Supplemental Data Files

Supplemental Data S1. A. Gene-protein-reactions in iRS605

LVS GENE	Protein	Abbreviation	Name	Equation
FTL_1542	Aas	AACPS1	acyl-[acyl-carrier-protein] synthetase (n-C14:0)	[c] : ACP + atp + ttdca --> amp + myrsACP + ppi
FTL_1542	Aas	AACPS2	acyl-[acyl-carrier-protein] synthetase (n-C14:1)	[c] : ACP + atp + ttdcea --> amp + ppi + tdeACP
FTL_1542	Aas	AACPS3	acyl-[acyl-carrier-protein] synthetase (n-C16:0)	[c] : ACP + atp + hdca --> amp + palmACP + ppi
FTL_1542	Aas	AACPS4	acyl-[acyl-carrier-protein] synthetase (n-C16:1)	[c] : ACP + atp + hdcea --> amp + hdeACP + ppi
FTL_1542	Aas	AACPS5	acyl-[acyl-carrier-protein] synthetase (n-C18:1)	[c] : ACP + atp + ocdcea --> amp + octeACP + ppi
FTL_1258	Aar1	AAD1	aryl-alcohol dehydrogenase	[c] : h + nadh + vrald --> nad + vralc
FTL_0583	YusK	ACACT10rr	acetyl-CoA C-acyltransferase (2-Methyl-3-acetoacetyl-CoA)	[c] : 2maacoa + coa <==> accoa + ppcoa
FTL_0583	YusK	ACACT2r	acetyl-CoA C-acyltransferase (butanoyl-CoA)	[c] : accoa + btcoa <==> 3ohcoa + coa
FTL_0583	YusK	ACACT3r	acetyl-CoA C-acyltransferase (hexanoyl-CoA)	[c] : accoa + hxcoa <==> 3oocoa + coa
FTL_0583	YusK	ACACT4r	acetyl-CoA C-acyltransferase (octanoyl-CoA)	[c] : accoa + occoa <==> 3odcoa + coa
FTL_0583	YusK	ACACT5r	acetyl-CoA C-acyltransferase (decanoyl-CoA)	[c] : accoa + dccoa <==> 3oddcoa + coa
FTL_0583	YusK	ACACT6r	acetyl-CoA C-acyltransferase (dodecanoyl-CoA)	[c] : accoa + ddcoa <==> 3otdcoa + coa
FTL_0583	YusK	ACACT7r	acetyl-CoA C-acyltransferase (tetradecanoyl-CoA)	[c] : accoa + tdcoa <==> 3ohdcoa + coa
FTL_0015	AckA	ACKr	acetate kinase	[c] : ac + atp <==> actp + adp
FTL_1137	FabF	ACMAT1	Acyl-[acyl-carrier-protein]:malonyl-[acyl-carrier-protein] C-acyltransferase (decarboxylating)	[c] : acACP + h + malACP --> ACP + actACP + co2
FTL_1141	FabHec	ACOATA	Acetyl-CoA ACP transacylase	[c] : ACP + accoa <==> acACP + coa
FTL_0753	AaC	ACODA	acetylornithine deacetylase	[c] : acorn + h2o --> ac + orn-L
FTL_1772	AcnA	ACONT	aconitase	[c] : cit <==> icit
FTL_1732	AcpT	ACP1e	acid phosphatase, extracellular (secreted)	[e] : fmn + h2o --> pi + ribflv
FTL_1262	PabABC	ADCL	4-aminobenzoate synthase	[c] : 4adcho --> 4abz + h + pyr
FTL_1262	PabABC	ADCS	4-amino-4-deoxychorismate synthase	[c] : chor + gln-L --> 4adcho + glu-L
FTL_0795	Adk	ADK1	adenylate kinase	[c] : amp + atp <==> (2) adp
FTL_0499	SpeD	ADMDC	Adenosylmethionine decarboxylase	[c] : amet + h <==> ametam + co2
FTL_0795	Adk	ADNK1	adenosine kinase	[c] : adn + atp --> adp + amp + h
FTL_1661	NupCec	ADNt2	adenosine transport in via proton symport	adn[e] + h[e] --> adn[c] + h[c]
FTL_1782	Apt	ADPT	adenine phosphoribosyltransferase	[c] : ade + prpp --> amp + ppi
FTL_1850	PurB	ADSL1r	adenylsuccinate lyase	[c] : dcamp <==> amp + fum
FTL_1850	PurB	ADSL2r	adenylosuccinate lyase	[c] : 25aics <==> aicar + fum
FTL_1930	PurA	ADSS	adenylosuccinate synthetase	[c] : asp-L + gtp + imp --> dcamp + gdp + (2) h + pi
