Added Ehrlich and Ester Forming Pathways

Table S1 Added Genes to current GSMM

Gene Name	Gene Short Name
YPL095C	EEB1
YBR177C	EHT1
YGR015C	EAT1

Table S2 Added Metabolites Added to current GSMM

NAME	MIRIAM	COMPOSITION	COMPARTMENT	REPLACEMENT ID	CHARGE
hexanoyl-CoA	chebi/CHEBI:27540;kegg.compound/C00642;metanetx.chemical/MNXM553;sbo/SBO:0000247	C27H46N7O17P3S	m	s_4207	-4
ethyl hexanoate	chebi/CHEBI:86055;metanetx.chemical/MNXM52763;sbo/SBO:0000247	C8H16O2	m	s_4208	0
ethyl hexanoate	chebi/CHEBI:86055;metanetx.chemical/MNXM52763;sbo/SBO:0000247	C8H16O2	c	s_4209	0
ethyl hexanoate	chebi/CHEBI:86055;metanetx.chemical/MNXM52763;sbo/SBO:0000247	C8H16O2	e	s_4210	0
octanoyl-CoA	chebi/ChEBI:15533;kegg.compound/C01944;metanetx.chemical/MNXM342;sbo/SBO:0000247	C29H46N7O17P3S	m	s_4211	-4
ethyl octanoate	chebi/ChEBI:87426;kegg.compound/C12292;metanetx.chemical/MNXM52785;sbo/SBO:0000247	C10H20O2	m	s_4212	0
ethyl octanoate	chebi/ChEBI:87426;kegg.compound/C12292;metanetx.chemical/MNXM52785;sbo/SBO:0000247	C10H20O2	c	s_4213	0
ethyl octanoate	chebi/ChEBI:87426;kegg.compound/C12292;metanetx.chemical/MNXM52785;sbo/SBO:0000247	C10H20O2	e	s_4214	0
butanoyl-CoA	chebi/ChEBI:57371;kegg.compound/C00136 ;metanetx.chemical/MNXM233;sbo/SBO:0000247	C25H38N7O17P3S	m	s_4215	-4
ethyl butanoate	chebi/ChEBI:88764;metanetx.chemical/MNXM11527;sbo/SBO:0000247	C6H12O2	m	s_4216	0
ethyl butanoate	chebi/ChEBI:88764;metanetx.chemical/MNXM11527;sbo/SBO:0000247	C6H12O2	c	s_4217	0
ethyl butanoate	chebi/ChEBI:88764;metanetx.chemical/MNXM11527;sbo/SBO:0000247	C6H12O2	e	s_4218	0
hexan-1-ol	chebi/ChEBI:87393;metanetx.chemical/MNXM18358;sbo/SBO:0000247	C6H14O	c	s_4219	0
hexyl acetate	chebi/ChEBI:87510;metanetx.chemical/MNXM99284;sbo/SBO:0000247	C8H16O2	m	s_4220	0
hexyl acetate	chebi/ChEBI:87510;metanetx.chemical/MNXM99284;sbo/SBO:0000247	C8H16O2	c	s_4221	0
hexyl acetate	chebi/ChEBI:87510;metanetx.chemical/MNXM99284;sbo/SBO:0000247	C8H16O2	e	s_4222	0
decanoyl-CoA	chebi/ChEBI:61430;kegg.compound/C05274;metanetx.chemical/MNXM486;sbo/SBO:0000247	C31H50N7O17P3S	c	s_4223	-4
ethyl decanoate	chebi/ChEBI:87430;metanetx.chemical/MNXM100679;sbo/SBO:0000247	C12H24O2	m	s_4224	0
ethyl decanoate	chebi/ChEBI:87430;metanetx.chemical/MNXM100679;sbo/SBO:0000247	C12H24O2	c	s_4225	0
ethyl decanoate	chebi/ChEBI:87430;metanetx.chemical/MNXM100679;sbo/SBO:0000247	C12H24O2	e	s_4226	0

