Supplementary Data 2. Biomass composition of *C. acetobutylicum* ATCC 824 used in the model

1. Atomic weights

Elements	AW
C	12.0107
H	1.00794
O	15.9994
N	14.0067
P	30.9738
S	32.066

2. Macromolecular composition

Macromolecular composition of *C. acetobutylicum* was assumed to be same with that of *B. subtilis*. The macromolecular composition of *B. subtilis* was adopted from Dauner and Sauer, 2001.

Components	Proportion (% g/g)
Protein	52.84
RNA	6.55
DNA	2.6
Lipids	7.6
Lipoteichoic Acid	3.04
Cell Wall Components	22.42
Trace Components	4.94

3. Nucleotide composition

The nucleotide composition of *C. acetobutylicum* was calculated from its genome sequence. The rRNA and tRNA composition were assumed to be average composition of all rDNA and tDNA genes, respectively. The mRNA composition was taken as for genomic DNA. It was assumed that the proportions of mRNA, rRNA, and tRNA were 5%, 75%, and 20%, respectively. Energy requirement for polymerization was adopted from Ingraham et al., 1983.

(1) DNA(chromosomal+ pSOL)

Bases	# of bases	Double strand	Composition (mol/mol DNA)	MW (g/mol)	mmol/g DNA
A	1427820	2854782	0.345	313.2	1.118
G	640100	1278098	0.155	329.2	0.501
T	1426962	2854782	0.345	304.2	1.118
C	637998	1278098	0.155	289.2	0.501
Sum	4132880	8265760			

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(2) rRNA

Bases	# of bases	Composition (mol/mol rRNA)
A	14140	0.284
G	14727	0.295
U	10565	0.212
C	10443	0.209
Sum	49875	

(3) tRNA

Bases	# of bases	Composition (mol/mol tRNA)
A	1101	0.205
G	1627	0.302
U	1315	0.244
C	1337	0.249
Sum	5380	

(4) mRNA

Bases	Composition (mol/mol mRNA)
A	0.345
G	0.155
U	0.345
C	0.155

(5) Total RNA

Nucleotides	Composition				MW (g/mol)	mmol/g RNA
	rRNA 75%	tRNA 20%	mRNA 5%	Weighted mean		
A	0.284	0.205	0.345	0.271	329.2	1.050
G	0.295	0.302	0.155	0.290	345.2	1.124
U	0.212	0.244	0.345	0.225	305.2	0.873
C	0.209	0.249	0.155	0.214	306.2	0.832

4. Phospholipid composition

The phospholipid composition of *C. acetobutylicum* was somewhat complicated because anaerobic biosynthesis of plasmalogen was not characterized. Therefore, it was assumed that fatty acids and fatty aldehydes were same. The proportion of plasmalogen was calculated from Johnstone and Goldfine, 1983. Acyl chain composition and alk-1-enyl chain composition were calculated respectively and were averaged to weighted mean. Polar group composition was tabulated from Johnstone and Goldfine, 1992.

Molar ratio of plasmalogens to total polar lipids: 0.287

(1) Acyl chain composition

Fatty acids	g/g total acyl chain	MW (g/mol)	mmol/g total acyl chain	mol/mol total acyl chain
C14	0.08	227.4	0.352	0.091
C16	0.645	255.4	2.525	0.653
C16:1	0.056	253.4	0.221	0.057
C18	0.03	283.5	0.106	0.027
C18:1	0.09	281.5	0.320	0.083
C17:cyc	0.01	265.4	0.038	0.010
C19:cyc	0.09	293.5	0.307	0.079
Average molecular weight		258.5		

(2) Alk-1-enyl chain composition

Fatty acids	g/g total alk-1-enyl chain	MW (g/mol)	mmol/g total alk-1-enyl chain	mol/mol total alk-1-enyl chain
C14	0.023	211.4	0.109	0.029
C16	0.175	239.4	0.731	0.192
C16:1	0.077	237.4	0.324	0.085
C18	0.057	267.5	0.213	0.056
C18:1	0.15	265.5	0.565	0.149
C17:cyc	0.05	249.4	0.200	0.053
C19:cyc	0.46	277.5	1.658	0.436
Average molecular weight		263.1		

