Additional Table 1 - Validation of the Y. lipolytica model

Validation of the Y. lipolytica model with respect to experimental evidence of Y. lipolytica growth under different media conditions and gene knockouts. Expected Growth was obtained by the referenced literature. Simulated Growth was obtained using flux balance analysis (FBA), optimizing over the biomass function of our model, and converted to a qualitative phenotype/no phenotype value by thresholding. In both cases, the symbols represent '+': growth; '-':no growth; 'n/a': condition cannot be simulated with current model, but are provided for future model improvements. The "Result" column compares the two: TP/FP: True/False Positives, TN/FN: True/False Negatives. The simulated models shows a sensitivity of 0.68, a specificity of 0.61 and an accuracy (geometric mean between sensitivity and specificity) of 0.65.

Ref	Media	Y. lipolytica	S. cerevisiae	Gene	Exp.	Simul.	Result
[00]	MAIDO	knocked locus	ortholog	name	Growth		
[33]	YNBO	YALIOC06347g	YGL124C	MON1	+	n/a	n/a
[33]	YNBC16	YALI0C06347g	YGL124C	MON1	+	n/a	n/a
[33]	YNBT	YALI0C06347g	YGL124C	MON1	+	n/a	n/a
[33]	YNBD	YALI0D27126g	YDR353W	TRR1	+	_	FN
			YHR106W	TRR2			
[33]	YNBD	YALI0E14729g	YOR153W	PDR5	+	+	TP
[33]	YNBO	YALI0E14729g	YOR153W	PDR5	+	-	FN
[33]	YNBC10	YALI0E14729g	YOR153W	PDR5	+	+	TP
[33]	YNBC16	YALI0E14729g	YOR153W	PDR5	-	-	TN
[33]	YNBT	YALI0E14729g	YOR153W	PDR5	+	-	FN
[33]	YNBD	YALI0E09405g	YGL153W	PEX14	+	n/a	n/a
[33]	YNBO	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
[33]	YNBC10	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
[33]	YNBC16	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
			YLL051C				
[33]	YNBD	YALI0D26081g	YOL152W	FRE3-7	+	n/a	n/a
[၁၁]	INDD	TALIOD20001g	YOR381W	THES-1			
			YOR384W				
	YNBO		YLL051C			n/a	n/a
[99]		YALI0D26081g	YOL152W	FRE3-7	+		
[33]		TALIUD20001g	YOR381W				
			YOR384W				
	YNBC10		YLL051C	FRE3-7	-	n/a	n/a
[99]		VAI 10D96091 m	YOL152W				
[33]		YALI0D26081g	YOR381W				
			YOR384W				
			YLL051C	FRE3-7	+	n/a	n/a
[99]	YNBC16	YALI0D26081g	YOL152W				
[33]		TALIUD20001g	YOR381W				
			YOR384W				
	YNBT		YLL051C	152W R381W FRE3-7	+	n/a	n/a
[99]		YALI0D26081g	YOL152W				
[33]		TALIUD20001g	YOR381W				
			YOR384W				
[33]	YNBD	YALI0F04095g	YDL066W	IDP1	-	+	FP
[33]	YNBO	YALI0F04095g	YDL066W	IDP1	-	-	TN
[33]	YNBT	YALI0F04095g	YDL066W	IDP1	-	-	TN
[33]	YNBD	YALI0E09405g	YGL153W	PEX14	+	n/a	n/a
[33]	YNBO	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
[33]	YNBC10	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
[33]	YNBC16	YALI0E09405g	YGL153W	PEX14	-	n/a	n/a
[33]	YNBT	YALI0E09405g	YGL153W	PEX14	+	n/a	n/a
[33]	YNBD	YALI0C21582g	YGL059W	PKP2	+	n/a	n/a
[33]	YNBO	YALI0C21582g	YGL059W	PKP2	-	n/a	n/a
[33]	YNBC10	YALI0C21582g	YGL059W	PKP2	_	n/a	$\frac{n/a}{n/a}$
[33]	YNBC16	YALI0C21582g	YGL059W	PKP2	+	n/a	$\frac{n/a}{n/a}$
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Ref	Media	Y. lipolytica	S. cerevisiae	Gene	Exp.	Simul.	Resul