ethyl acetate	chebi/CHEBI:27750;kegg.compound/C00849;metanetx.chemical/MNXM8595;sbo/SBO:0000247	C4H8O2	m	s_4227	0
propanal	chebi/CHEBI:17153;kegg.compound/C00479;metanetx.chemical/MNXM821;sbo/SBO:0000247	C3H6O	c	s_4228	0
propanal	chebi/CHEBI:17153;kegg.compound/C00479;metanetx.chemical/MNXM821;sbo/SBO:0000247	C3H6O	m	s_4229	0
propanal	chebi/CHEBI:17153;kegg.compound/C00479;metanetx.chemical/MNXM821;sbo/SBO:0000247	C3H6O	e	s_4230	0
propanol	chebi/CHEBI:28831;kegg.compound/C05979;metanetx.chemical/MNXM6396;sbo/SBO:0000247	C3H8O	c	s_4231	0
propanol	chebi/CHEBI:28831;kegg.compound/C05979;metanetx.chemical/MNXM6396;sbo/SBO:0000247	C3H8O	m	s_4232	0
propanol	chebi/CHEBI:28831;kegg.compound/C05979;metanetx.chemical/MNXM6396;sbo/SBO:0000247	C3H8O	e	s_4233	0
methional	chebi/CHEBI:49017;metanetx.chemical/MNXM6829;sbo/SBO:0000247	C4H8OS	c	s_4234	0
methional	chebi/CHEBI:49017;metanetx.chemical/MNXM6829;sbo/SBO:0000247	C4H8OS	m	s_4235	0
methional	chebi/CHEBI:49017;metanetx.chemical/MNXM6829;sbo/SBO:0000247	C4H8OS	e	s_4236	0
methionol	chebi/CHEBI:49019;metanetx.chemical/MNXM14592;sbo/SBO:0000247	C4H10OS	c	s_4237	0
methionol	chebi/CHEBI:49019;metanetx.chemical/MNXM14592;sbo/SBO:0000247	C4H10OS	m	s_4238	0
methionol	chebi/CHEBI:49019;metanetx.chemical/MNXM14592;sbo/SBO:0000247	C4H10OS	e	s_4239	0
(4-hydroxyphenyl) acetaldehyde	chebi/CHEBI:15621;sbo/SBO:0000247	C8H8O2	c	s_4240	0
(4-hydroxyphenyl) acetaldehyde	chebi/CHEBI:15621;sbo/SBO:0000247	C8H8O2	m	s_4241	0
(4-hydroxyphenyl) acetaldehyde	chebi/CHEBI:15621;sbo/SBO:0000247	C8H8O2	e	s_4242	0
tyrosol	chebi/CHEBI:1879;kegg.compound/C06044;sbo/SBO:0000247	C8H10O2	c	s_4243	0
tyrosol	chebi/CHEBI:1879;kegg.compound/C06044;sbo/SBO:0000247	C8H10O2	m	s_4244	0
tyrosol	chebi/CHEBI:1879;kegg.compound/C06044;sbo/SBO:0000247	C8H10O2	e	s_4245	0

Table S3 Added Reactions to current GSMM

ID	**NAME**	**EQUATION**	**EC-NUMBER**	**GENE ASSOCIATION**
r_4629	alcohol acyltransferase (hexanoyl-CoA)	hexanoyl-CoA[m] + ethanol[m] <=> ethyl hexanoate[m] + coenzyme A[m]	2.3.1.84	YBR177C or YPL095C
r_4630	alcohol acyltransferase (octanoyl-CoA)	octanoyl-CoA[m] + ethanol[m] <=> ethyl octanoate[m] + coenzyme A[m]	2.3.1.84	YBR177C or YPL095C
r_4631	alcohol acyltransferase (butyryl-CoA)	butanoyl-CoA[m] + ethanol[m] <=> ethyl butanoate[m] + coenzyme A[m]	2.3.1.84	YBR177C or YPL095C
r_4632	alcohol acyltransferase	acetyl-CoA[m] + hexan-1-ol[m]	2.3.1.84	YBR177C or

