-sn-phosphatidyl)-sn-glycerol 1-phosphate used for cardiolipin biosynthesis
CMP	CMP
CO2	Carbon dioxide
CO2e	Carbon dioxide (extracellular)
CO2m	Carbon dioxide (mitochondrial)
COA	Coenzyme A
COAm	Coenzyme A (mitochondrial)
COUM	Coumarate
COUMe	Coumarate (extracellular)
CPAD5P	1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose 5-phosphate
CTP	CTP
CYS	L-Cysteine
CYSe	L-Cysteine (extracellular)
CYST	Cystine
CYTD	Cytidine
CYTS	Cytosine
D6PDGC	6-phospho-2-dehydro-D-gluconate
D6PGC	6-Phospho-D-gluconate
D6PGL	d-Glucono-1,5-lactone 6-phosphate
DA	Deoxyadenosine
DADP	dADP
DAGLY	Diacylglycerol
DAGLYP	Diacylglycerol-3-Phosphate
DAMP	dAMP
DAONA	7,8-diaminononanoate
DATP	dATP
DC	Deoxycytidine
DCDA	4-methylcholesta-8,24-diene-3-ol-4-carboxylate
DCDOL	4,4-Dimethylcholesta-8,24-diene-3-ol
DCDP	dCDP
DCMP	dCMP
DCTOL	4,4-Dimethylcholesta-8,14,24-triene-3-ol
DCTP	dCTP
DG	Deoxyguanosine
DGDG	Digalactosyl diglyceride
DGDMIPC	Digalactosyl-dimannosyl-inositol-P-ceramide
DGDP	dGDP

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Abbreviation	Full name
DGLC	D-Glucose
DGLCe	D-Glucose (extracellular)
DGMP	dGMP
DGTP	dGTP
DHBA	2,3-dihydroxybenzoate
DHCHDDC	(1R,6S)-dihydroxycyclohexa-2,4-diene-1,4-dicarboxylate
DHF	7,8-Dihydrofolate
DHMVAm	(R)-2,3-dihydroxy-3-methylbutanoate (mitochondrial)
DHP	2-Amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine
DHPLYSm	protein-dihydrolipoyllysine
DHPT	Dihydropteroate
DHSK	3-Dehydroshikimate
DHSKe	3-Dehydroshikimate (extracellular)
DHVALm	(R)-2,3-dihydroxy-3-methylbutanoate (mitochondrial)
DIMGP	D-erythro-1-(Imidazol-4-yl)glycerol 3-phosphate
DIN	Deoxyinosine
DMAND	D-mandelate
DMANDe	D-mandelate (extracellular)
DMIPC	Di-mannosyl-inositol-P-ceramide
DMNAD	Deamido-NAD
DMPP	Dimethylallyl diphosphate
DMT	Dimethylterephthalate
DMTe	Dimethylterephthalate (extracellular)
DNA	Deoxyribonucleic acid
DOROA	(S)-Dihydroorotate
DPCOA	Dephospho-CoA
DPTH	2-[3-Carboxy-3-(methylammonio)propyl]-L-histidine
DQT	3-Dehydroquinate
DR1P	Deoxy-ribose 1-phosphate
DSAM	S-Adenosylmethioninamine
DT	Thymidine
DTB	Dethiobiotin
DTBe	dethiobiotin (extracellular)
DTDP	dTDP
DTMP	dTMP

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Abbreviation	Full name
DTTP	dTTP
DU	Deoxyuridine
DUDP	dUDP
DUMP	dUMP
DUTP	dUTP
E	D-Erythrose
E4P	D-Erythrose 4-phosphate
Ee	D-Erythrose (extracellular)
EOL	Erythritol
EOLe	Erythritol (extracellular)
EPST	Episterol
ERGOD	Ergosta-5,7-dienol
ERGOSE	Ergosterolester
ERGOST	Ergosterol
ERGOT	Ergosta-5,7,22,24-tetraenol
ETH	Ethanol
ETHe	Ethanol (extracellular)
ETHm	Ethanol (mitochondrial)
EU	L-Erythrulose
EU1P	L-Erythrulose 1-phosphate
EUe	L-Erythrulose (extracellular)
F26P	D-Fructose 2,6-bisphosphate
F6P	beta-D-Fructose 6-phosphate
FADH2m	FADH2 (mitochondrial)
FADm	FAD (mitochondrial)
FALD	Formaldehyde
FDP	beta-D-Fructose 1,6-bisphosphate
FER	Ferulic acid
FERCOA	trans-feruloyl-CoA
FERe	Ferulic acid (extracellular)
FERHCOA	4-hydroxy-3-methoxyphenyl-beta-hydroxypropionyl-CoA
FERIm	Ferricytochrome c (mitochondrial)
FEROm	Ferrocytochrome c (mitochondrial)
FEST	Fecosterol
FGAM	2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine
FGAR	5'-Phosphoribosyl-N-formylglycinamide
FGT	S-Formylglutathione
FKYN	L-Formylkynurenine

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Abbreviation	Full name
FOR	Formate
FORe	Formate (extracellular)
FORm	Formate (mitochondrial)
FPP	trans,trans-Farnesyl diphosphate
FRU	D-Fructose
FRUe	D-Fructose (extracellular)
FTHF	10'-Formyltetrahydrofolate
FTHFm	10-Formyltetrahydrofolate (mitochondrial)
FUACAC	4-Fumarylacetoacetate
FUM	Fumarate
FUMe	Fumarate (extracellular)
FUMm	Fumarate (mitochondrial)
G	D-Glycerate
G1P	alpha-D-Glucose 1-phosphate
G6P	alpha-D-Glucose 6-phosphate
GA6P	D-Glucosamine 6-phosphate
GABA	4-Aminobutanoate
GABAe	4-Aminobutanoate (extracellular)
GABAm	4-Aminobutanoate (mitochondrial)
GAG	Galactosaminogalactan
GAL1P	alpha-D-Galactose 1-phosphate
GALCER	Galactosylceramide
GALCERA	Galactosylceramide(Comp. A)
GALCERB	Galactosylceramide(Comp. B)
GALN14LAC	D-Galactono-1,4-lactone
GALNT	D-Galactonate
GALNTe	D-Galactonate (extracellular)
GALOL	Galactitol
GALOLe	Galactitol (extracellular)
GALUNT	D-Galacturonate
GALUNTe	D-Galacturonate (extracellular)
GALUNTP	1-phospho-alpha-D-glucuronate
GAMYLe	Glucoamylase (secreted to the medium)
GAR	5'-Phosphoribosylglycinamide
GBAD	4-Guanidino-butanamide
GBAT	4-Guanidino-butanoate
GC	gamma-L-Glutamyl-L-cysteine
GDMIPC	Galactosyl-Dimannosyl-inositol-P-ceramide
GDP	GDP

