

This table provides the detailed biomass composition for *G. sulfurreducens*

This is captured in the model as the reaction, agg_GS13m

Table 2 Supplementary Information

ABBREVIATION	OFFICIALNAME	COEFFICIENT
Substrates		
26dap-M	meso-2,6-Diaminoheptanedioate	0.02
3pg	3-Phospho-D-glycerate	0.02
akg	2-Oxoglutarate	0.02
ala-D	D-Alanine	0.02
ala-L	L-Alanine	0.37
arg-L	L-Arginine	0.20
asn-L	L-Asparagine	0.16
asp-L	L-Aspartate	0.16
atp	ATP	46.72
ca2	Calcium	0.00
ctp	CTP	0.04
cys-L	L-Cysteine	0.06
datp	dATP	0.02
dctp	dCTP	0.02
dgtp	dGTP	0.02
dttp	dTTP	0.02
fa1	Fatty acid (Iso-C14:0)	0.00
fa3	Fatty acid (Iso-C15:0)	0.06
fa4	Fatty acid (Anteiso-C15:0)	0.00
fa9	Fatty acid (Iso-C17:1)	0.01
g3p	Glyceraldehyde 3-phosphate	0.19
g6p	D-Glucose 6-phosphate	0.03
gln-L	L-Glutamine	0.18
glu-D	D-Glutamate	0.02
glu-L	L-Glutamate	0.18
gly	Glycine	0.42
glycogen	glycogen	0.93
gtp	GTP	0.06
h2o	H2O	13.07
hdca	Hexadecanoate (n-C16:0)	0.23
hdcea	hexadecenoate (n-C16:1)	0.28
his-L	L-Histidine	0.06
ile-L	L-Isoleucine	0.20
k	K+	0.22
leu-L	L-Leucine	0.31
lys-L	L-Lysine	0.23
met-L	L-Methionine	0.10
mg2	Mg	0.03
myrt	Myristate; Fatty acid (n-C14:0) fa2	0.02
nad	Nicotinamide adenine dinucleotide	0.02
nadph	Nicotinamide adenine dinucleotide phosphate - r	0.06
nh4	Ammonium	0.06
ocdca	octadecanoate (n-C18:0)	0.00
ocdcea	octadecenoate (n-C18:1)	0.02
pep	Phosphoenolpyruvate	0.02
phe-L	L-Phenylalanine	0.13
ppi	Diphosphate	0.28
pro-L	L-Proline	0.15
r5p	alpha-D-Ribose 5-phosphate	0.02
ser-L	L-Serine	0.47
thr-L	L-Threonine	0.17
trp-L	L-Tryptophan	0.04
tyr-L	L-Tyrosine	0.09
uacgam	UDP-N-acetyl-D-glucosamine	0.03
uamr	UDP-N-acetylmuramate	0.02
udpg	UDPglucose	0.01
utp	UTP	0.04
val-L	L-Valine	0.29
Products		
adp	ADP	46.67
h	H+	46.71
nadh	Nicotinamide adenine dinucleotide - reduced	0.02
nadp	Nicotinamide adenine dinucleotide phosphate	0.06
pi	Phosphate	46.72

Table 3 (Supplementary Information)

