

BIOMASS COMPOSITIONS

Biomass composition of *M. maripaludis S2* used in our model

Table 1: Cellular composition of *M. maripaludis S2* from batch culture¹

Major cellular components	Cellular content % (g/gDCW)
Proteins	60.97
RNA	22.73
DNA	3.44
Phospholipids	10.09
Glycogen	0.34
Soluble pools	2.43

Table 2: Energy requirements during growth of *M. maripaludis* required for polymerization of macromolecules (Verduyn.²)

Cellular components	Cellular content (g/gDCW)	ATP per molecule (mmolATP/gpolymer)	Total (mmolATP/gcell)
Proteins	0.6097	37.7	22.9857
Glycogen	0.0034	12.8	0.0435
RNA	0.2273	26	5.9098
DNA	0.0344	26	0.8944
		Total ATP requirements	29.833

Proteins and Phospholipids Composition

Proteins and phospholipids compositions were adopted from the study of Stoyler et al.¹ which was determined after resuspending cell pellets in NaOH. The weight of water was excluded from molecular weight considering the removal of water during peptide bind formation.

Protein (mmol/g) – 60%

Amino acids	% Protein (g/g)	MW (g/mol)	Protein (mmol/g)
Alanine	6.824	71.09	0.96
Arginine	7.185	156.20	0.46
Asparagine	5.249	114.12	0.46
Aspartate	5.294	115.10	0.46
Cysteine	1.547	103.16	0.15
Glutamate	6.663	128.15	0.52
Glutamine	6.714	129.13	0.52
Glycine	4.394	57.07	0.77
Histidine	2.194	137.16	0.16

Isoleucine	4.979	113.18	0.44
Leucine	9.620	113.18	0.85
Lysine	6.922	128.19	0.54
Methionine	2.886	131.21	0.22
Phenylalanine	4.415	147.19	0.30
Proline	3.302	97.13	0.34
Serine	3.832	87.09	0.44
Threonine	4.854	101.12	0.48
Tryptophan	0.186	186.23	0.01
Tyrosine	4.243	163.19	0.26
Valine	6.643	99.15	0.67

0.77 Gly + 0.96 Ala + 0.67 Val + 0.85 Leu + 0.44 Ile + 0.44 Ser + 0.48 Thr + 0.30 Phe + 0.26 Tyr + 0.01 Trp + 0.15 Cys + 0.22 Met + 0.54 Lys + 0.46 Arg + 0.16 His + 0.46 Asp + 0.52 Glu + 0.46 Asn + 0.52 Gln + 0.34 Pro → Protein

DNA Composition

DNA composition was estimated using GC content present in the genomic sequence of *M. maripaludis* S2 by Hendrickson et al.³. When polymerized, each nucleotide will lose a water molecule of 18.0, and not considering methylation of any bases, the molecular weight of each will be reduced

DNA (mmol/g) - 3.44%

Bases	# of bases	Double strand	Composition (mol/molDNA)	MW (g/mol)	DNA mmol/g DNA
A	559092	1118184	0.3366	313.2	1.0746
T	552203	1104406	0.3324	304.2	1.0928
C	274207	548414	0.1651	289.2	0.5708
G	275635	551270	0.1659	329.2	0.5041
sum	1661137	3322274			

0.504 dGTP + 1.075 dATP + 0.571 dCTP + 1.093 dTTP → DNA + 3.242 ppi

RNA Composition

It has been assumed that RNA consists of 5% mRNA, 81% rRNA, 14% tRNA taken from total composition of *E. coli*. The nucleotide composition of mRNA was considered similar with CDS region of genomic DNA. Nucleotide composition of rRNA and tRNA has been calculated from the sequences of rRNA and tRNA from web Artemis. The molecular weight given in the table below is the weight of the nucleotide minus the weight of water molecule, which is lost during esterification