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Abbreviation	Full name
GDPm	GDP (mitochondrial)
GDPMAN	GDPmannose
GEN	Gentisate
GGM	Galactoglucomannan
GL	Glycerol
GL3P	Glycerol 3-phosphate
GLAC	D-Galactose
GLACe	D-Galactose (extracellular)
GLAL	Glycolaldehyde
GLC	alpha-D-Glucose
GLCe	alpha-D-Glucose (extracellular)
GLCN	D-Glucosamine
GLCN15LAC	d-Glucono-1,5-lactone
GLCN15LACe	d-Glucono-1,5-lactone (extracellular)
GLCNT	D-Gluconate
GLCNTe	D-Gluconate (extracellular)
GLCUNT	D-Glucuronate
GLCUNTe	D-Glucuronate (extracellular)
GLe	Glycerol (extracellular)
GLN	L-Glutamine
GLNe	L-Glutamine (extracellular)
GLU	L-Glutamate
GLUCER1	Glucocerebroside 1
GLUCER2	Glucocerebroside 2
GLUe	L-Glutamate (extracellular)
GLUGSAL	L-Glutamate 5-semialdehyde
GLUGSALm	L-Glutamate 5-semialdehyde (mitochondrial)
GLUm	L-Glutamate (mitochondrial)
GLUP	alpha-D-Glutamyl phosphate
GLX	Glyoxylate
GLY	Glycine
GLYA	Glycolate
GLYAL	D-Glyceraldehyde
GLYCOGEN	Glycogen
GLYCOGENe	Glycogen (extracellular)
GLYe	Glycine (extracellular)
GLYm	Glycine (mitochondrial)
GLYN	Glycerone (DHA/dihydroxyacetone)
GLYNe	Glycerone (DHA/dihydroxyacetone) (extracellular)

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Abbreviation	Full name
GMP	GMP
GN	Guanine
GNTAL	Gentisate aldehyde
GPP	Geranyl diphosphate
GSN	Guanosine
GTP	GTP
GTPm	GTP (mitochondrial)
GUA	Guaiacol
H+	Intracellular protons
H+$_P$O	Proton (energy metabolism)
H+$_P$Om	Proton (mitochondrial) (energy metabolism)
H+e	Protons (extracellular)
H2O	Water
H2O2	Hydrogen peroxide
H2O2e	Hydrogen peroxide (extracellular)
H2Oe	Water (extracellular)
H2Om	Water (mitochondria)
H2S	Hydrogen sulfide
H2SO3	Sulfite
H2SO3e	Sulfite (extracellular)
H3MCOA	(S)-3-Hydroxy-3-methylglutaryl-CoA
HACNm	But-1-ene-1,2,4-tricarboxylate (mitochondrial)
HAN	3-Hydroxyanthranilate
HCITm	2-Hydroxybutane-1,2,4-tricarboxylate (mitochondrial)
HCYS	L-Homocysteine
HICITm	Homoisocitrate (mitochondrial)
HIS	L-Histidine
HISe	L-Histidine (extracellular)
HISN	Histamine
HISOL	L-Histidinol
HISOLP	L-Histidinol phosphate
HIUR	5-hydroxyisourate
HKYN	3-Hydroxykynurenine
HNO2	Nitrite
HNO3	Nitrate
HNO3e	Nitrate (extracellular)
HOMOGEN	Homogentisate
HPLYSm	H-protein-lipoyllysine

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Abbreviation	Full name
HPSAMLYSm	H-protein-S-aminomethyldihydrolipoyllysine
HSER	L-Homoserine
HYXN	Hypoxanthine
HYXNe	Hypoxanthine (extracellular)
ICIT	Isocitrate
ICITe	Isocitrate (extracellular)
ICITm	Isocitrate (mitochondrial)
IDOL	L-Iditol
IDOLe	L-Iditol (extracellular)
IDP	IDP
IDPm	IDP (mitochondrial)
IGP	Indoleglycerol phosphate
ILE	L-Isoleucine
ILEe	L-Isoleucine (extracellular)
ILEm	L-Isoleucine (mitochondrial)
IMACP	3-(Imidazol-4-yl)-2-oxopropyl phosphate
IMASP	Iminoaspartate
IMP	IMP
INAC	Indoleacetate
IND	Indole
INDe	Indole (extracellular)
INS	Inosine
IPC	Inositol phosphorylceramide
IPPMALm	2-Isopropylmalate (mitochondrial)
IPPP	Isopentenyl diphosphate
ITP	ITP
ITPm	ITP (mitochondrial)
KDDGC	2-dehydro-3-deoxy-D-gluconate
KOJA	Kojic acid
KOJAe	Kojic acid (extracellular)
KYN	L-Kynurenine
KYNe	L-Kynurenine (extracellular)
LAC	D-Lactate
LACAL	D-Lactaldehyde
LACe	D-Lactate (extracellular)
LACm	(R)-Lactate (mitochondrial)
LACT	Lactose
LACTe	Lactose (extracellular)
LAOL	L-Arabitol

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Abbreviation	Full name
LAOLe	L-Arabitol (extracellular)
LARAB	L-Arabinose
LARABe	L-Arabinose (extracellular)
LEU	L-Leucine
LEUe	L-Leucine (extracellular)
LEUm	L-Leucine (mitochondrial)
LGT	S-D-Lactoylglutathione
LIPIDS	Artificial metabolite. The metabolites found in the biomass. Measured in grams
LIPOm	Lipoamide (mitochondrial)
LLAC	L-Lactate
LLACe	L-Lactate (extracellular)
LLACm	(S)-Lactate (mitochondrial)
LLCT	L-Cystathionine
LMAND	L-mandelate
LMANDe	L-mandelate (extracellullar)
LNST	Lanosterol
LPC	Lysophosphatidylcholine
LPE	Lysophosphatidylethanolamine
LPSE2m	(LipS2)-dihydrolipoyl transsuccinylase
LXUL	L-Xylulose
LXULe	L-Xylulose (extracellular)
LYS	L-Lysine
LYSe	L-Lysine (extracellular)
LYSm	L-Lysine (mitochondrial)
MACAC	maleylacetoacetate
MAGLY	Monoacylglycerol
MAGLYP	Monoacylglycerol-3-Phosphate
MAL	(S)-Malate
MALACP	Malonyl-[acyl-carrier protein]
MALCOA	Malonyl coenzyme A
MALe	(S)-Malate (extracellular)
MALm	(S)-Malate (mitochondrial)
MAN	D-Mannose
MAN1P	alpha-D-Mannose 1-phosphate
MAN6P	D-Mannose 6-phosphate
MANe	D-Mannose (extracellular)
MANNANe	Mannan (extracellular)
MELIe	Melibiose (extracellular)