	(acetyl-CoA)	<=> hexyl acetate[m] + coenzyme A[m]		YPL095C
r_4633	alcohol acyltransferase (decanoyl-CoA)	decanoyl-CoA[m] + ethanol[m] <=> ethyl decanoate[m] + coenzyme A[m]	2.3.1.84	YBR177C or YPL095C
r_4634	ethyl hexanoate transport, mitochondrial	ethyl hexanoate[m] <=> ethyl hexanoate[c]		
r_4635	ethyl octanoate transport, mitochondrial	ethyl octanoate[m] <=> ethyl octanoate[c]		
r_4636	ethyl butanoate transport, mitochondrial	ethyl butanoate[m] <=> ethyl butanoate[c]		
r_4637	hexyl acetate transport, mitochondrial	hexyl acetate[m] => hexyl acetate[c]		
r_4638	ethyl decanoate transport, mitochondrial	ethyl decanoate[m] => ethyl decanoate[c]		
r_4639	ethyl hexanoate transport	ethyl hexanoate[c] <=> ethyl hexanoate[e]		
r_4640	ethyl octanoate transport	ethyl octanoate[c] <=> ethyl octanoate[e]		
r_4641	ethyl butanoate transport	ethyl butanoate[c] <=> ethyl butanoate[e]		
r_4642	hexyl acetate transport	hexyl acetate[c] => hexyl acetate[e]		
r_4643	ethyl decanoate transport	ethyl decanoate[c] => ethyl decanoate[e]		
r_4644	ethyl hexanoate exchange	ethyl hexanoate[e] <=>		
r_4645	ethyl octanoate exchange	ethyl octanoate[e] <=>		
r_4646	ethyl butanoate exchange	ethyl butanoate[e] <=>		
r_4647	hexyl acetate exchange	hexyl acetate[e] <=>		
r_4648	ethyl decanoate exchange	ethyl decanoate[e] <=>		
r_4649	mitochondrial ethanol O-acetyltransferase	ethanol[m] + acetyl-CoA[m] => ethyl acetate[m] + coenzyme A[m]	2.3.1.268	YGR015C
r_4650	ethyl acetate transport, mitochondrial	ethyl acetate[m] => ethyl acetate[c]		
r_4651	pyruvate decarboxylase (aldedyde-forming)	H+[c] + 2-oxobutanoate[c] => carbon dioxide[c] + propanal[c]	4.1.1.1	YGR087C or YLR044C or YLR134W
r_4652	aldehyde dehydrogenase (1-propanol, NAD)	propanal[c] + H+[c] + NADH[c] => propanol[c] + NAD[c]	1.1.1.-; 1.1.1.1; 1.1.1.284	YBR145W or YDL168W or YOL086C
r_4653	aldehyde dehydrogenase (1-propanol, NAD)	propanal[m] + H+[m] + NADH[m] => propanol[m] + NAD[m]	1.1.1.1	YGL256W or YMR083W
r_4654	aldehyde dehydrogenase (1-propanol, NADP)	propanal[c] + H+[c] + NADPH[c] => propanol[c] + NADP(+)[c]	1.1.1.-; 1.1.1.2	YCR105W or YDR368W or YMR318C
r_4655	1-propyl alcohol transport, mitochondrial	propanol[c] <=> propanol[m]		
r_4656	propanal transport, cytosol	propanal[c] <=> propanal[e]		
r_4657	1-propyl alcohol transport, cytosol	propanol[c] <=> propanol[e]		
r_4658	propanal exchange	propanal[e] =>		
r_4659	propanol exchange	propanol[e] =>		
r_4660	2-oxo acid decarboxylase	H+[c] + 4-methylthio-2-oxobutanoate[c] => carbon dioxide[c] + methional[c]	4.1.1.1	YHR137W

r_4661	aldehyde dehydrogenase (methionol, NAD)	methional[c] + H+[c] + NADH[c] => methionol[c] + NAD[c]	1.1.1.-; 1.1.1.1; 1.1.1.284	YBR145W or YDL168W or YOL086C
r_4662	aldehyde dehydrogenase (methionol, NAD)	methional[m] + H+[m] + NADH[m] => methionol[m] + NAD[m]	1.1.1.1	YGL256W or YMR083W
r_4663	aldehyde dehydrogenase (methionol, NADP)	methional[c] + H+[c] + NADPH[c] => methionol[c] + NADP(+)[c]	1.1.1.-; 1.1.1.2	YCR105W or YDR368W or YMR318C
r_4664	methionol transport, mitochondrial	methionol[c] <=> methionol[m]		
r_4665	methional transport, cytosol	methional[c] <=> methional[e]		
r_4666	methionol transport, cytosol	methionol[c] <=> methionol[e]		
r_4667	methional exchange	methional[e] =>		
r_4668	methionol exchange	methionol[e] =>		
r_4669	pyruvate decarboxylase (hydroxy-phenyl)	H+[c] + 3-(4-hydroxyphenyl)pyruvate[c] => carbon dioxide[c] + (4-hydroxyphenyl)acetaldehyde[c]	4.1.1.1	YGR087C or YLR044C or YLR134W
r_4670	aldehyde dehydrogenase (tyrosol, NAD)	(4-hydroxyphenyl)acetaldehyde[c] + H+[c] + NADH[c] => tyrosol[c] + NAD[c]	1.1.1.-; 1.1.1.1; 1.1.1.284	YBR145W or YDL168W or YOL086C
r_4671	aldehyde dehydrogenase (tyrosol, NAD)	(4-hydroxyphenyl)acetaldehyde[m] + H+[m] + NADH[m] => tyrosol[m] + NAD[m]	1.1.1.1	YGL256W or YMR083W
r_4672	aldehyde dehydrogenase (tyrosol, NADP)	(4-hydroxyphenyl)acetaldehyde[c] + H+[c] + NADPH[c] => tyrosol[c] + NADP(+)[c]	1.1.1.-; 1.1.1.2	YCR105W or YDR368W or YMR318C
r_4673	tyrosol transport, mitochondrial	tyrosol[c] <=> tyrosol[m]		
r_4674	(4-hydroxyphenyl)acetaldehyde transport, cytosol	(4-hydroxyphenyl)acetaldehyde[c] <=> (4-hydroxyphenyl)acetaldehyde[e]		
r_4675	tyrosol transport, cytosol	tyrosol[c] <=> tyrosol[e]		
r_4676	(4-hydroxyphenyl)acetaldehyde exchange	(4-hydroxyphenyl)acetaldehyde[e] =>		
r_4677	tyrosol exchange	tyrosol[e] =>		