FTL_0786	NagA	AGDC	N-acetylglucosamine-6-phosphate deacetylase	[c] : acgam6p + h2o --> ac + gam6p
FTL_1294	Adhapr	AGLYPR	acylglycerone-phosphate reductase	[c] : nadp + pgly3p --> h + nadph + pamglyc
FTL_0088	PlsC2	AGPAT	1-acylglycerol-3-phosphate O-acyltransferase	[c] : 12dag3p + coa --> 1ag3p + acoa
FTL_0463	Mtn	AHCYSNS	adenosylhomocysteine nucleosidase	[c] : ahcys + h2o --> ade + rhcys
FTL_1929	PurH	AICART	phosphoribosylaminoimidazolecarboxamide formyltransferase	[c] : 10fthf + aicar <==> fprica + thf
FTL_0399	PurK	AIRC1	phosphoribosylaminoimidazole carboxylase (ATP-dependent)	[c] : air + atp + co2 + h2o --> 5aizc + adp + (2) h + pi
FTL_0399	PurK	AIRC2	phosphoribosylaminoimidazole carboxylase	[c] : air + atp + hco3 --> 5caiz + adp + h + pi
FTL_0398	PurE	AIRC3	phosphoribosylaminoimidazole carboxylase (mutase rxn)	[c] : 5aizc <==> 5caiz
FTL_0777	Pho8	AKP1	alkaline phosphatase (Dihydroneopterin)	[c] : ahdt + (3) h2o --> dhnpt + (2) h + (3) pi
FTL_1910	DdlB	ALAALA	D-alanine-D-alanine ligase (reversible)	[c] : (2) ala-D + atp <==> adp + alaala + h + pi
FTL_1338	Alrec	ALAR	alanine racemase	[c] : ala-L <==> ala-D
FTL_0703	GlyA	ALATA_L	L-alanine transaminase	[c] : akg + ala-L <==> glu-L + pyr
FTL_1106	AlaS	ALATRS	Alanyl-tRNA synthetase	[c] : ala-L + atp + trnaala --> alatrna + amp + ppi
FTL_1009	AdhD	ALDD14	aldehyde dehydrogenase (tetradecanal, NAD)	[c] : h2o + nad + ttdcal --> (2) h + nadh + ttdca
FTL_1271	BioA	AMAOT	adenosylmethionine-8-amino-7-oxononanoate transaminase	[c] : 8aonn + amet <==> amob + dann
FTL_1261	TrpG	ANPRT	anthranilate phosphoribosyltransferase	[c] : anth + prpp --> ppi + pran
FTL_1273	BioF	AOXS	8-amino-7-oxononanoate synthase	[c] : ala-L + h + pmcoa <==> 8aonn + co2 + coa
FTL_1594	ApaH	AP4AH	bis(5'-nucleosyl)-tetraphosphatase	[c] : ap4a + h2o --> (2) adp + (2) h
FTL_1594	ApaH	AP5AH	Ap5A hydrolase	[c] : ap5a + h2o --> adp + atp + (2) h
FTL_0882	CutE	APAT	apolipoprotein N-acyl transferase	[c] : accoa + h2o + thdp <==> acamoxm + coa
FTL_0078	RibD	APRAUR	5-amino-6-(5-phosphoribosylamino)uracil reductase	[c] : 5apru + h + nadph --> 5aprbu + nadp
FTL_1609	ArnT	ARA4NT	4-amino-4-deoxy-L-arabinose transferase	[c] : (2) ara4n-L + (2) h + lipa --> ara4n-lipa + (2) h2o
FTL_0501	SpeA	ARGDC	arginine decarboxylase	[c] : arg-L + h --> agm + co2
FTL_1598	ArgS	ARGTRS	Arginyl-tRNA synthetase	[c] : arg-L + atp + trnaarg --> amp + argtrna + ppi
FTL_0696	YqiZ	ARGabc	L-arginine transport via ABC system	arg-L[e] + atp[c] + h2o[c] --> adp[c] + arg-L[c] + h[c] + pi[c]
FTL_1220	RocE	ARGt2	L-arginine transport in via proton symport	arg-L[e] + h[e] --> arg-L[c] + h[c]
FTL_0494	Asd	ASAD	aspartate-semialdehyde dehydrogenase	[c] : aspsa + nadp + pi <==> 4pasp + h + nadph
FTL_0494	Asd	ASADi	aspartate-semialdehyde dehydrogenase, irreversible	[c] : 4pasp + h + nadph --> aspsa + nadp + pi