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Abbreviation	Full name
MET	L-Methionine
METe	L-Methionine (extracellular)
METH	Methanethiol
METHF	5,10-Methenyltetrahydrofolate
METHFm	5,10-Methenyltetrahydrofolate (mitochondrial)
METHOL	Methanol
METHOLe	Methanol (extracellular)
METTHF	5,10-Methylenetetrahydrofolate
METTHFm	5,10-Methylenetetrahydrofolate (mitochondrial)
MGC181	Monoglucosyloxyoctadecenoic acid
MGDG	Monogalactosyl diglyceride
MI1P	1L-myo-Inositol 1-phosphate
MIPC	Mannose-inositol-P-ceramide
MLT	Maltose
MLTe	Maltose (extracellular)
MNT	D-Mannitol
MNT1P	D-Mannitol 1-phosphate
MNTe	D-Mannitol (extracellular)
MTHF	5-Methyltetrahydrofolate
MTHFm	5-Methyltetrahydrofolate (mitochondrial)
MTHGXL	Methylglyoxal
MTPHTH	Monomethylterephthalate
MUCL	Muconolactone
MUCO	cis,cis-muconate
MVL	(R)-Mevalonate
MYOI	myo-Inositol
NAD	NAD+
NADH	NADH
NADHm	NADH (mitochondrial)
NADm	NAD+ (mitochondrial)
NADP	NADP+
NADPH	NADPH
NADPHm	NADPH (mitochondrial)
NADPm	NADP+ (mitochondrial)
NAG	N-Acetyl-D-glucosamine
NAGA1P	N-Acetyl-D-glucosamine 1-phosphate
NAGA6P	N-Acetyl-D-glucosamine 6-phosphate
NAGLUm	N-Acetyl-L-glutamate (mitochondrial)
NAGLUPm	N-Acetyl-L-glutamate 5-phosphate (mitochondrial)

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Abbreviation	Full name
NAGLUSm	N-Acetyl-L-glutamate 5-semialdehyde (mitochondrial)
NAHISN	N-acetylhistamine
NAMN	Nicotinate D-ribonucleotide
NAMR	Nicotinamide D-ribonucleoside
NAORNm	N2-Acetyl-L-ornithine (mitochondrial)
NAR	Nicotinate D-ribonucleoside
NFAN	N-formylanthranilate
NH3	Ammonia
NH3e	Ammonia (extracellular)
NH3m	Ammonia (mitochondrial)
NH4OH	Ammonium hydroxide
NICA	Nicotinate
NICAe	Nicotinate (extracellular)
NICD	Nicotinamide
NICDe	Nicotinamide (extracellular)
NIG	Nigeran (alpha-1,3-Glucose-alpha-1,4-Glucose)
NMN	Nicotinamide D-ribonucleotide
NPRAN	N-(5-Phospho-D-ribosyl)anthranilate
O2	Oxygen
O2e	Oxygen (extracellular)
O2m	Oxygen (mitochondrial)
OA	Oxaloacetate
OAe	Oxaloacetate (extracellular)
OAEL	3-Oxoadipate enol-lactone
OAHSER	O-Acetyl-L-homoserine
OAm	Oxaloacetate (mitochondrial)
OBUT	2-Oxobutanoate
OBUTm	2-Oxobutanoate (mitochondrial)
OGT	Oxidized glutathione
OICAP	3-Carboxy-4-methyl-2-oxopentanoate
OICAPm	3-Carboxy-4-methyl-2-oxopentanoate (mitochondrial)
OIVALm	(R)-2-Oxoisovalerate (mitochondrial)
OMP	Orotidine 5'-phosphate
OMVAL	3-Methyl-2-oxobutanoate
OMVALm	3-Methyl-2-oxobutanoate (mitochondrial)
ORN	L-Ornithine
ORNe	L-Ornithine (extracellular)

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Abbreviation	Full name
ORNm	L-Ornithine (mitochondrial)
OROA	Orotate
OTA	Ochratoxin A
OTAe	Ochratoxin A (extracellular)
OTHIO	Oxidized thioredoxin
OTHIOm	Oxidized thioredoxin (mitochondrial)
OXAL	Oxalate
OXALe	Oxalate (extracellular)
OXAm	Oxaloglutarate (mitochondrial)
OXGLY	Oxaloglycolate
P5C	(S)-1-Pyrroline-5-carboxylate
P5Cm	(S)-1-Pyrroline-5-carboxylate (mitochondrial)
PABA	4-Aminobenzoate
PANT	(R)-Pantoate
PAP	Adenosine 3',5'-bisphosphate
PAPS	3'-Phosphoadenylylsulfate
PC	Phosphatidylcholine
PCAGL3P	1-acyl-sn-glycerol-3-phosphate used for phosphatidylcholine
PCAT3P2	1-acyl-sn-glycerone phosphate used for phosphatidylcholine
PCC	Protocatechuate
PCCDPDG	Cdp-diacylglycerol used for phosphatidylcholine
PCCe	Protocatechuate (extracellular)
PCPA	Phosphatidate used for phosphatidylcholine
PCPDME	Phosphatidyl-N-dimethylethanolamine
PCPE	Phosphatidylethanolamine used for phosphatidylcholine
PCPMME	Phosphatidyl-N-methylethanolamine
PCPS	Phosphatidylserine used for phosphatidylcholine
PE	Phosphatidylethanolamine
PEAGL3P	1-acyl-sn-glycerol-3-phosphate used for phosphatidylethanolamine
PEAT3P2	1-acyl-sn-glycerone phosphate used for phosphatidylethanolamine
PECDPDG	Cdp-diacylglycerol used for phosphatidylethanolamine
PECTATEe	Pectate (extracellular)
PENAL	Pentanal

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Abbreviation	Full name
PENN	Pentylamine
PENNe	Pentylamine (extracellular)
PEP	Phosphoenolpyruvate
PEPA	Phosphatidate used for phosphatidylethanolamine
PEPS	Phosphatidylserine used for phosphatidylethanolamine
PG	Phosphatidylglycerol
PHAC	Phenylacetate
PHACe	Phenylacetate (extracellular)
PHAL	Phenylacetaldehyde
PHALe	Phenylacetaldehyde (extracellular)
PHE	L-Phenylalanine
PHEe	L-Phenylalanine (extracellular)
PHEN	Prephenate
PHP	3-Phosphonooxypyruvate
PHPYR	Phenylpyruvate
PHPYRe	Phenylpyruvate (extracellular)
PHSER	O-Phospho-L-homoserine
PI	Orthophosphate
PIe	Orthophosphate (extracellular)
PIm	Orthophosphate (mitochondrial)
PINS	1-Phosphatidyl-D-myo-inositol
PINSP	1-Phosphatidyl-1D-myo-inositol 3-phosphate
PMVL	(R)-5-Phosphomevalonate
PNTO	(R)-Pantothenate
POOL	Artificial metabolite. A group of small molecules found in the biomass
PPI	Pyrophosphate
PPIm	Pyrophosphate (mitochondrial)
PPMVL	(R)-5-Diphosphomevalonate
PRAM	5-Phosphoribosylamine
PRBAMP	N1-(5-Phospho-D-ribosyl)-AMP
PRBATP	N1-(5-Phospho-D-ribosyl)-ATP
PRCP	5-Phosphoribosyl monophosphate
PRFICA	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide
PRFP	5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4-carboxamide

