Electronic Supplementary Material (ESI) for Molecular BioSystems.


# BIOMASS COMPOSITIONS

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

Table 1: Cellular composition of *M. maripaludis S2* from batch culture[1]

| 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 |

0.789 UTP + 0.708 CTP + 0.82 ATP + 0.783 GTP → RNA + 3.107 ppi

**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:

(n)UDP-Glucose -> Glycogen + UDP

**Phospholipid – 10.09%**

20.8 acetyl-CoA + 1.95 D-Glyceraldehyde 3-phosphate + 0.65 L-Serine + 0.80 CDP-2,3-bis-O-(geranylgeranyl)-sn-glycerol + 44.2 ATP + 38.35 NADH -> 20.8 CoA + 44.2 ADP + 0.65 $CO_2$ + Phospholipid + 38.35 NAD

**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.