

## S6 Nutrients and Target metabolites

### S6.1 *E. coli*

Nutrients <i>E. coli</i>			
Name	MetaCyc-Id	Name	MetaCyc-Id
Ag <sup>+</sup>	AG+	ammonia	AMMONIA
NH <sub>4</sub> <sup>+</sup>	AMMONIUM	arsenate	ARSENATE
Br <sup>-</sup>	BR-	Ca <sup>2+</sup>	CA+2
Cd <sup>2+</sup>	CD+2	chlorate	CHLORATE
chlorite	CHLORITE	chloride	CL-
Co <sup>2+</sup>	CO+2	tetrathionate	CPD-14
hyponitrous acid	CPD-1541	phosphite	CPD-27
molybdate	CPD-3	iodide	CPD-387
Cr <sup>6+</sup>	CPD-4762	phosphoramidate	CPD-494
PbS	CPD-527	PbSO <sub>4</sub>	CPD-530
trithionate	CPD-552	trimetaphosphate	CPD-610
selenide	CPD-678	S <sup>2-</sup>	CPD-7046
arsenite	CPD-763	HS <sup>-</sup>	CPD-846
As <sub>3</sub> H <sub>3</sub> O <sub>6</sub>	CPD0-1119	Cr <sup>3+</sup>	CR+3
Cu <sup>+</sup>	CU+	Cu <sup>2+</sup>	CU+2
fluoride	F-	Fe <sup>2+</sup>	FE+2
Fe <sup>3+</sup>	FE+3	β-D-glucose	GLC
H <sub>2</sub> SO <sub>4</sub>	H <sub>2</sub> SO <sub>4</sub>	HCl	HCL
Hg <sup>2+</sup>	HG+2	Hg <sup>0</sup>	HG0
hydrogen sulfide	HS	bisulfite	HSO3
hydrazine	HYDRAZINE	H <sub>2</sub>	HYDROGEN-MOLECULE
H <sub>2</sub> O <sub>2</sub>	HYDROGEN-PEROXIDE	hydroxylamine	HYDROXYLAMINE
I <sub>2</sub>	IODINE-MOLECULE	K <sup>+</sup>	K+
Li <sup>+</sup>	LI+	Mg <sup>2+</sup>	MG+2
Mn <sup>2+</sup>	MN+2	Mn <sup>+3</sup>	MN+3
Na <sup>+</sup>	NA+	ammonium hydroxide	NH4OH
Ni <sup>2+</sup>	NI+2	nitrate	NITRATE
nitric oxide	NITRIC-OXIDE	nitrite	NITRITE
N <sub>2</sub>	NITROGEN-MOLECULE	nitrous oxide	NITROUS-OXIDE
OH <sup>-</sup>	OH	oxygen	OXYGEN-MOLECULE
PPP <sub>i</sub>	P3I	phosphonate	PHOSPHONATE
phosphoramidate	PHOSPHORAMIDATE	diphosphate	PPI
H <sup>+</sup>	PROTON	thiosulfate	S2O3
S <sup>0</sup>	S8	selenate	SELENATE
selenite	SELENITE	selenophosphate	SEPO3
sulfite	SO3	sulfate	SULFATE
sulphur dioxide	SULFUR-DIOXIDE	O <sub>2</sub> <sup>-</sup>	SUPER-OXIDE
H <sub>2</sub> O	WATER		

Target metabolites <i>E. coli</i>	
Name	MetaCyc-Id
L-alanine	L-ALPHA-ALANINE
L-arginine	ARG
L-asparagine	ASN
L-aspartate	L-ASPARTATE
L-cysteine	CYS
L-glutamate	GLT
L-glutamine	GLN
glycine	GLY
L-histidine	HIS
L-isoleucine	ILE
L-leucine	LEU
L-lysine	LYS
L-methionine	MET
L-phenylalanine	PHE
L-proline	PRO
L-serine	SER
L-threonine	THR
L-tryptophan	TRP
L-tyrosine	TYR

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Target metabolites E. coli – continued from previous page	
Name	MetaCyc-Id
L-valine	VAL
ATP	ATP
CTP	CTP
UTP	UTP
GTP	GTP
dATP	DATP
dGTP	DGTP
dUTP	DUTP
dTTP	TTP

## S6.2 *Chlamydomonas reinhardtii*

The calculations of producible metabolites with the method of network expansion for photoautotrophic organisms bears an additional technical finesse. If the only carbon containing compound in the seed is  $\text{CO}_2$ , the reactions of the Calvin-Benson cycle cannot operate, since for the fixation of  $\text{CO}_2$ , the acceptor molecule ribulose-1,5-bisphosphate (RuBP) is required. With steady state analysis of the Calvin cycle it is easy to show that there exist steady state fluxes producing all intermediate compounds exclusively from  $\text{CO}_2$  and inorganic material (orthophosphate and water). Precisely the same results are obtained when including  $\text{CO}_2$  and RuBP in the seed. The adequate correction to obtain realistic results with the method of network expansion is therefore given by the addition of RuBP to the seed. The pentose phosphate pathway, which is structurally similar and in parts identical to the Calvin cycle, has been discussed in this context in <sup>1</sup>.