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Abbreviation	Full name
PRLP	N-(5'-Phospho-D-1'-ribulosylformimino)-5-amino-1-(5"-phospho-D-ribosyl)-4-imidazolecarboxamide
PRO	L-Proline
PROe	L-Proline (extracellular)
PROm	L-Proline (mitochondrial)
PROP	Propanoate
PROPACP	Propanoyl-[acyl-carrier protein]
PROPAL	Propionaldehyde
PROPALe	Propionaldehyde (extracellular)
PROPCOA	Propanoyl-CoA
PROPCOAm	Propanoyl-CoA (mitochondrial)
PROPe	Propanoate (extracellular)
PROPm	Propanoate (mitochondrial)
Protein	Protein
PRPP	5-Phospho-alpha-D-ribose 1-diphosphate
PS	Phosphatidylserine
PSAGL3P	1-acyl-sn-glycerol-3-phosphate used for phosphatidylserine
PSAT3P2	1-acyl-sn-glycerone phosphate used for phosphatidylserine
PSCDPDG	Cdp-diacylglycerol used for phosphatidylserine
PSNIG	Pseudonigeran (1,3-alpha-glucan)
PSPA	Phosphatidate used for phosphatidylserine
PYR	Pyruvate
PYRe	Pyruvate (extracellular)
PYRm	Pyruvate (mitochondrial)
QH2m	Ubiquinol (mitochondrial)
Qm	Ubiquinone (mitochondrial)
QT	Quinate
QTe	Quinate (extracellular)
QUIN	Quinolinate
QUINe	Quinolinate (extracellular)
R1P	D-Ribose 1-phosphate
R5P	D-Ribose 5-phosphate
RAFFe	Raffinose (extracellular)
RES	Resocinol
RESe	Resocinol (extracellular)
RGT	Glutathione
RHA	L-Rhamnose

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Abbreviation	Full name
RHAe	Extracellular rhamnose
RHAMN	L-rhamnulose
RHAMNP	L-rhamnulose 1-phosphate
RIB	D-Ribose
RIBe	D-Ribose (extracellular)
RIBOL	Ribitol
RIBOLe	Ribitol (extracellular)
RL	D-Ribulose
RL5P	D-Ribulose 5-phosphate
RLe	D-Ribulose (extracellular)
RNA	Ribonucleic acid
RTHIO	Reduced thioredoxin
RTHIOm	Reduced thioredoxin (mitochondrial)
S	Sulfur
S23E	(S)-2,3-Epoxysqualene
S7P	Sedoheptulose 7-phosphate
SACPm	Saccharopine (mitochondrial)
SAH	S-Adenosyl-L-homocysteine
SAICAR	1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole
SALI	Salicylate
SALIe	Salicylate (extracellular)
SAM	S-Adenosyl-L-methionine, S-Adenosyl-L-methionine; Acylcarnitine
SAMOB	S-adenosyl-4-methylthio-2-oxobutanoate
SEDAG	1,2-diacyl-sn-glycerol (for Sterolesters)
SEDAGP	1,2-diacyl-sn-glycerol 3-phosphate (for Sterolesters)
SEMAG	Monoacylglycerol(for Sterolesters)
SEMAGP	Monoacylglycerol-3-phosphate (for Sterolesters)
SER	L-Serine
SERe	L-Serine (extracellular)
SLF	Sulfate
SLFe	Sulphate (extracellular)
SME	Shikimate
SME3P	Shikimate 3-phosphate
SMEe	Shikimate (extracellular)
SOR	L-Sorbose
SORe	L-Sorbose (extracellular)
SOT	D-Sorbitol

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Abbreviation	Full name
SOTe	D-Sorbitol (extracellular)
SQL	Squalene
STACe	Stachyose
STARe	Starch (extracellular)
SUCC	Succinate
SUCCe	Succinate (extracellular)
SUCCm	Succinate (mitochondrial)
SUCCOAm	Succinyl coenzyme A (mitochondrial)
SUCCSALm	Succinate-semialdehyde (mitochondrial)
SUCe	Sucrose (extracellular)
T3P1	D-Glyceraldehyde 3-phosphate
T3P2	Glycerone phosphate (DHAP)
TAGLY	Triacylglycerol
TANAe	Tannic acid (extracellular)
TAR	Tartrate
TARe	Tartrate (extracellular)
TDPE1m	(thiamine diphosphate)-alpha-ketoglutarate dehydrogenase
TGDMIPC	Trigalactosyldimannosylinositol-P-ceramide
THF	Tetrahydrofolate
THFG	Tetrahydrofolyl-[Glu](n)
THFm	Tetrahydrofolate (mitochondrial)
THR	L-Threonine
THRe	L-Threonine (extracellular)
THRm	L-Threonine (mitochondrial)
THY	Thymine
TPHTH	Terephthalate
TPHTHe	Terephthalate (extracellular)
TRE	alpha,alpha-Trehalose
TRE6P	alpha,alpha-Trehalose 6-phosphate
TREe	alpha,alpha-Trehalose (extracellular)
TRP	L-Tryptophan
TRPe	L-Tryptophan (extracellular)
TYR	L-Tyrosine
TYRe	L-Tyrosine (extracellular)
UDP	UDP
UDPG	UDPglucose
UDPGAL	UDPgalactose
UDPGALU	UDP-galacturonate

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Abbreviation	Full name
UDPNAG	UDP-N-acetyl-D-glucosamine
UDPNAGAL	UDP-N-acetyl-D-galactosamine
UGC	(-)-Ureidoglycolate
UMP	UMP
URA	Uracil
URAe	Uracil (extracellular)
UREA	Urea
UREAC	Urea-1-carboxylate
UREAe	Urea (extracellular)
UREAm	Urea (mitochondrial)
URI	Uridine
URIC	Ureate
URIe	Uridine (extracellular)
UTP	UTP
VAL	L-Valine
VALe	L-Valine (extracellular)
VALm	L-Valine (mitochondrial)
VAN	Vanillate
VANe	Vanillate (extracellular)
VANIN	Vanillin
XAN	Xanthine
XANe	Xanthine (extracellular)
XMP	Xanthosine 5'-phosphate
XOL	Xylitol
XOLe	Xylitol (extracellular)
XTSINE	Xanthosine
XUL	D-Xylulose
XUL5P	D-Xylulose 5-phosphate
XULe	D-Xylulose (extracellular)
XYL	D-Xylose
XYLANe	Xylan (extracellular)
XYLe	D-Xylose (extracellular)
ZYMST	Zymosterol

Suppl. Table III: Protein composition of *A. niger*. The measured values are from Christias et al. (1975). It is assumed that the ASP/ASN and GLU/GLN ratios are 3:1 as in Oura (1972). Polymerization cost is calculated from (Ingraham et al., 1983). A large proportion of the weight of a glucoprotein can be sugar (Leskovac et al. (2005) reports as much as 10-16% of the weight of glucose oxidase) but data on an average ratio of sugar/protein is neither available nor easily estimated.