001	VNDD	knocked locus	ortholog	name	Growth	Growth	mD.
33]	YNBD	YALIOE34672g	YJR095W	ACR1	+	+	TP
33]	YNBO	YALI0E34672g	YJR095W	ACR1	-	-	TN
33]	YNBC10	YALIOE34672g	YJR095W	ACR1	-	+	FP
33]	YNBC16	YALI0E34672g	YJR095W	ACR1	-	-	TN
33]	YNBT	YALI0E34672g	YJR095W	ACR1	-	-	TN
33]	YNBD	YALI0B13970g	YIL155C	GUT2	+	+	TP
33]	YNBC10	YALI0B13970g	YIL155C	GUT2	+	+	TP
33]	YNBC16	YALI0B13970g	YIL155C	GUT2	+	-	FN
33]	YNBD	YALI0E06831g		PEX20	+	n/a	n/a
33]	YNBO	YALI0E06831g		PEX20	-	n/a	n/a
33]	YNBC10	YALI0E06831g		PEX20	-	n/a	n/a
33]	YNBC16	YALI0E06831g		PEX20	-	n/a	n/a
33]	YNBT	YALI0E06831g		PEX20	+	n/a	n/a
33]	YNBD	YALI0F18216g	YFL001W	DEG1	+	+	TP
33]	YNBC16	YALI0F18216g	YFL001W	DEG1	+	-	FN
33]	YNBT	YALI0F18216g	YFL001W	DEG1	+	-	FN
33]	YNBD	YALI0E03058g	YPR128C	PMP34	+	+	TP
33]	YNBO	YALI0E03058g	YPR128C	PMP34	+	-	FN
33]	YNBC10	YALI0E03058g	YPR128C	PMP34	-	+	FP
33]	YNBC16	YALI0E03058g	YPR128C	PMP34	+	-	FN
33]	YNBT	YALI0E03058g	YPR128C	PMP34	+	-	FN
33]	YNBD	YALI0C16885g	YER065C	ICL1	+	+	TP
33]	YNBO	YALI0C16885g	YER065C	ICL1	-	-	TN
33]	YNBC10	YALI0C16885g	YER065C	ICL1	-	-	TN
33	YNBC16	YALI0C16885g	YER065C	ICL1	-	-	TN
33	YNBT	YALI0C16885g	YER065C	ICL1	-	-	TN
	YNBD	YALI0E14729g	YOL075C	PDR5	+	+	TP
33]			YNR070W				
-			YDR011W				
	YNBO	YALI0E14729g	YOL075C		+	-	FN
33]			YNR070W	PDR5			
-			YDR011W				
	YNBC10	YALI0E14729g	YOL075C	PDR5	+	+	TP
33]			YNR070W				
-			YDR011W				
	YNBC16	YALI0E14729g	YOL075C	PDR5	-	-	TN
33]			YNR070W				
-			YDR011W				
	YNBT	YALI0E14729g	YOL075C	PDR5	+ -		FN
33]			YNR070W			-	
			YDR011W				
34]	Lactose	n/a		-	n/a	n/a	
34]	D-Galactose	n/a		-	+	FP	
35]	YNBD	YALI0A15972g	YLR377C	FBP1	+	+	TP
-	Ethanol	YALI0A15972g	YLR377C	FBP1	+	-	FN
[35]	Littation						

Ref	Media	Y. lipolytica	S. cerevisiae	Gene	Exp.	Simul.	Result
		knocked locus	ortholog	name	Growth	Growth	
[35]	Acetate	YALIOA15972g	YLR377C	FBP1	+	-	FN
[36]	YNBD	YALI0C24101g	YGL062W	PYC1	+	+	TP
[36]	Ethanol	YALI0C24101g	YGL062W	PYC1	+	+	TP
[36]	Aspartate	YALI0C24101g	YGL062W	PYC1	+	+	TP
[36]	Glutamate	YALI0C24101g	YGL062W	PYC1	+	+	TP
[36]	YNBD	YALI0C16885g	YER065C	ICL1	+	+	TP
[36]	Ethanol	YALI0C16885g	YER065C	ICL1	-	-	TN
[36]	Aspartate	YALI0C16885g	YER065C	ICL1	+	+	TP
[36]	Glutamate	YALI0C16885g	YER065C	ICL1	+	+	TP
[36]	YNBD	YALI0C24101g	YGL062W	ICL1		+	FP
[90]	TNDD	YALI0C16885g	YER065C	PYC1	_	T	1.1
[36]	Ethanol	YALI0C24101g	YGL062W	ICL1	_		TN
[90]	Editation	YALI0C16885g	YER065C	PYC1	_	_	111