Table S4. Experimentally measured consumption/production rates of the different metabolites analyzed from Quiros et al. 2013 and constraints used in the study.

	240 g L^{-1} Glucose		280 g L^{-1} Glucose		Constraint: Lower and Upper Bound
Reaction Constraint	16 °C (Case III)	28 °C (Case IV)	16 °C (Case I)	28 °C (Case II)	
	mmol gDW^{-1} h^{-1}	mmol gDW^{-1} h^{-1}	mmol gDW^{-1} h^{-1}	mmol gDW^{-1} h^{-1}	mmol gDW^{-1} h^{-1}
Glucose[ex]	-4.76	-20.51	-4.19	-16.31	LB = EV and UB =1000
Glycerol[ex]	0.38	1.37	0.34	1.39	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Ethanol[ex]	8.29	25.7	6.79	21.47	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Succinic acid[ex]	0.02	0.04	0.01	0.03	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Acetic acid[ex]	0.12	0.29	0.12	0.36	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Lactic acid[ex]	-	0.1157	-	0.0424	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Ala[ex]	-0.0353	-0.0925	-0.0178	-0.0705	LB = EV and UB =1000
Arg[ex]	-0.0724	-0.1427	-0.0568	-0.1426	LB = EV and UB =1000
Asp[ex]	-0.013	-0.0335	-0.0148	-0.0322	LB = EV and UB =1000
Cys[ex]	-	-0.0045	-	-0.0032	LB = EV and UB =1000
Gln[ex]	-0.0852	-0.2004	-0.0614	-0.1552	LB = EV and UB =1000
Glu[ex]	-0.0181	-0.053	-0.0092	-0.0449	LB = EV and UB =1000
Gly[ex]	-0.0015	-0.0049	-0.0008	-0.0033	LB = EV and UB =1000
His[ex]	0.0017	0.0007	0.0006	0.0007	LB = EV and UB =1000
Ile[ex]	-0.0112	-0.0244	-0.0093	-0.0223	LB = EV and UB =1000
Leu[ex]	-0.0182	-0.0392	-0.0164	-0.0359	LB = EV and UB =1000
Lys[ex]	-0.0095	-0.017	-0.0129	-0.0187	LB = EV and UB =1000
Met[ex]	-0.0087	-0.018	-0.0077	-0.0168	LB = EV and UB =1000
NH_4[ex]	-0.0657	-0.5219	-0.0555	-0.494	LB = EV and UB =1000
Phe[ex]	-0.0066	-0.0206	-0.005	-0.0181	LB = EV and UB =1000
Ser[ex]	-0.0389	-0.0733	-0.0327	-0.0625	LB = EV and UB =1000
Thr[ex]	-0.0324	-0.0635	-0.0285	-0.0552	LB = EV and UB =1000
Trp[ex]	-0.0033	-0.0129	-0.0016	-0.0099	LB = EV and UB =1000
Tyr[ex]	-0.0003	-0.0051	-0.0006	-0.0025	LB = EV and UB =1000
Val[ex]	-0.0119	-0.0234	-0.0092	-0.0253	LB = EV and UB =1000
Amyl alcohol[ex]	0.0024	0.0095	0.0021	0.0067	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Isoamyl alcohol[ex]	0.0062	0.0242	0.0053	0.019	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Propanol[ex]	0.0081	0.0248	0.0069	0.0253	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV

Isobutanol[ex]	0.0024	0.0183	0.0025	0.0101	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
Phenyl ethanol[ex]	0.0009	0.0046	0.0009	0.0035	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV
CO_2[ex]	9.04	25.78	6.88	21.31	2) LB = 1000 and UB =1000 3) LB = 1000 and UB =EV

The values in the constraint column correspond to the parts (e.g. 2) Validation of Model Predictions) of the results section. (Experimental Value = EV)