Amino acid	**Amount** $\left[{}^{\text{mmole}}/_{\text{g protein}}\right]$
ALA	1.048
ARG	0.419
ASN	0.213
ASP	0.638
CYS	0.080
GLU	0.913
GLN	0.304
GLY	0.875
HIS	0.208
ILE	0.402
LEU	0.715
LYS	0.660
MET	0.107
PHE	0.317
PRO	0.448
SER	0.638
THR	0.510
TRP	0.128
TYR	0.208
VAL	0.544
Polymerization cost:	
ATP	39.729

Suppl. Table IV: RNA composition of *A. niger*. The measured values are from Uryson and Belozerskii (1960). Polymerization cost is calculated from (Ingraham et al., 1983).

Ribonucleotide	**Amount** $^{\text{mmole}}/_{\text{g RNA}}$
AMP	0.773
GMP	0.931
CMP	0.773
UMP	0.615
Polymerization cost:	
ATP	7.424

Suppl. Table V: DNA composition of *A. niger*. The measured values are from Uryson and Belozerskii (1960) and in accordance with the ratio of the genome sequence of CBS 513.88 (Pel et al., 2007). Polymerization cost is calculated from Ingraham et al. (1983).

Deoxyribonucleotides	**Amount** $^{\text{mmol}}/_{\text{g DNA}}$
dAMP	0.782
dCMP	0.814
dTMP	0.782
dGMP	0.814
Polymerization cost:	
ATP	10.849

Suppl. Table VI: Small molecules in the biomass of *A. niger*. The references from which the values are calculated, are found next to each component.

Component	**Reference**	**Amount** $^{\text{mmol}}/_{\text{g DW}}$
Isocitrate	Promper et al. (1993)	0.075
Citrate	Promper et al. (1993)	2.498
Succinate	Promper et al. (1993)	0.107
Fumarate	Promper et al. (1993)	0.008
Malate	Promper et al. (1993)	0.087
NAD	Fuhrer et al. (1980)	1.128
NADH	Fuhrer et al. (1980)	0.120
NADP	Fuhrer et al. (1980)	0.104
NADPH	Fuhrer et al. (1980)	0.060
Trehalose	Witteveen and Visser (1995)	13.692
Mannitol	Witteveen and Visser (1995)	32.791
Glycerol	Witteveen and Visser (1995)	42.363
Erythritol	Witteveen and Visser (1995)	36.636
Arabitol	Witteveen and Visser (1995)	1.521

Suppl. Table VII: Cell wall composition of *A. niger*. The references from which the values are calculated, are found next to each component.

Cell wall component	**Reference**	**Amount** $^{\text{mmol}}/_{\text{g cell wall}}$
Galactosaminogalactan	Bardalaye and Nordin (1976)	0.04
Nigeran	(Johnston, 1965; Damveld et al., 2005)	0.25
Pseudonigeran (α-1,3-glucan)	Horisberger et al. (1972)	0.33
Galactoglucomannan	Bardalaye and Nordin (1977); Horisberger et al. (1972)	0.37
1,4-α-glucan	Stagg and Feather (1973)	0.38
Chitin	Ram et al. (2004); Stagg and Feather (1973); Blumenthal and Roseman (1957)	1.57
1,3-β-glucan	Stagg and Feather (1973); Ram et al. (2004)	2.64

Suppl. Table VIII: Lipid composition of *A. niger*. The amounts are sorted into categories of neutral lipids, sphingolipids and phospholipids. The references from which the values are calculated, are found next to each component.

Lipids	**Reference**	**Amount** mmol/g DW
Neutral lipids		
Triacylglycerols	Morozova et al. (2002)	0.010083
Diacylglycerols	Morozova et al. (2002)	0.001009
Monoacylglycerols	Morozova et al. (2002)	0.008912
C14:0 acyl	Morozova et al. (2002)	0.000223
C16:0 acyl	Morozova et al. (2002)	0.001480
C18:0 acyl	Morozova et al. (2002)	0.000245
C18:1 acyl	Morozova et al. (2002)	0.001678
C18:2 acyl	Morozova et al. (2002)	0.001664
C18:3 acyl	Morozova et al. (2002)	0.000047
Ergosterol	Nemec and Jernejc (2002)	0.034062
Ergosterol esters	Nemec and Jernejc (2002)	0.010038
Glucolipids		
Monogalactosyldiglyceride	Chattopadhyay et al. (1985a)	0.030053
Monoglucosyloxyoctadecenoic acid	Brennan et al. (1974)	0.012374
Digalactosyldiglyceride	Chattopadhyay et al. (1985a)	0.007859
Sphingolipids		
Trigalactosyldimannosylinositolphosphorylceramide (GPSL G)	Byrne and Brennan (1976)	0.000005
Cerebrin 1 (with C18 or C20 Phytosphingosin)	Byrne and Brennan (1976)	0.000030
Cerebrin 2 (with C18 or C20 sphingosin)	Byrne and Brennan (1976)	0.000031
Cerebroside (Galactosylceramide)	Byrne and Brennan (1976)	0.000025
Glucocerebroside 1	Byrne and Brennan (1976)	0.000024
Glucocerebroside 2	Byrne and Brennan (1976)	0.000024
Phospholipids		
Cardiolipin	Chattopadhyay et al. (1985a)	0.001746
Phosphatidylcholine	Chattopadhyay et al. (1985a)	0.015312
Phosphatidylserine	Chattopadhyay et al. (1985a)	0.000359
Phosphatidylethanolamine	Chattopadhyay et al. (1985a)	0.034807

Suppl. Table IX: Carbon sources found in literature available to the model. Substrates that are only found as carbon sources together with glucose are indicated by $*$.

C-source		Reference
Acetate		Ruijter et al. (1999)
Alanine	$*$	Nomachi and Komano (1980)
Anthranilic acid	$*$	Reddy and Vaidyanathan (1975)
Arabinose		vanKuyk et al. (2001); de Groot et al. (2003); de Vries et al. (2002b); Witteveen et al. (1994)
Arabitol		vd Veen et al. (1993)
Aspartic acid	$*$	Nomachi and Komano (1980)
Benzoate	$*$	Reddy and Vaidyanathan (1975)
Benzyl-vanillic acid	$*$	Milstein et al. (1988)
Citrate		Muller (1975a)
Coumaric acid	$*$	Milstein et al. (1988)
Dethiobiotin	$*$	Tepper et al. (1966); Li et al. (1968)
D-galacturonic acid		de Vries et al. (2002b); de Vries et al. (2002)
D-glucuronic acid		de Vries et al. (2002b); de Vries et al. (2002)
Dihydroxyacetone		Witteveen et al. (1990)
Dimethylterephthalate		Ganji et al. (1995)
DL-mandelic acid	$*$	Jamaluddin et al. (1970)
D-xylose		Ngiam et al. (2000)
Ferulic acid		Milstein et al. (1988)
Fructose		Ruijter et al. (1999); de Vries et al. (2002b)
Fumarate		Muller (1975a)
Galactose		Ademark et al. (2001); Basten et al. (2005); de Vries et al. (2002b)
Gluconate		Elzainy et al. (1973); Ruijter et al. (1999)
Gluconic acid lactone		Lakshminarayana et al. (1969a)
Glucose		Numerous
Glutamate	$*$	Nomachi and Komano (1980)
Glycerol		Tereshina et al. (2004)
Indole	$*$	Kamath and Vaidyanathan (1990)
Lactose		Arisan-Atac et al. (1996)
L-rhamnose		Fries and Kallstromer (1965)

