





## Supplementary Material A

### Dynamic genome-based metabolic modeling of the predominant cellulolytic rumen bacterium *Fibrobacter succinogenes* S85

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**Table S1.** Compounds present in the biomass reaction of the large-scale metabolic network of *F. succinogenes* S85. The Table was built based on the biomass reaction modelled for *E. coli*.

<b>List of input compounds of biomass reaction</b>			
<b>MetaCyc id</b>	<b>Name</b>	<b>Class</b>	<b>Coefficient</b>
ATP	ATP	nucleic acid	40.1701
CTP	CTP	nucleic acid	0.12988
DATP	dATP	nucleic acid	0.023503
DCTP	dCTP	nucleic acid	0.023503
DGTP	dGTP	nucleic acid	0.023503
GTP	GTP	nucleic acid	0.2091
TTP	dTTP	nucleic acid	0.023503
UTP	UTP	nucleic acid	0.14027
ARG	L-arginine	amino acid	0.28828
ASN	L-asparagine	amino acid	0.23468
CYS	L-cysteine	amino acid	0.08898
GLN	L-glutamine	amino acid	0.25601
GLT	L-glutamate	amino acid	0.25601
GLY	glycine	amino acid	0.5958
HIS	L-histidine	amino acid	0.092623
ILE	L-isoleucine	amino acid	0.28255
L-ALPHA-ALANINE	L-alanine	amino acid	0.50006
L-ASPARTATE	L-aspartate	amino acid	0.23468
LEU	L-leucine	amino acid	0.43866
LYS	L-lysine	amino acid	0.33355
MET	L-methionine	amino acid	0.14934
PHE	L-phenylalanine	amino acid	0.18056
PRO	L-proline	amino acid	0.21543
S-ADENOSYLMETHIONINE	S-adenosyl-L-methionine	amino acid	0.004668
SER	L-serine	amino acid	0.2097
THR	L-threonine	amino acid	0.24665
TRP	L-tryptophan	amino acid	0.055157
TYR	L-tyrosine	amino acid	0.13425
VAL	L-valine	amino acid	0.4116
SPERMIDINE	spermidine	amine	0.004668
CPD-9649	all-trans-undecaprenyl diphosphate	lipid	0.092476
PROTOHEME	protoheme	organic heterocycle compound	0.004668
Glycogens	glycogen	carbohydrates	0.154187
5-METHYL-THF	5-methyltetrahydropteroyl mono-L-glutamate	cofactor	0.004668
10-FORMYL-THF	10-formyl-tetrahydrofolate mono-L-glutamate	cofactor	0.004668

CO-A	coenzyme A	cofactor	0.004668
PYRIDOXAL_PHOSPHATE	pyridoxal 5'-phosphate	cofactor	0.004668
THF	5,6,7,8-tetrahydrofolate	cofactor	0.004668
CPD-12125	menaquinol-7	acceptor	0.004668
FAD	FAD	acceptor	0.004668
NAD	NAD <sup>+</sup>	acceptor	0.004668
NADP	NADP <sup>+</sup>	acceptor	0.004668
REDUCED-MENAQUINONE	menaquinol-8	acceptor	0.004668
CA+2	Ca <sup>2+</sup>	ion	0.004668
CO+2	Co <sup>2+</sup>	ion	0.004668
FE+2	Fe <sup>2+</sup>	ion	0.004668
FE+3	Fe <sup>3+</sup>	ion	0.004668
MG+2	Mg <sup>2+</sup>	ion	0.004668
MN+2	Mn <sup>2+</sup>	ion	0.004668
Na+	Na <sup>+</sup>	ion	0.004668
ZN+2	Zn <sup>2+</sup>	ion	0.004668
ADENOSYLCOBALAMIN	adenosylcobalamin	vitamin	0.004668
BIOTIN	biotin	vitamin	0.004668
RIBOFLAVIN	riboflavin	vitamin	0.004668
KCL	potassium chloride	salt	0.004668
WATER	H <sub>2</sub> O		34.7965
<b>List of output compounds of biomass reaction</b>			
MetaCyc id	Name	Class	Coefficient
Bio	external biomass		1.0
ADP	ADP	nucleic acid	40.0
Pi	phosphate	ion	39.9953
PPI	diphosphate	ion	0.60238
PROTON	H <sup>+</sup>	ion	40.0

