**Table S9.** Biomass composition calculations for *P. chrysogenum*.

(g/gDW)
0.45
0.08
0.01
0.035
0.01
0.005
0.22
0.03
0.04
0.02
0.02

<sup>&</sup>lt;sup>a</sup>If nothing else is stated the composition is taken from Table 4.13 in Physiological Engineering Aspects of Penicillin chrysogenum [1] <sup>b</sup>This proportion is assumed to contain mono-, di-, and triacylglycerides as well as free fatty acids

### AMINO ACIDS AND PROTEIN

		Protein	Scaled protein	Protein	Free amino acid	Scaled free amino	
		composition	composition	composition	pool (mol/mol	acid composition	
	Molecular weight	(mol/mol amino	(mol/mol amino	(mmol/g	free amino	(mol/mol free amino	Amino acid pool composition
	(g/mol)	acids) <sup>a</sup>	acids) <sup>d</sup>	protein)	acids) <sup>e,f</sup>	acids) <sup>d</sup>	(mmol/g free amino acids)
L-alanine	89.09	0.071	0.071753411	0.583943653	0.13	0.1363398	1.04484604
L-2-aminoadipate	161.15	0	0	0	0.006	0.00629261	0.04822366
L-arginine	174.2	0.0675	0.068216271	0.555157698	0.026	0.02726796	0.20896921
L-asparagine <sup>b</sup>	132.12	0.017125	0.017306721	0.140845564	0.034	0.0356581	0.27326743
L-aspartate <sup>b</sup>	133.11	0.051375	0.051920162	0.422536693	0.058	0.06082853	0.46616208
L-cysteine	121.16	0.018	0.018191006	0.148042053	0.005	0.00524384	0.04018639
L-glutamate <sup>c</sup>	147.13	0.088125	0.089060131	0.724789217	0.254	0.266387	2.04146841
L-glutamine <sup>c</sup>	146.15	0.029375	0.02968671	0.241596406	0.166	0.17409544	1.33418802
glycine	75.07	0.0755	0.076301162	0.620954166	0.032	0.03356057	0.25719287
L-histidine	155.16	0.025	0.025265285	0.205613962	0.028	0.0293655	0.22504376
L-isoleucine	131.18	0.042	0.04244568	0.345431457	0.013	0.01363398	0.1044846
L-leucine	131.18	0.0845	0.085396665	0.694975193	0.016	0.01678028	0.12859644
L-lysine	146.19	0.0755	0.076301162	0.620954166	0.022	0.02307289	0.1768201

L-methionine	149.21	0.054	0.054573017	0.444126159	0.005	0.00524384	0.04018639
L-phenylalanine	165.19	0.0335	0.033855483	0.27552271	0.005	0.00524384	0.04018639
L-proline	115.13	0.0515	0.052046488	0.423564762	0.0515	0.05401154	0.41391978
L-serine	105.09	0.0515	0.052046488	0.423564762	0.047	0.04929208	0.37775203
L-threonine	119.12	0.0535	0.054067711	0.440013879	0.031	0.0325118	0.24915559
L-tryptophan	204.23	0.007	0.00707428	0.057571909	0.002	0.00209754	0.01607455
L-tyrosine	118.19	0.0235	0.023749368	0.193277125	0.006	0.00629261	0.04822366
L-valine	117.15	0.07	0.070742799	0.575719094	0.016	0.01678028	0.12859644
TOTAL		0.9895	1		0.9535	1	

Molecular weight of protein (g/mol)	122.8772852
Molecular weight of free amino acid	
pool (g/mol)	130.4879339

<sup>&</sup>lt;sup>a</sup>Data from Table 4.11 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]. Averaged composition from two studies (Jørgensen 1993;[2]

# **DNA AND**

RNA

	RNA composition (mmol/g RNA) <sup>a</sup>		DNA composition (mmol/g DNA) <sup>a</sup>
AMP	0.79	dAMP	0.79
GMP	0.89	dGMP	0.86
CMP	0.61	dCMP	0.86
UMP	0.81	dTMP	0.79

<sup>&</sup>lt;sup>a</sup>Following the reasoning in section 4.3.3 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]

#### FREE RIBONUCLEOTIDES

	Free ribonucleotide	Molecular weigh	t Composition (mmol/g free
	composition (mmol/g DW) <sup>a</sup>	(g/mol)	ribonucleotides)
GTP	0.0033	532.18	0.213396447
ATP	0.0225	507.18	1.454975775
UTP	0.00145	484.14	0.093765105
CTP	0.0033	483.16	0.213396447

bThe pool of aspartate and asparagine is measured. A ratio of 3:1 aspartate/asparagine is assumed (Oura, 1972)

The pool of glutamate and glutamine is measured. A ratio of 3:1 glutamate/glutamine is assumed (Oura, 1972)

<sup>&</sup>lt;sup>d</sup>Scaled composition to deal with the molecular balance not closing

<sup>&</sup>lt;sup>e</sup>Data from Table 4.7 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]. Original data from Jørgensen (1993)

<sup>&</sup>lt;sup>f</sup>Proline cannot be measured with the applied method. Assumes the same composition as in protein

<sup>a</sup>Following the reasoning in section 4.3.2 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]. Average values are used.