This table lists all the non-gene associated reactions incorporated in the model

No	Note	Abbreviation	OfficialName	Flux	Confidence Level	Subsystem
1	Required for cysteine synthesis	CTL	cystathionine g-lyase	0.0037	3	Amino Acid Metabolism
2	Required for cysteine synthesis	CYSTS	cystathionine b-synthase	0.0037	1	Amino Acid Metabolism
3	Spontaneous Reaction	G5SADs	L-glutamate 5-semialdehyde dehydratase (spontaneous)	0.0090	4	Amino Acid Metabolism
4	Spontaneous Reaction	OMCDC	2-Oxo-4-methyl-3-carboxypentanoate decarboxylation	0.0228	2	Amino Acid Metabolism
5	Required for lysine synthesis	THDPS	tetrahydrodipicolinate succinylase	0.0154	1	Amino Acid Metabolism
6	Required for lysine synthesis	SDPDS	succinyl-diaminopimelate desuccinylase	0.0154	1	Amino Acid Metabolism
7	Required for serine synthesis	PSP_L	phosphoserine phosphatase (L-serine)	0.0648	1	Amino Acid Metabolism
8	Required for threonine synthesis	HSK	homoserine kinase	0.0228	1	Amino Acid Metabolism
9	Required for glycogen synthesis	GLGC	glucose-1-phosphate adenylyltransferase	0.0556	2	Carbohydrate Metabolism
10	Based on biochemical data	FNOR	ferredoxin-NADP reductase	12.2486	2	Energy Metabolism
11	Required for fatty acid synthesis	ODACPHL	Oleoyl-[acyl-carrier-protein] hydrolase	0.0002	1	Fatty Acid Synthesis
12	Required for fatty acid synthesis	TDACPHL	Oleoyl-[acyl-carrier-protein] hydrolase	0.0013	1	Fatty Acid Synthesis
13	Required for fatty acid synthesis	HDACPHL	Oleoyl-[acyl-carrier-protein] hydrolase	0.0136	1	Fatty Acid Synthesis
14	Required for peptidoglycan synthesis	G1PACT	glucosamine-1-phosphate N-acetyltransferase	0.0034	1	Lipid & Cell Wall Metabolism
15	Required for peptidoglycan synthesis	UAGT3	UDP-N-acetylmuramoylpentapeptide-lysine N6-glycinetransferase (uaagtm3a)	0.0000	1	Lipid & Cell Wall Metabolism
16	Required for peptidoglycan synthesis	UDCPDP	undecaprenyl-diphosphatase	0.0000	1	Lipid & Cell Wall Metabolism
17	Required for peptidoglycan synthesis	PPTGS2	Peptidoglycan subunit synthesis	0.0000	2	Lipid & Cell Wall Metabolism
18	Required for sulfur reduction	PSULF	Poly sulfide formation (first step)	0.0000	4	Nonenzymatic Chemical Reactions
19	Spontaneous Reaction	NH4DIS	nh4 Dissociation	-0.0037	4	Nonenzymatic Chemical Reactions
20	Spontaneous Reaction	NH4OHD	NH4OH dissociation	0.0000	4	Nonenzymatic Chemical Reactions
21	Required for sulfate assimilation	BPNT	3',5'-bisphosphate nucleotidase	0.0100	1	Other
22	Spontaneous Reaction	H2td	hydrogen transport	0.0000	1	Transport
23	Spontaneous Reaction	N2t	nitrogen transport diffusion	0.0000	1	Transport
24	Required for malate transport	MALt6	malate symporter	0.0000	1	Transport
25	Spontaneous Reaction	CO2t	CO2 transport out via diffusion	-24.8950	4	Transport
26	Required for formate transport	FORT2	formate transport in via proton symport	0.0000	3	Transport
27	Spontaneous Reaction	H2Ot5	H2O transport via diffusion	21.5258	4	Transport
28	Required for Fe(III) reduction	FERCYT	Fe (III) Reductase: G sulfurreducens	98.5477	1	Transport
29	Required for fatty acid synthesis	OIVD2	2-oxoisovalerate dehydrogenase (acylating; 3-methyl-2-oxobutanoate)	0.0001	1	Valine, leucine, and isoleucine metabolism
30	Required for fatty acid synthesis	OIVD3	2-oxoisovalerate dehydrogenase (acylating; 3-methyl-2-oxopentanoate)	0.0002	1	Valine, leucine, and isoleucine metabolism
31	Required for fatty acid synthesis	OIVD1	2-oxoisovalerate dehydrogenase (acylating; 4-methyl-2-oxopentanoate)	0.0044	1	Valine, leucine, and isoleucine metabolism
32	Required for menaquinone synthesis	OCTDPS	Octaprenyl pyrophosphate synthase	0.0000	1	Vitamins & Cofactor Biosynthesis
33	Required for menaquinone synthesis	IPDPS	1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate reductase (ipdp)	0.0000	1	Vitamins & Cofactor Biosynthesis
34	Required for menaquinone synthesis	DMPPS	1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate reductase (dmpp)	0.0000	1	Vitamins & Cofactor Biosynthesis
35	Required for menaquinone synthesis	OXGDC2	2-oxoglutarate decarboxylase	0.0000	1	Vitamins & Cofactor Biosynthesis
36	Required for menaquinone synthesis	MECDPDH	2C-methyl-D-erythritol 2,4-cyclodiphosphate dehydratase	0.0000	1	Vitamins & Cofactor Biosynthesis
37	Required for menaquinone synthesis	ICHORSi	Isochorismate Synthase	0.0000	1	Vitamins & Cofactor Biosynthesis
38	Required for menaquinone synthesis	SHCHCS2	2-succinyl-6-hydroxy-2,4-cyclohexadiene 1-carboxylate synthase	0.0000	1	Vitamins & Cofactor Biosynthesis
39	Required for menaquinone synthesis	DHNAOT	1,4-dihydroxy-2-naphthoate octaprenyltransferase	0.0000	1	Vitamins & Cofactor Biosynthesis
40	Required for menaquinone synthesis	AMMQT8_2	S-adenosylmethionine:2-demethylmenaquinone methyltransferase	0.0000	1	Vitamins & Cofactor Biosynthesis
41	Required for menaquinone synthesis	SUCBZL	o-succinylbenzoate-CoA ligase	0.0000	1	Vitamins & Cofactor Biosynthesis
42	Required for menaquinone synthesis	SUCBZS	O-succinylbenzoate-CoA synthase	0.0000	1	Vitamins & Cofactor Biosynthesis
43	Required for menaquinone synthesis	NPHS	naphthoate synthase	0.0000	1	Vitamins & Cofactor Biosynthesis
44	Required for nucleotide metabolism	ADNK1	adenosine kinase	0.0000	1	Nucleotide Metabolism
45	Non-growth associated maintenance	ATPM	ATP drain	0.4500	1	Energy Metabolism
46	Added to simulate citrate transport	CIT6	Citrate transporter	0.0000	1	Transport
47	Added to simulate B12 synthesis in free living ge	CO1DAMAT	cob(I)yrinic acid a,c-diamide adenylyltransferase	0.0000	1	Vitamins & Cofactor Biosynthesis