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C-source		Reference
Maltose		Pedersen et al. (2000b)
Mannitol		Tereshina et al. (2004)
Mannose		Adya and Elbein (1977); de Vries et al. (2002b)
Methanol		Kirimura et al. (1999)
m-hydroxybenzoic acid	∗	Premkumar et al. (1969); Kumar et al. (1973)
Phenylacetic acid	∗	Sugumaran et al. (1973)
Phenylalanine	∗	Kishore et al. (1974, 1976)
Resorcinol		Shailubhai et al. (1983)
Rhamnose		de Vries et al. (2002b)
Salicylate		Shailubhai et al. (1983)
Sorbitol		Desai et al. (1967, 1969a); vd Veen et al. (1991)
Succinate		Muller (1975a)
Sucrose		Arisan-Atac et al. (1996); de Graaff et al. (1992)
Tannic acid		Bhardwaj et al. (2003)
Tartrate		Patil and Ramakrishnan (1966)
Trehalose		Tereshina et al. (2004)
Tryptophan	∗	Sreeleela et al. (1969); Subramanian and Vaidyanathan (1984)
Vanillic acid	∗	Milstein et al. (1988)
Xylitol		vd Veen et al. (1993)
Xylose		Ngiam et al. (2000)

Suppl. Table X: Sole carbon sources that are utilizable by *A. niger* *i*MA871, but with no available reference.

Carbon source
3-hydroxybenzoate
Arginine
Asparagine
Benzonitrile
Benzoylamine
Butanoate
Citrulline
Decanoate
D-Erythrose
D-Lactate
D-mandelate
Dodecanoate
D-Ribose
D-Ribulose
D-Xylulose
Eicosanoate
Ethanol
GABA
Galactitol
Galactonate
Galacturonate
Glutamine
Glycine
Heptadecanoate
Heptadecenoate
Hexadecadienoate
Hexadecanoate
Hexadecenoate
Hexanoate
Isocitrate
L-Arabinose
L-Arabitol
L-Erythrulose
L-Iditol
L-Lactate
L-mandelate
L-Sorbose

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Carbon source
L-Xylulose
Malate
Melibiose
Nonadecadienoate
Nonadecanoate
Nonadecenoate
Octadecadienoate
Octadecanoate
Octadecatrienoate
Octadecenoate
Octanoate
Ornithine
Oxalate
Oxaloacetate
Pentadecanoate
Phenylpyruvate
Proline
Propanoate
Protocatechuate
Pyruvate
Raffinose
Ribitol
Serine
Stachyose
Terephthalate
Tetradecanoate
Tetradecenoate
Threonine
Tyrosine

Suppl. Table XI: Compounds utilizable by *A. niger* *i*MA871 as sole nitrogen source. Compounds, where the use as sole nitrogen source has found described in literature, are followed by one or more references.

Nitrogen source	**Reference**
Alanine	Lenouvel et al. (2001)
Ammonia	Basten et al. (2001)
Anthranilate	Kamath et al. (1987)
Arginine	Lenouvel et al. (2001)
Asparagine	Lenouvel et al. (2001); Laine et al. (1972)
Aspartate	
Butylamine	Schilling and Lerch (1995a)
Citrulline	Lenouvel et al. (2002)
GABA	Kumar and Punekar (1998)
Glutamate	Lenouvel et al. (2001)
Glutamine	
Glycine	Morton and Broadbent (1955)
Nitrate	Pedersen and Nielsen (2000)
Ornithine	Lenouvel et al. (2002)
Pentylamine	Schilling and Lerch (1995a)
Phenylalanine	
Proline	Lenouvel et al. (2001)
Serine	
Threonine	
Tryptophan	
Tyrosine	
Urea	Smith et al. (1993)
Xanthin	Taha and Sharabash (1956)

Suppl. Table XII: Enzymatic activities that were found in the literature, but not added to the reaction list of *A. niger* *i*MA871. References, EC-number and enzyme name is added to the reactions where possible.

Reaction	EC-no	Enzyme	Source
Degradation of biopolymers			
RNA + H2O ⇆ 3'-phosphomononucleotides	3.1.27.1	RNase I	Nomachi and Komano (1980)
RNA-bound phospho-guanine + H2O ⇆ RNA + 3'-phospho-guanine	3.1.27.3	RNase II	Nomachi and Komano (1980)
Extracellular RNA + H2O ⇆ ribonucleotides	3.1.27.1	ribonuclease	Xiong et al. (2005)
Dinucleoside monophosphates + H2O ⇆ Nucleotide 5'-phosphate + Nucleoside	3.1.4.1	Cyclic-ribonucleotide phosphomutase-5'-phosphodiesterase (phosphodiesterase I/5'-exonuclease activity)	Chohnan et al. (1994)
DNA + H2O ⇆ Nucleotide monophosphates	3.1.4.1	Phosphodiesterase I (5'-exonuclease)	Chohnan et al. (1994)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.11.5	prolyl aminopeptidase (papA)	Basten et al. (2005)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.14.5	dipeptidyl-peptidase IV (dapB)	Javing et al. (2005)

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Reaction	EC-no	Enzyme	Source
Extracellular proteins + H2O ⇆ Amino acid components	3.4.16.5	Carboxypeptidase I	dal Degan et al. (1992)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.16.5	Carboxypeptidase II	dal Degan et al. (1992)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.16.5	Serine-type carboxypeptidase F (pepF)	Krishnan and Vijayalakshmi (1985); van den Hombergh et al. (1994)
Extracellular proteins + H2O ⇆ Amino acid components	PEPC	carboxypeptidase C (pepC)	Frederick et al. (1993)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.21.61	Kexin	Jalving et al. (2000)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.23.18	Aspergillopepsin A (I) (pepA)	Mattern et al. (1992)
Extracellular proteins + H2O ⇆ Amino acid components	3.4.23.19	Aspergillopepsin B (II) (pepB)	Mattern et al. (1992); Huang et al. (2000)
removes AAs from peptide end	3.4.11.2	lysine aminopeptidase	Basten et al. (2001)
Peptide with N-terminal aromatic amino acid + H2O ⇒ Peptide + aromatic AA	No EC	phenylalanine peptidase	Basten et al. (2003)
Extracellular tri-acyl glycerol + H2O ⇆ Di-acyl glycerol + Fatty acid	3.1.1.3	Lipase (extracellular)	Namboodiri and Chattopadhyaya (2000)
Extracellular diacyl glycerol + H2O ⇆ Mono-acyl glycerol + Fatty acid	3.1.1.3	Lipase (extracellular)	Namboodiri and Chattopadhyaya (2000)