[36]	Aspartate	YALI0C24101g	YGL062W	ICL1	+	+	TP
[90]	Aspartate	YALI0C16885g	YER065C	PYC1	+	+	11
[36]	Glutamate	YALI0C24101g	YGL062W	ICL1		-	TP
[90]		YALI0C16885g	YER065C	PYC1	+	+	
[37]	YNBC10	YALI0E19514g	YCR077C	PAT1	-	n/a	n/a
[37]	YNBD	YALI0E19514g	YCR077C	PAT1	+	n/a	n/a
[37]	Glycerol	YALI0E19514g	YCR077C	PAT1	+	n/a	n/a
[00]	YNBD	YALI0D24431g		ACL1	+	+	TP
[38]		YALI0E34793g					1P
[00]	YNBO	YALI0D24431g		ACL1	+	-	ENI
[38]		YALI0E34793g		ACLI			FN
[39]	Acetate	YALI0C16885g	YER065C	ICL1	-	-	TN
[39]	YNBO	YALIOC16885g	YER065C	ICL1	-	-	TN
[39]	YNBD	YALIOC16885g	YER065C	ICL1	+	+	TP
[39]	Acetate	YALI0E15708g	YNL117W	MLS1	+	+	TP
[39]	YNBO	YALI0E15708g	YNL117W	MLS1	+	-	FN
[39]	YNBD	YALI0E15708g	YNL117W	MLS1	+	+	TP
[00]			YCR005C	CITTO .			(TED)
[39]	Acetate	YALI0E02684g	YNR001C	CIT2	+	+	TP
[00]	YNBO	N/A I TOFFOOO /	YCR005C	CITTO	+		ENT
[39]		YALI0E02684g	YNR001C	CIT2		-	FN
[00]	TOTO	N/A I TOFFOOO /	YCR005C	OTT.			TED.
[39]	YNBD	YALI0E02684g	YNR001C	CIT2	+	+	TP
[40]	YNBD	YALI0B13970g	YIL155C	GUT2	+	+	TP
[40]	Glycerol	YALI0B13970g	YIL155C	GUT2	-	+	FP
[40]	YNBO	YALI0B13970g	YIL155C	GUT2	+	_	FN
		YALI0B13970g		GUT2			
	YNBD	YALI0E32835g YALI0F10857g	YIL155C YGL205W	POX1	+	+	
				POX2			
[40]		YALI0D24750g		POX3			TP
		YALI0E27654g		POX4			
		YALI0C23859g		POX5			
		YALI0E06567g		POX6			
0 1	inued on next pa	Ü	1	1			

D.C	N. 1:	Y. lipolytica	S. cerevisiae	Gene	Exp.	Simul.	D 14
Ref	Media	knocked locus	ortholog	name	Growth	Growth	Result
[40]	Glycerol	YALI0B13970g		GUT2			
		YALI0E32835g		POX1			
		YALI0F10857g	YIL155C YGL205W	POX2			
		YALI0D24750g		POX3	-	+	FP
		YALI0E27654g		POX4		'	
		YALI0C23859g		POX5			
		YALI0E06567g		POX6			
		YALI0B13970g		GUT2			
		YALI0E32835g		POX1			
		YALI0F10857g		POX2			
[40]	YNBO	YALI0D24750g	YIL155C	POX3	_	_	TN
[40]	INDO	YALI0E27654g	YGL205W	POX4		_	111
		YALI0C23859g		POX5			
				POX6			
		YALI0E06567g					
		YALIOE32835g		POX1			
		YALIOF10857g	7777 4880	POX2			
[40]	YNBD	YALI0D24750g	YIL155C	POX3	+	+	TP
[-]		YALI0E27654g	YGL205W	POX4			
		YALI0C23859g		POX5			
		YALI0E06567g		POX6			
	Glycerol	YALI0E32835g		POX1	+		
		YALI0F10857g		POX2			
[40]		YALI0D24750g	YIL155C YGL205W	POX3		+	TP
[40]		YALI0E27654g		POX4			11
		YALI0C23859g		POX5			
		YALI0E06567g		POX6			
		YALI0E32835g	YIL155C	POX1	-	-	TN
		YALI0F10857g		POX2			
[40]	VNDO	YALI0D24750g		POX3			
[40]	YNBO	YALI0E27654g	YGL205W	POX4			
		YALI0C23859g		POX5			
		YALI0E06567g		POX6			