Nutrients <i>Chlamydomonas reinhardtii</i>			
Name	MetaCyc-Id	Name	MetaCyc-Id
$\text{NH}_4^+$	AMMONIUM	$\text{Ca}^{2+}$	CA+2
$\text{CO}_2$	CARBON-DIOXIDE	chloride	CL-
$\text{Co}^{2+}$	CO+2	$\text{Cu}^{2+}$	CU+2
EDTA	EDTA	$\text{Fe}^{2+}$	FE+2
$\text{HCO}_3^-$	HCO3	$\text{K}^+$	K+
$\text{Mg}^{2+}$	MG+2	$\text{Mn}^{2+}$	MN+2
$\text{Mo}^{2+}$	MO+2	$\text{Na}^+$	NA+
phosphate	Pi	sulfate	SULFATE
$\text{H}_2\text{O}$	WATER	$\text{Zn}^{2+}$	ZN+2
D-ribulose-1,5-bisphosphate	d-ribulose-1,5-p.2		

Target metabolites <i>Chlamydomonas reinhardtii</i>			
Name	MetaCyc-Id	producible by draft	unreachable
2-hydroxyglutarate	2-HYDROXYGLUTARIC_ACID		
2-keto-isovalerate	2-KETO-ISOVALERATE	×	
$\alpha$ -ketoglutarate	2-KETOGLUTARATE	×	
2-phosphoglycerate	2-PG	×	
3- $\beta$ -D-glucosyl-D-glucose	3-BETA-D-GLUCOSYLGLUCOSE		
2-isopropylmalate	3-CARBOXY-3-HYDROXY-ISOCAPROATE	×	
4-aminobutyrate	4-AMINO-BUTYRATE	×	
4-hydroxy-L-proline	4-HYDROXY-L-PROLINE		
4-hydroxyphenylacetate	4-HYDROXYPHENYLACETATE		
5-oxoproline	5-OXOPROLINE	×	
adenine	ADENINE	×	
adenosine	ADENOSINE	×	
adipate	ADIPATE		×
$\alpha$ -D-glucose 6-phosphate	ALPHA-GLC-6-P	×	
$\alpha$ -tocopherol	ALPHA-TOCOPHEROL	×	
arachidate	ARACHIDIC_ACID		×
L-arginine	ARG	×	
L-asparagine	ASN	×	
$\beta$ -alanine	B-ALANINE	×	
benzoate	BENZOATE		
$\beta$ -tocopherol	BETA-TOCOPHEROL	×	

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Target metabolites Chlamydomonas reinhardtii – continued from previous page			
Name	MetaCyc-Id	producible by draft	unreachable
caffeate	CAFFEATE		
cholesterol	CHOLESTEROL		
cis-aconitate	CIS-ACONITATE	×	
citrate	CIT	×	
D-lysine	CPD-219		
6-phospho-D-gluconate	CPD-2961	×	
N-acetyl-D-galactosamine	CPD-3604		×
D-Ribonate	CPD-373		
N-acetyl-L-phenylalanine	CPD-439		
galactinol	CPD-458		
α-aminoadipate	CPD-468	×	
formyl phosphate	CPD-495		
glycerol 2-phosphate	CPD-536		
N-acetylputrescine	CPD-569		
lumichrome	CPD-605		
2-phosphoglycolate	CPD-67	×	
margarate	CPD-7830		×
cerotate	CPD-7832		×
myristate	CPD-7836		×
pentadecanoate	CPD-8462		×
pelargonate	CPD-8505		×
L-cysteine	CYS	×	
L-cystine	CYSTINE		
D-galactonate	D-GALACTONATE		
galacturonate	D-GALACTURONATE		
D-myo-Inositol (1)-monophosphate	D-MYO-INOSITOL-1-MONOPHOSPHATE		
D-xylulose	D-XYLULOSE	×	
dihydrouracil	DI-H-URACIL	×	
dodecanoate	DODECANOATE		×
ergosterol	ERGOSTEROL		
ethanolamine	ETHANOL-AMINE	×	
fructose	FRU	×	
fructose-1,6-bisphosphate	FRUCTOSE-16-DIPHOSPHATE	×	
fructose-6-phosphate	FRUCTOSE-6P	×	
fumarate	FUM	×	
&gamma;-tocopherol	GAMA-TOCOPHEROL	×	
D-glyceraldehyde-3-phosphate	GAP	×	
β-D-glucose	GLC	×	
α-D-glucose 1-phosphate	GLC-1-P	×	
L-glutamine	GLN	×	
L-glutamate	GLT	×	
D-gluconate	GLUCONATE	×	
glycine	GLY	×	
glycerate	GLYCERATE	×	
glycerol	GLYCEROL	×	
sn-glycerol-3-phosphate	GLYCEROL-3P	×	
glycolate	GLYCOLLATE	×	
GMP	GMP	×	
guanine	GUANINE	×	
hexanoate	HEXANOATE		×
L-histidine	HIS	×	
homoserine	HOMO-SER	×	
hydrogen sulfide	HS	×	
hydroquinone	HYDROQUINONE		
hydroxy-urea	HYDROXY-UREA		×
L-soleucine	ILE	×	
kojic acid	KOJIC-ACID		×
L-alanine	L-ALPHA-ALANINE	×	
L-aspartate	L-ASPARTATE	×	
citrulline	L-CITRULLINE	×	
L-dehydro-ascorbate	L-DEHYDRO-ASCORBATE	×	
L-lactate	L-LACTATE		
L-methionine sulfoxide	L-METHIONINE_SULFOXIDE		×
L-ornithine	L-ORNITHINE	×	
L-threonate	L-THREONATE	×	
L-leucine	LEU	×	
linoleate	LINOLEIC_ACID		×
linolenate	LINOLENIC_ACID		×
malate	MAL	×	
maleate	MALEATE		
maltose	MALTOSE		