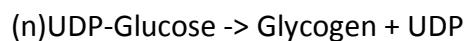
RNA (mmol/g) – 22.73%

Nucleotides	MW (g/mol)	Composition (mol/mol RNA)	RNA (mmol/g)
A	329.2	0.2410	0.7896
U	306.2	0.2719	0.8260
C	305.2	0.2704	0.7832
G	345.2	0.2167	0.7077

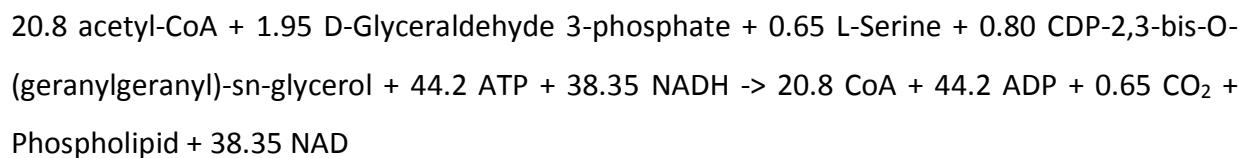


Glycogen – 0.34%

Presence of enzyme glycogen synthase (UDPGlc) in *M. maripaludis* S2 associated with EC number 2.7.1.11 has been demonstrated by Yu et al.⁴ for glycogen formation and is given by reaction:



Phospholipid – 10.09%



Soluble pool

For simplification, it was assumed that the selected soluble pool molecules are equally present in the cell. Adding soluble pool components in biomass equation also make sure that the essential vitamins and cofactors needed for enzyme activity are produced during the growth.

Soluble pool (mmol/g) – 2.43%

Molecules	MW (g/mol)	Pool composition (g/gDCW)	Pool molecules (mmol/g)
Coenzyme F430	905.286	0.00111	0.001
Putrescine	88.151	0.00111	0.013
Spermine	202.215	0.00111	0.005
Cofactor 420	773.592	0.00111	0.001
Cofactor 420-0	515.364	0.00111	0.002
Cofactor 420-1	644.478	0.00111	0.002
Cofactor 420-3	902.706	0.00111	0.001

AMP	347.221	0.00111	0.003
Coenzyme B	327.334	0.00111	0.003
Coenzyme M	142.197	0.00111	0.008
Siroheme	916.661	0.00111	0.001
Vitamin B ₁₂	1579.581	0.00111	0.001
Coenzyme A	767.534	0.00111	0.001
Pyridoxal phosphate	247.141	0.00111	0.004
Acetyl COA	809.570	0.00111	0.001
NAD	664.433	0.00111	0.002
NADH	665.441	0.00111	0.002
NADP	744.413	0.00111	0.001
NADPH	745.421	0.00111	0.001
Biotin	244.310	0.00111	0.005
Riboflavin	376.364	0.00111	0.003
Nicotinic acid	123.109	0.00111	0.009
THMPT	776.683	0.00111	0.0014

0.2273 RNA + 0.0344 DNA + 0.1009 Phospholipid + 0.6097 Proteins + 0.0034 Glycogen + 0.0243 Soluble pool + 30 ATP -> BIOMASS + 30 ADP + 30 Pi

References

1. S. Stolyar, S. Van Dien, K. L. Hillesland, N. Pinel, T. J. Lie, J. A. Leigh and D. A. Stahl, *Molecular systems biology*, 2007, **3**, 92.
2. C. Verduyn, A. H. Stouthamer, W. A. Scheffers and J. P. Dijken, *Antonie van Leeuwenhoek*, 1991, **59**, 49-63.
3. E. Hendrickson, R. Kaul, Y. Zhou, D. Bovee, P. Chapman, J. Chung, E. C. de Macario, J. Dodsworth, W. Gillett and D. Graham, *Journal of bacteriology*, 2004, **186**, 6956-6969.
4. J.-P. Yu, J. Ladapo and W. B. Whitman, *Journal of bacteriology*, 1994, **176**, 325-332.