[41]	YNBD	YALI0D02629g	YOR222W YPL134C	ODC1	-	+	FP
F 4 4 1	YNBD+ pu-		YOR222W	0.7.01			
[41]	trescine	YALI0D02629g	YPL134C	ODC1	+	+	TP
[42]	YNBD	YALI0B07667g	YDR007W	TRP1	-	+	FP
[42]	YNBD+ trypto- phane	YALI0B07667g	YDR007W	TRP1	+	+	TP
	2-Keto-D-						
[32]	Gluconate	n/a	, media only		-	n/a	n/a
[32]	a,a-Trehalose	n /o	modia only		_	+	FP
[32]	Arbutin	n/a, media only n/a, media only			-	·	
		, ,			-	n/a	n/a
[32]	Butane 2,3 diol	n/a, media only			-	n/a	n/a
[32]	Cellobiose	n/a, media only			-	n/a	n/a
[32]	Citrate	n/a, media only			+	+	TP
[32]	D-Arabinose	n/a, media only			-	-	TN
Cont	inued on next page						

Ref	Media	Y. lipolytica knocked locus	S. cerevisiae ortholog	Gene name	Exp. Growth	Simul. Growth	Result
[32]	D-Galactonate	n/a, media only			-	n/a	n/a
[32]	D-Galactose	n/a, media only			-	+	FP
	D-	/ 1. 1					TEN.
[32]	Galacturonate	n/a, media only			-	-	TN
[32]	D-glucarate	n/a, media only			-	n/a	n/a
[32]	D-Glucitol	n/a	, media only		+	+	TP
[32]	D-Gluconate	n/a	, media only		+	n/a	n/a
[32]	D-Glucono-1,5-	n/a	, media only		+	n/a	n/a
	lactone	·				,	,
[32]	D-Glucosamine		, media only		-	+	FP
[32]	D-Glucose	/	, media only		+	+	TP
[32]	D-Glucuronate		, media only		-	n/a	n/a
[32]	D-Mannitol		, media only		+	n/a	n/a
[32]	D-Ribose		, media only		-	+	FP
[32]	D-Xylose		, media only		-	+	FP
[32]	DL-Lactate	n/a	, media only		+	+	TP
[32]	Erythritol	n/a	, media only		+	n/a	n/a
[32]	Ethanol	n/a	, media only		+	+	TP
[32]	Galactitol	n/a	, media only		-	n/a	n/a
[32]	Glycerol	n/a	n/a, media only			+	TP
[32]	Inulin	n/a, media only			-	n/a	n/a
[32]	L-Arabinitol	n/a, media only			-	-	TN
[32]	L-Arabinose	n/a, media only			-	-	TN
[32]	L-Rhamnose	n/a	, media only		-	n/a	n/a
[32]	L-Sorbose	n/a	, media only		-	-	TN
[32]	Lactose		, media only		-	n/a	n/a
[32]	Maltose		, media only		-	-	ŤN
[00]	Me-a-D-					,	,
[32]	Glucoside	n/a	, media only		-	n/a	n/a
[32]	Melezitose	n/a	, media only		-	n/a	n/a
[32]	Melibiose	n/a	, media only		-	-	TN
[32]	Methanol	n/a	, media only		-	n/a	n/a
[32]	myo-Inositol	n/a	, media only		-	-	TN
[32]	Propane 1,2 diol	n/a	, media only		-	n/a	n/a
[32]	Quinic acid		, media only		-	n/a	n/a
[32]	Raffinose	n/a	, media only		-	n/a	n/a
[32]	Ribitol	n/a	, media only		-	n/a	n/a
[32]	Salicin	n/a, media only		-	n/a	n/a	
[32]	Starch	n/a, media only		-	n/a	n/a	
[32]	Succinate	n/a, media only			+	+	TP
[32]	Sucrose	n/a	, media only		-	+	FP
[32]	Xylitol	,	, media only		-	+	FP
	all results:	,		N: 25, FN:	18, FP: 1		