(3) Average fatty acid and aldehyde composition (mol/total fatty acids or aldehydes) in phospholipids

Fatty acids and aldehydes	Ratio	Average MW
C14	0.073	222.8
C16	0.521	250.8
C16:1	0.065	248.8
C18	0.036	278.9
C18:1	0.102	276.9
C17:cyc	0.022	260.8
C19:cyc	0.182	288.9
Sum	1.000	
Average MW of total fatty acid and aldehyde	259.4	

(4) Polar lipid composition

Polar groups	g/g total polar group	MW			mmol/g
		Backbone	# of fatty acid chains	Total	
Phosphatidylethanolamine	0.56	181.1	2	700.0	0.800
Phosphatidylglycerol	0.29	212.1	2	731.0	0.397
Cardiolipin	0.15	332.2	4	1369.9	0.109

5. Amino acid composition

The amino acid composition of *C. acetobutylicum* is not available from literature. Therefore, we cultured *C. acetobutylicum* ATCC 824 in the bioreactor containing chemically defined medium, and the culture in exponential phase was sampled. Six samples of the culture were analyzed using HCl hydrolysis, PITC derivatization, and HPLC by Korea Basic Science Institute and were averaged. Energy requirement for polymerization was taken as for *E. coli* (Ingraham et al., 1983).

Amino acids	Molar ratio	MW (g/mol)	mmol/g protein
Gly	0.115	57.1	1.078
Ala	0.083	71.1	0.775
Val	0.125	99.1	1.172
Leu	0.046	113.2	0.429
Ile	0.046	113.2	0.436
Met	0.083	131.2	0.783
Pro	0.049	97.1	0.457
Phe	0.020	147.2	0.185
Tyr	0.085	163.2	0.801
Trp	0.005	186.2	0.043
Ser	0.045	87.1	0.427
Thr	0.044	101.1	0.410
Asn	0.017	114.1	0.156
Asp	0.017	115.1	0.156
Gln	0.014	129.1	0.127
Glu	0.014	128.1	0.127
Cys	0.130	103.2	1.216
Lys	0.036	128.2	0.336
Arg	0.014	156.2	0.133
His	0.016	137.2	0.146
Average molecular weight		106.5	

6. Peptidoglycan composition

There is no published data of the peptidoglycan composition of *C. acetobutylicum* . Therefore, the culture samples were analyzed in DSMZ. The type of peptidoglycan was determined as A1γ. Based on this result, the molar ratio was calculated from the structure of peptidoglycan. Energy requirement for polymerization was adopted from Ingraham et al., 1983.

Components	Molar ratio	MW (g/mol)	mmol/g peptidoglycan
N-acetylmuramate	1.000	275.3	1.106
N-acetylglucosamine	1.000	203.2	1.106
Alanine	2.000	71.1	2.213
Diaminopimelic acid	1.000	154.2	1.106
Glutamate	1.000	129.1	1.106
Average molecular weight		903.9	
ATP per each polymerization:		4.425	

7. Carbohydrate composition

The components of carbohydrates were also determined from analysis in DSMZ. The molar ratio of carbohydrates was assumed to be identical to *S. antibioticus* (Zaretskaia and Polin, 1987) except glucose was used instead of N-acetylglucosamine. The polysaccharide is made from activated building blocks, so there is no need for additional ATP during polymerization.

Components	Molar ratio	MW (g/mol)	mmol/g
Glucose	1	162	2.058
Galactose	2	162	4.115

8. Teichoic acid composition

There is no published data of teichoic acid of clostridial species. Therefore, the teichoic acid composition was adopted from the model of *S. coelicolor* (Borodina et al., 2003).

Components	Molar ratio	MW (g/mol)	mmol/g teichoic acid
Polyglycerophosphate chain	1	1848.7	0.518
Lysine	0.25	128.2	0.129
N-acetylglucosamine	0.25	203.2	0.129
Energy requirement for polymerization (ATP):		0.129	

References

Number	Authors	Year	issue;volume/page	Journal/Publisher
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6	Oh, Y.K., Palsson, B.O., Park, S.M., Schilling, C.H., and Mahadevan, R.	2007	282(39):28791-28799	J. Biol. Chem.
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