48	Added to simulate B12 synthesis in free living ge	CO2DAMR	cob(II)yrinic acid a,c-diamide reductase	0.0000	1	Vitamins & Cofactor Biosynthesis
49	Added to simulate to fumarate transport	FUMt4	Fumarate transporter	0.0000	1	Putative Transporters
50	Added to simulate B12 synthesis in free living ge	HGBAMCOC	hydrogenobyirinic acid a,c-diamide cobaltochelataase	0.0000	1	Vitamins & Cofactor Biosynthesis
51	Added to simulate B12 synthesis in free living ge	PC3BS	Uncharacterized reaction	0.0000	1	Vitamins & Cofactor Biosynthesis
52	Added to simulate B12 synthesis in free living ge	PC6AR	precorrin-6A reductase	0.0000	1	Vitamins & Cofactor Biosynthesis
53	Added to simulate B12 synthesis in free living ge	PMDPHT	pyrimidine phosphatase	0.0000	1	Vitamins & Cofactor Biosynthesis
54	Added to simulate pantothenate synthesis	PNTK	pantothenate kinase	0.0000	1	Vitamins & Cofactor Biosynthesis
55	Added to simulate B12 synthesis	PRE6AS	precorrin-6A synthase	0.0000	1	Vitamins & Cofactor Biosynthesis