**Table S2.** Seeds and targets used for the GEM metabolic network reconstruction.**Seeds**

<b>Name</b>	<b>Metacyc compound Name</b>	<b>Id Metacyc</b>
Cellulose	CELLULOSE	CELLULOSE
Cellobiose	Cellobiose	CELLOBIOSE
Glucose	Glucopyranose	Glucopyranose
Biotine	biotin	BIOTIN
p-aminobenzoic acid	4-aminobenzoate	P-AMINO-BENZOATE
Ammonia (NH3)	ammonia	AMMONIUM
Water	water	WATER
Acetic acid	acetate	ACET
isobutyric acid	isobutanoate	ISOBUTYRATE
n-butyric acid	butanoate	BUTYRIC_ACID
DL-a-methyl butyric acid	2-methylbutanoate	CPD-7076
isovaleric acid	isovalerate	ISOVALERATE
n-valeric acid	valerianic acid	5-AMINOPENTANOATE
propionic acid	propanoate	PROPIONATE
hemin	hemin	CPD-11678
cysteine	L-cysteine	CYS
K2HPO4	dipotassium phosphate	CPD0-2433
MgSO4	magnesium sulfate	CPD0-2390
CaCl2	calcium chloride	CPD0-1589
MnSO4·6H2O	manganese sulfate	CPD0-1608
CoCl2·6H2O	cobalt dichloride	CPD0-1695
FeSO4·7H2O	iron sulfate	CPD0-2386
ADP	ADP	ADP
ATP	ATP	ATP
Bio		
CARBON-DIOXIDE	CARBON-DIOXIDE	CARBON-DIOXIDE
CL-	chloride	CL-
CA+2	calcium(II)	CA+2
CO+2	cobalt(II)	CO+2
CO-A	coenzyme A	CO-A
COB-I-ALAMIN	COB-I-ALAMIN	COB-I-ALAMIN
cob(II)inamide	cob(II)inamide	CPD-20903
flavin adenine dinucleotide	FAD	FAD
FE+2	iron(II)	FE+2
FE+3	iron(III)	FE+3
flavin mononucleotide	flavin mononucleotide	FMN
potassium(I)	potassium(I)	K+
potassium chloride	potassium chloride	KCL
MG+2	magnesium(II)	MG+2
MN+2	manganese(II)	MN+2
Na+	SodiumI	Na+
NACL	Sodium chloride	NACL
NAD	NAD	NAD
NADH	NADH	NADH
NADP	NADP	NADP

NADPH	NADPH	NADPH
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	ammonium sulfate	NH <sub>4</sub> SO <sub>4</sub>
<b>Targets</b>		
<b>Name</b>	<b>Metacyc compound Name</b>	<b>Id Metacyc</b>
Acetic acid	acetate	ACET
Acetyl CoA	acetyl-CoA	ACETYL-COA
Alanine	L-alanine	L-ALPHA-ALANINE
Arginine	L-arginine	ARG
Asparagine	L-asparagine	ASN
Aspartate	L-aspartate	L-ASPARTATE
biotin	biotin	BIOTIN
Citrate	citrate	CIT
Cysteine	L-cysteine	CYS
Folate	folate	CPD-12826
Formate	formate	FORMATE
Fructose-6-P,	β-D-fructofuranose 6-phosphate	FRUCTOSE-6P
Fructose-1-6-P	β-D-fructose 1,6-bisphosphate	FRUCTOSE-16-DIPHOSPHATE
Glyceraldehyde-3-P	D-glyceraldehyde-3-P	GAP
1,3-PP Glycerate	3-phospho-D-glyceroyl-phosphate	DPG
3-P Glycerate	3-phospho-D-glycerate	G3P
2-P Glycerate	2-phospho-D-glycerate	2-PG
Glycine	glycine	GLY
Glycogen (futyle cycle : synthetized and degraded Gaudet)	a glycogen	Glycogens
Glutamate	L-glutamate	GLT
Glutamine	L-glutamine	GLN
Histidine	L-histidine	HIS
Isocitrate	D-threo-isocitrate	THREO-DS-ISO-CITRATE
Isoleucine	L-isoleucine	ILE
Leucine	L-leucine	LEU
Lysine	L-lysine	LYS
Malate	(S)-malate	MAL
Meso 2,6 diaminopimelic acid	meso-diaminopimelate	MESO-DIAMINOPIMELATE
Methionine	L-methionine	MET
Oxaloacetate	oxaloacetate	OXALACETIC_ACID
2-oxoglutarate	2-oxoglutarate	2-KETOGLUTARATE
Pantothenate	(R)-pantothenate	PANTOTHENATE
Phenylalanine	L-phenylalanine	PHE
Phosphoenolpyruvate (PEP)	phosphoenolpyruvate	PHOSPHO-ENOL-PYRUVATE
Proline	L-proline	PRO
Pyruvate	pyruvate	PYRUVATE
Ribose-5-P	D-ribose 5-phosphate	RIBOSE-5P
Ribulose-5-P	D-ribulose 5-phosphate	RIBULOSE-5P