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Target metabolites <i>Chlamydomonas reinhardtii</i> – continued from previous page			
Name	MetaCyc-Id	producible by draft	unreachable
D-mannitol	MANNITOL	×	
L-methionine	MET	×	
methyl- $\beta$ -D-galactoside	METHYL-BETA-D-GALACTOSIDE		×
myo-inositol	MYO-INOSITOL	×	
N-acetyl-L-ornithine	N-ALPHA-ACETYLORNITHINE	×	
nicotinamide	NIACINAMIDE	×	
hydroxypyruvate	OH-PYR	×	
oxalate	OXALATE	×	
L-phenylalanine	PHE	×	
phenylpyruvate	PHENYL-PYRUVATE	×	
phenylacetaldehyde	PHENYLACETALDEHYDE		
phosphoenolpyruvate	PHOSPHO-ENOL-PYRUVATE	×	
phosphoryl-ethanolamine	PHOSPHORYL-ETHANOLAMINE	×	
phytol	PHYTOL		
picolinate	PICOLINATE		×
diphosphate	PPI	×	
prephenate	PREPHENATE	×	
L-proline	PRO	×	
putrescine	PUTRESCINE	×	
pyrrole-2-carboxylate	PYRROLE-2-CARBOXYLATE		×
pyruvate	PYRUVATE	×	
L-rhamnose	RHAMNOSE		
D-ribose	RIBOSE	×	
D-ribose-5-phosphate	RIBOSE-5P	×	
(S)-citramalate	S-CITRAMALATE		
L-serine	SER	×	
shikimate	SHIKIMATE	×	
sinapate	SINAPATE		
squalene	SQUALENE	×	
stearate	STEARIC_ACID		×
succinate	SUC	×	
succinate semialdehyde	SUCC-S-ALD	×	
sucrose	SUCROSE	×	
tetracosanoate	TETRACOSANOATE		×
L-threonine	THR	×	
trehalose	TREHALOSE	×	
L-tryptophan	TRP	×	
L-tyrosine	TYR	×	
uracil	URACIL	×	
urea	UREA	×	
uridine	URIDINE	×	
L-valine	VAL	×	
D-xylose	XYLOSE		
4-hydroxybenzoate	4-hydroxybenzoate		
phosphate	Pi	×	
D-isocitrate	threo-d(s)-iso-citrate	×	

### S6.3 *B. subtilis*

Nutrients			
Name	MetaCyc-Id	Name	MetaCyc-Id
NH <sub>4</sub> <sup>+</sup>	AMMONIUM	Ca <sup>2+</sup>	CA+2
citrate	CIT	chloride	CL-
MnCl <sub>2</sub>	CPD-8604	Fe <sup>3+</sup>	FE+3
$\beta$ -D-glucose	GLC	K <sup>+</sup>	K+
Mg <sup>2+</sup>	MG+2	Na <sup>+</sup>	NA+
NO <sub>3</sub> <sup>-</sup>	NITRATE	SO <sub>4</sub> <sup>2-</sup>	SULFATE
L-tryptophan	TRP	H <sub>2</sub> O	WATER
phosphate	Pi		

## References

- [1] K. Kruse and O. Ebenhöf, *Genome Informatics*, 2008, **20**, 91–101.