# LIPIDS

		Fatty acid	Scaled fatty acid					
		composition	composition					
	Molecular	(mol/mol total fatty						
	weight (g/mol) <sup>a</sup>	acids) <sup>b</sup>	acids) <sup>c</sup>	Free fatty acid co	emposition (mmol/g	g free fatty acids)		
pentadecanoyl	225.3925	0.0125	0.011927481	0.042968034				
palmitoyl	239.4192	0.2425	0.23139313	0.833579865				
hexadecenoyl	237.4032	0.03	0.028625954	0.103123282				
stearoyl	267.4726	0.09	0.085877863	0.309369847				
octadecenoyl	265.4566	0.047	0.044847328	0.161559809				
octadecadienoyl	263.4406	0.48	0.458015267	1.649972517				
arachidate	295.526	0.146	0.139312977	0.501866641				
TOTAL		1.048	1					
		Phospholipid composition	Phospholipid composition	Acylglyceride composition	Acylglyceride composition	Ergosterol/ergosterol ester composition	Ergosterol/ergostero l ester composition	Glucolipid
		(mol/mol total	(mmol/g total	(mol/mol	(mmol/g total	(mol/mol total	(mmol/g total	composition
Average molecular w	eights (g/mol):	phospholipid) <sup>d</sup>	phospholipid)	acylglyceride) <sup>d.f</sup>	acylglyceride)	ergosterol) <sup>d</sup>	ergosterol)	(mol/gDW) <sup>d.e</sup>
acyl group	261.589634							
free fatty acids	277.589634			0.210607316	0.379742043			
monoglycerides	352.677734			0.351683043	0.634113001			
diglycerides	613.259368			0.039816898	0.07179309			
triglycerides	873.8410021			0.397892743	0.717432831			
phosphatidylserine	779.308468	0.006873576	0.00886945					
phosphatidylcholines	779.393868	0.293170461	0.378298093					
phosphatidylethanolam								
ines	736.305768	0.666430527	0.859941335					
ergosterol	396.6516					0.77238095	1.69394811	
ergosterol ester	657.233234					0.22761905	0.49920296	
digalactosyl-	(75.050124							0.007070
diacylglycerol	675.958134							0.007859
trigalactosyldimannosy		0.572227.05	0.00012252					
linositol-P-ceramide	2038.883868 596.9949	9.57323E-05	0.00012353					0.00003
cerebrin 1 cerebrin 2	580.9949							0.00003
galactosylceramides	747.1284							0.000031
glucocerebroside 1	928.2966							0.000023
gracocereoroside I	940.4900							0.000024

glucocerebroside 2 926.2806			0.00002
cardiolipin 1502.506836 0.033429704 0.043136656	136656		

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caratonpin	1302.300030
Molecular weight of	
phospholipid (g/mol)	774.972082
Molecular weight of	
acylglycerides (g/mol)	554.6062653
Molecular weight of	
sterol esters (g/mol)	455.9649434

<sup>&</sup>lt;sup>a</sup>Composition calculated only for the acyl chain, not for the fatty acid (lacks the carboxyl group)

The free fatty acid proportion differ between *Penicillium chrysogenum* and *Aspergillius niger* but it is assumed that the proportion relative to the acylglycerides is the same

CELLWALL AND STORAGE <sup>a</sup> UDP-N-acetyl-D-	Molecular weight of monomer in cell wall (without UDP/GDP) (g/mol) <sup>b</sup>	Cell wall monomer composition (mol/mol total monomers) <sup>b</sup>	Cell wall monomer composition (mmol/g cell wall monomers)
glucosamine	214.1596	0.27184466	1.54208087
UDP-glucose UDP-D-galactose	162.1442 162.1442	0.495145631 0.145631068	2.808790156 0.826114752
GDP-mannose trehalose	162.1442 162.1442	0.058252427 0.029126214	0.330445901 0.16522295
Molecular weight of cell wall and storage (mmol/g)	176.28430	087	

<sup>&</sup>lt;sup>a</sup>The cell wall composition of *Penicillium chrysogenum* is not well researched and there is conflicting data. The cell wall composition if therefore expressed as a polymerization of the monomers.

<sup>&</sup>lt;sup>b</sup>Total fatty acid composition for growth on glucose as sole carbon source [3]

<sup>&</sup>lt;sup>c</sup>Scaled composition to deal with the molecular balance not closing

<sup>&</sup>lt;sup>d</sup>Assumes the same composition as in the A. niger model

<sup>&</sup>lt;sup>e</sup>No reliable data could be found on the percentage of glucolipids in *Penicillium chrysogenum*. It is therefore assumed that the composition and amount is the same as in *Aspergillius niger* (see the A. niger model [4])

<sup>&</sup>lt;sup>b</sup>Following the reasoning in section 4.3.3 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]

## POLYMERISATION COSTS<sup>a</sup>

DNA 11.22 RNA 7.44

Protein (mmol ATP/g protein) 34.9942627

<sup>&</sup>lt;sup>a</sup>Following the reasoning in section 4.3.3 in Physiological Engineering Aspects of *Penicillin chrysogenum* [1]

## References

- 1. Nielsen JH (1995) Physiological engineering aspects of penicillium chrysogenum. Denmark: Polyteknisk forlag. x, 223 p. p.
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- 3. Divakaran P, Modak MJ (1968) Fatty acid composition of mycelium of Penicillium chrysogenum grown in different carbohydrates as a sole source of carbon. Experientia 24: 1102.
- 4. Andersen MR, Nielsen ML, Nielsen J (2008) Metabolic model integration of the bibliome, genome, metabolome and reactome of Aspergillus niger. Mol Syst Biol 4: 178.