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Reaction	EC-no	Enzyme	Source
Degradation of complex carbon sources			
Glycyrrhizinate + H2O ⇆ 1,2-beta-D-glucuronosyl-D-glucuronate + Glycyrrhetinate	3.2.1.128	glycyrrhizinate beta-glucuronidase	Sasaki et al. (1988)
1,2-beta-D-glucuronosyl-D-glucuronate + H2O ⇆ 2 D-Glucuronate	3.2.1.15	Polygalacturonase	Behere et al. (1993); Acuña-Argüelles et al. (1995); de Vries and Visser (2001); de Vries et al. (2002a)
Extracellular phytate + 4 H2O ⇆ myo-inositol-di-phosphate + 4 Phosphate	3.1.3.8	3-phytase	Skowronski (1978); van Hartingsveldt et al. (1993); Martinelli and Kinghorn (1994); Wyss et al. (1998, 1999); Nagashima et al. (1999); Dvorakova et al. (2000); Vohra and Satyanarayana (2003); Vats and Banerjee (2005)
Extracellular phytate + 5 H2O ⇆ Inositol-monophosphate + 5 Phosphate	3.1.3.26	6-phytase	Wyss et al. (1999); Vohra and Satyanarayana (2003); Casey and Walsh (2003)
Aromatic degradations			

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Reaction	EC-no	Enzyme	Source
2-chlorobenzoate + NADPH + O2 ⇆ 2-chloro-4-hydroxybenzoate + NADP + H2O	1.14.13.1	benzoate 4-monooxygenase (benzoate-para-hydroxylase A, bphA)	Sahasrabudhe and Modi (1985)
3-chlorobenzoate + NADPH + O2 ⇆ 3-chloro-4-hydroxybenzoate + NADP + H2O	1.14.13.1	benzoate 4-monooxygenase (benzoate-para-hydroxylase A, bphA)	Sahasrabudhe and Modi (1985)
2-hydroxybenzoate + NADPH + O2 ⇆ 2,4-dihydroxybenzoate + NADP + H2O	1.14.13.1	benzoate 4-monooxygenase	Faber et al. (2001); Malonek et al. (2004)
3-Hydroxyanthranilate + Dihydrobiopterin + H2O ⇆ Anthranilate + Tetrahydrobiopterin + O2	1.14.16.3	anthranilate 3-monooxygenase	Subba Rao et al. (1971)
Phenylacetate + O2 + NADPH ⇆ 3-hydroxy-phenylacetate + H2O + NADP	No EC	Phenylacetate hydroxylase	Sugumaran and Vaidyanathan (1978)
3-hydroxybenzylalcohol + NADP ⇆ 3-hydroxybenzaldehyde + NADPH	No EC	3-hydroxy benzylalcohol dehydrogenase	Sugumaran et al. (1973)
3-hydroxybenzaldehyde + NAD ⇆ 3HBA + NADH	No EC	3-hydroxy benzylaldehyde dehydrogenase	Sugumaran et al. (1973)
Orcinol + NADH + O2 ⇆ 2,3,5-trihydroxytoluene + NAD + H2O	1.14.13.6	orcinol 2-monooxygenase	Sahasrabudhe et al. (1986)

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Reaction	EC-no	Enzyme	Source
4-nitrophenyl phosphate + H2O ⇆ 4-nitrophenol + Phosphate	3.1.3.41	4-nitrophenylphosphatase	Versaw et al. (1991)
2-hydroxymuconate semialdehyde ⇆ Catechol + O2	1.13.11.2	catechol 2,3-dioxygenase	Sahasrabudhe et al. (1986)
Miscellaneous			
Sulcaton + NADH ⇆ sulcatol + NAD	1.1.1.260	sulcatone reductase	Belan et al. (1987)
Propanal + NADPH ⇆ Propanol + NADP	1.1.1.78	Methylglyoxal reductase II	Inoue et al. (1988)
Butanal + NAD + H2O ⇆ Butanate + NADH	1.2.1.3	Aldehyde dehydrogenase (NAD+)	Kazimirova and Novotel'nov (1956)
Heptanal + NAD + H2O ⇆ Heptanate + NADH	1.2.1.3	Aldehyde dehydrogenase (NAD+)	Kazimirova and Novotel'nov (1956)
Quercitin + O2 ⇒ 2-protocatechuoylphloroglucinol carboxylic acid + CO	1.13.11.2	Flavonol 2,4 dioxygenase	Hund et al. (1999)
Phloretin + H2O ⇆ Phloretate + 1,3,5-Trihydroxybenzene	3.7.1.4	phloretin hydrolase	Minamikawa et al. (1970)
2',3'-Cyclic AMP ⇆ cyclic AMP	3.1.4.16	Cyclic-ribonucleotide phosphomutase-5'-phosphodiesterase	Chohnan et al. (1994)
2',3'-Cyclic CMP ⇆ cyclic CMP	3.1.4.16	Cyclic-ribonucleotide phosphomutase-5'-phosphodiesterase	Chohnan et al. (1994)

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Reaction	EC-no	Enzyme	Source
2',3'-Cyclic GMP ⇆ cyclic GMP	3.1.4.16	Cyclic-ribonucleotide phosphomutase-5'-phosphodiesterase	Chohnan et al. (1994)
2',3'-Cyclic IMP ⇆ cyclic IMP	3.1.4.16	Cyclic-ribonucleotide phosphomutase-5'-phosphodiesterase	Chohnan et al. (1994)
Carbaryl ⇆ 1-hydroxynaphthalene + N-methylcarbamate	No EC	Carbaryl hydrolase	Qing et al. (2003)
Methionine + Glyoxalate ⇆ 4-methylthio-2-oxobutanoate + Glycine	2.6.1.73	L-methionine-glyoxylate transaminase	Oganesyan et al. (2004)
Diacetyl + NADPH ⇆ Acetoin + NADP	1.1.1.72	Glycerol dehydrogenase (NADP+)	Schuurink et al. (1990)
Methylglyoxal + NADPH ⇆ 1-Hydroxy-2-propanone + NADP	1.1.1.72	Glycerol dehydrogenase (NADP+)	Schuurink et al. (1990)
4-hydroxyphenylacetaldehyde oxime + NADPH + O2 ⇆ 4-hydroxymandelonitrile + NADP + 2 H2	1.13.14.6	NADPH-cytochrome P450 reductase (cprA)	van den Brink et al. (1996); Malonek et al. (2004)
2 Superoxide + 2 H+ ⇒ O2 + H2O2	1.15.1.1	Cu,Zn superoxide dismutase	Sugumaran and Vaidyanathan (1978); Holdom et al. (1996)
R-CH2-NH2 + H2O + O2 ⇆ R-CHO + H2O2 + NH3	1.4.3.4	amine oxidase (flavin-containing)	Schilling and Lerch (1995a)