Serine Succinyl CoA	L-serine succinyl-CoA	SER SUC-COA
Succinate	succinate	SUC
Threonine	L-threonine	THR
Tryptophan	L-tryptophan	TRP
Tyrosine	L-tyrosine	TYR
Valine	L-valine	VAL
Xylulose-5-P	D-xylulose 5-phosphate	XYLULOSE-5-PHOSPHATE
UDP-N-acetyl- $\alpha$ -D-muramoyl-L-alanyl- $\gamma$ -D-glutamyl-L-lysyl-D-alanyl-D-alanine	C3	C3
UDP-N-acetyl- $\alpha$ -D-muramoyl-L-alanyl- $\gamma$ -D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine	C1	C1
UDP-N-acetyl- $\alpha$ -D-muramoyl-L-alanine	CPD0-1456	CPD0-1456
ditrans,octakis-undecaprenyldiphospho-N-acetyl-(N-acetyl- $\beta$ -D-glucosaminy)muramoyl-L-alanyl- $\gamma$ -D-glutamyl-L-lysyl-D-alUDP-OHMYR-ACETYLGLUCOSAMINE anyl-D-alanine	CPD-7695	CPD-7695
UDP-N-acetyl- $\alpha$ -D-muramoyl-L-alanyl- $\gamma$ -D-glutamyl-meso-2,6-diaminopimelate	UDP-AAGM-DIAMINOHEPTANEDIOATE	UDP-AAGM-DIAMINOHEPTANEDIOATE
Adénine	adenine	ADENINE
Guanine	guanine	GUANINE
Cytosine	cytosine	CYTOSINE
Thymine	thymine	THYMINE
DCTP	2'-deoxycytidine-5'-triphosphate deoxycytidine-triphosphate deoxy-CTP	DCTP
TTP	thiamine thiothiazolone diphosphate	TTP
GTP	GTP	GTP
NADP	NADP	NADP
5-METHYL-THF	5-methyltetrahydropteroyl mono-L-glutamate	5-METHYL-THF
PYRIDOXAL_PHOSPHATE	PYRIDOXAL_PHOSPHATE	PYRIDOXAL_PHOSPHATE
CO-A	coenzyme A	CO-A
SPERMIDINE	SPERMIDINE	SPERMIDINE
THF	Oxolane	CPD-24834

CTP	cytidine-triphosphate	CTP
CPD-9649	all-trans-undecaprenyl diphosphate	CPD-9649
FAD	flavin adenine dinucleotide	FAD
PROTOHEME	PROTOHEME	PROTOHEME
ATP	ATP	ATP
S-ADENOSYLMETHIONINE	S-ADENOSYLMETHIONINE	S-ADENOSYLMETHIONINE
DGTP	DGTP	DGTP
ADENOSYLCOBALAMIN	ADENOSYLCOBALAMIN	ADENOSYLCOBALAMIN
10-FORMYL-THF	10-FORMYL-THF	10-FORMYL-THF
CPD-12125	menaquinol-7	CPD-12125
UTP	UTP	UTP
Glutamates	Glutamates	Glutamates
ACP	ACP	ACP
NAD	NAD	NAD
RIBOFLAVIN	RIBOFLAVIN	RIBOFLAVIN
REDUCED-MENAQUINONE	REDUCED-MENAQUINONE	REDUCED-MENAQUINONE
DATP	deoxy-ATP	DATP
PPI	diphosphate	PPI
Pi	phosphate	Pi
PROTON	PROTON	PROTON
ADP	ADP	ADP

**Table S3:** Comparison of the two draft models obtained via Pathway Tools from the two annotated *F. succinogenes* genomes NC\_017448 and NC\_013410

<b>Common reactions</b>	
<b>common reactions found with Pathway Tools in NC_017448 and NC_013410 genomes</b>	<b>817</b>
<b>Specific reactions</b>	
<b>6 specific reactions to NC_013410</b>	<b>4 specific reactions to NC_017448</b>
1.2.7.8-RXN (gene: FISUC_RS06185) 3.8.1.11-RXN (gene: FISUC_RS04815) ALDOSE-1-EPIMERASE-RXN (gene: FISUC_RS03645) ALDOSE1EPIM-RXN (gene: FISUC_RS03645) RXN-6263 (gene: FISUC_RS04815) RXN-6264 (gene: FISUC_RS04815)	RXN0-5190 (genes: FSU_RS06885 or FSU_RS05220) RXN-17391 (genes: FSU_RS06885 or FSU_RS05220) RXN-17392 (genes: FSU_RS06885 or FSU_RS05220) RXN-17393 (genes: FSU_RS06885 or FSU_RS05220)