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Reaction	EC-no	Enzyme	Source
R-CH2-NH2 + H2O + O2 ⇆ R-CHO + H2O2 + NH3	1.4.3.6	amine oxidase (copper-containing)	Schilling and Lerch (1995a)
Glycerol triacetate + H2O ⇆ Glycerol + 3 Acetate	3.1.1.3	triacylglycerol lipase	Hannan (1959)
Chlorogenate + H2O ⇒ Caffeate + Quinate	3.1.1.42	chlorogenic acid hydrolase	Schobel and Pollmann (1980); Asther et al. (2005)
Several epoxides to their di-ols	3.3.2.3	epoxide hydrolase	Morisseau et al. (1999); Arand et al. (1999)
Serine + Glyoxylate ⇆ 3-hydroxypyruvate + Glycine	2.6.1.45	L-serine-glyoxylate transaminase	Oganesyan et al. (2004)
Serine + Pyruvate ⇆ 3-Hydroxypyruvate + Alanine	2.6.1.51	L-serine-pyruvate transaminase	Oganesyan et al. (2004)
Methionine + Pyruvate ⇆ 4-methylthio-2-oxobutanoate + Alanine	2.6.1.41	L-methionine-pyruvate transaminase	Oganesyan et al. (2004)
Valine + Glyoxylate ⇆ (R)-2-Oxoisovalerate + Glycine	No EC	L-valine-glyoxylate transaminase	Oganesyan et al. (2004)
Leucine + Glyoxylate ⇆ 4-Methyl-2-oxopentanoate + Glycine	No EC	L-leucine-glyoxylate transaminase	Oganesyan et al. (2004)
Methylamine + H2O + O2 ⇒ NH3 + Methanal + H2O2	1.4.3.4	amine oxidase (flavin-containing)	Schilling and Lerch (1995b)
2-Phenylethylamine + H2O + O2 ⇒ 2-phenylethanal + NH3 + H2O2	1.4.3.4	amine oxidase (flavin-containing)	Schilling and Lerch (1995a)

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Reaction	EC-no	Enzyme	Source
Dopamine + H2O + O2 ⇒ (3,4-dihydroxyphenyl)acetaldehyde + NH3 + H2O2	1.4.3.4	amine oxidase (flavin-containing)	Schilling and Lerch (1995a)
Ethylamine + H2O + O2 ⇒ Acetaldehyde + NH3 + H2O2	1.4.3.4	amine oxidase (flavin-containing)	Schilling and Lerch (1995a)
Sinigrin + H2O ⇒ D-Glucose + isothiocyanate	3.2.1.147	Myrosinase	Ohtsuru et al. (1973)
UDP-N-acetyl-D-glucosamine + Dolichyl phosphate ⇆ UMP + N-acetyl-D-glucosaminyl-diphosphodolichol	2.7.8.15	UDP-N-acetylglucosamine: dolichyl-phosphate N-acetylglucosaminephosph	Sorensen et al. (2003)
Nitrophenylsulphate + H2O ⇆ Nitrophenol + Sulphate	3.1.6.1	arylsulfatase	Sakurai et al. (1980)

Suppl. Table XIII: Pathways that were reported in literature to be present, but not included in the reaction list of *A. niger* *i*MA871.

Compound	Source
Degradation	
2-heptanone	(Baltazar et al., 1999)
2-nonanone	(Baltazar et al., 1999)
Anthracene	Yogambal and Karegoudar (1997)
Caproic acid	Lewis (1970)
Carbaryl	Qing et al. (2003)
Ceramide-phosphoinositol	Hackett and Brennan (1977)
Cerebrosine	Wagner and Fiegert (1969)
Dolichol	Sorensen et al. (2003)
Naphthalene	Yogambal and Karegoudar (1997)
Orcinol	Sahasrabudhe et al. (1986)
PAH	Sack et al. (1997)
Phenenthrene	Yogambal and Karegoudar (1997); Sack et al. (1997)
Pyrene	Wunder et al. (1994)
Secondary metabolites	
1,1-heptanediol diacetate	Abo-Dahab (2002)
1,4-diaza-2,5-dioxo-3-isobutylbicyclo (4.3.0) nonane	Abo-Dahab (2002)
4,9-dimethyl-furano(2,3h) coumarin	Abo-Dahab (2002)
Amphetamine	Abo-Dahab (2002)
Asperazine	Varoglu et al. (1997); Varoglu and Crews (2000)
Aspergillin	Rawat (1968); Ray and Eakin (1975)
Asperic acid	Varoglu and Crews (2000)
Aspernigrin A	Hiort et al. (2004)
Aspernigrin B	Hiort et al. (2004)
Aurasperone B	Bouras et al. (2005)
Aurasperone C	Bouras et al. (2005)
Aurasperone D	Blumenthal (2004); Samson et al. (2004)
Aurasperone E	Bouras et al. (2005)
Aurasperone F	Bouras et al. (2005)
Bicoumanigrin	Hiort et al. (2004)
Butanoic acid 2-[(difluoroacetyl)amino]-butyl ester	Abo-Dahab (2002)
Cycloleucomelone	Hiort et al. (2004)
Dihydroergotamine	Abo-Dahab (2002)

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Compound	Source
Flavasperone (Asperxanthone)	Bycroft et al. (1962)
Fonsecin	Bouras et al. (2005)
hexylitaconic acid	Varoglu and Crews (2000)
Kotanin	Samson et al. (2004)
Malformin A1 (Formerly known as A)	Yukioka and Winnick (1966); Schuster et al. (2002); Blumenthal (2004); Kobbe et al. (1977); Yukioka and Winnick (1966)
Malformin A2	Schuster et al. (2002); Blumenthal (2004); Kobbe et al. (1977); Yukioka and Winnick (1966)
Malformin B	Schuster et al. (2002); Blumenthal (2004); Kobbe et al. (1977); Yukioka and Winnick (1966)
Malformin C	Kobbe et al. (1977); Varoglu and Crews (2000)
Melanin	McGovern and Bentley (1975)
Mlaviolin	McGovern and Bentley (1975)
Nerolidol-epoxyacetate	Abo-Dahab (2002)
n-heptanal	Abo-Dahab (2002)
Nigerazine B	Blumenthal (2004)
Nigragillin	Blumenthal (2004)
N-methylmorpholine	Abo-Dahab (2002)
Ochratoxin A	Abarca et al. (1994); Varga et al. (2003); O'Callaghan et al. (2003); Samson et al. (2004); Blumenthal (2004)
Orobol	Nishioka et al. (1989)
Phatalimide	Abo-Dahab (2002)
Phenol-3,5-dimethoxyphenyl acetate	Abo-Dahab (2002)
Pyranonigrin A	Samson et al. (2004); Hiort et al. (2004)
Pyranonigrin B	Samson et al. (2004); Hiort et al. (2004)
Pyranonigrin C	Samson et al. (2004); Hiort et al. (2004)
Pyranonigrin D	Samson et al. (2004); Hiort et al. (2004)
Pyrophen	Varoglu and Crews (2000)
Roridine E	Abo-Dahab (2002)

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