FTL_0600	WbtH	ASNS1	asparagine synthase (glutamine-hydrolysing)	[c] : asp-L + atp + gln-L + h2o --> amp + asn-L + glu-L + h + ppi
FTL_0672	PanD	ASP1DC	aspartate 1-decarboxylase	[c] : asp-L + h --> ala-B + co2
FTL_0028	PyrBec	ASPCT	aspartate carbamoyltransferase	[c] : asp-L + cbp --> cbasp + h + pi
FTL_1388	NadB	ASPO1	L-aspartate oxidase	[c] : asp-L + nad --> (2) h + iasp + nadh
FTL_1388	NadB	ASPO6	L-aspartate oxidase	[c] : asp-L + o2 --> h + h2o2 + iasp
FTL_1388	NadB	ASPO7	L-aspartate oxidase	[c] : asp-L + h2o + o2 --> h2o2 + nh4 + oaa
FTL_0649	YbdL	ASPTA1	aspartate transaminase	[c] : akg + asp-L --> glu-L + oaa
FTL_0020	AspS	ASPTRS	Aspartyl-tRNA synthetase	[c] : asp-L + atp + trnaasp --> amp + asptrna + ppi
FTL_0863	GltP	ASPt2	L-aspartate transport in via proton symport	asp-L[e] + h[e] --> asp-L[c] + h[c]
FTL_0345	YocS	BILEt4	Bile acid transport in via sodium symport	bilea[e] + na1[e] --> bilea[c] + na1[c]
FTL_0957	PenP	BLACT	beta-lactamase	[c] : h2o + pencil <==> h + pencilca
FTL_1272	BioBec	BTSsf	biotin synthase	[c] : (2) amet + dtbt + s --> btn + (2) dad-5 + (2) met-L
FTL_1211	SsuA	BUTSabc	butanesulfonate transport via ABC system	atp[c] + buts[e] + h2o[c] --> adp[c] + buts[c] + h[c] + pi[c]
FTL_1442	FabI	C120SN	Fatty acid biosynthesis (n-C12:0)	[c] : actACP + (14) h + (4) malACP + (10) nadph --> (4) ACP + (4) co2 + ddcaACP + (5) h2o + (10) nadp
FTL_1442	FabI	C140SN	Fatty acid biosynthesis (n-C14:0)	[c] : actACP + (17) h + (5) malACP + (12) nadph --> (5) ACP + (5) co2 + (6) h2o + myrsACP + (12) nadp
FTL_1442	FabI	C160SN	Fatty acid biosynthesis (n-C16:0)	[c] : actACP + (20) h + (6) malACP + (14) nadph --> (6) ACP + (6) co2 + (7) h2o + (14) nadp + palmACP
FTL_0708	Erg27	C3STKR1	C-3 sterol keto reductase (4-methylzymosterol)	[c] : 4mzym_int2 + h + nadph --> 4mzym + nadp
FTL_0708	Erg27	C3STKR2	C-3 sterol keto reductase (zymosterol)	[c] : h + nadph + zym_int2 --> nadp + zymst
FTL_1504	KatG	CAT	catalase	[c] : (2) h2o2 --> (2) h2o + o2
FTL_0329	PssA1	CDPDSP	CDPdiacylglycerol-serine O-phosphatidyltransferase	[c] : cdpdag + ser-L --> cmp + h + ps
FTL_0151	IspE	CDPMEK	4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol kinase	[c] : 4c2me + atp --> 2p4c2me + adp + h
FTL_1288	Scs7	CERS2'24	Ceramide-2' synthase (24C)	[c] : cer1_24 + h + nadph + o2 --> cer2'_24 + h2o + nadp
FTL_1288	Scs7	CERS2'26	Ceramide-2' synthase (26C)	[c] : cer1_26 + h + nadph + o2 --> cer2'_26 + h2o + nadp
FTL_1288	Scs7	CERS324	Ceramide-3 synthase (24C)	[c] : cer2_24 + h + nadph + o2 --> cer3_24 + h2o + nadp
FTL_1288	Scs7	CERS326	Ceramide-3 synthase (26C)	[c] : cer2_26 + h + nadph + o2 --> cer3_26 + h2o + nadp
FTL_1731	LicB	CHLt6	choline transport in/out via proton symport	chol[e] + h[e] <==> chol[c] + h[c]
FTL_0663	LicA	CHOLK	Choline kinase	[c] : atp + chol --> adp + cholp + h
FTL_0377	AroC	CHORS	chorismate synthase	[c] : 3psme --> chor + pi
FTL_0356	UbiC	CHRPL	chorismate pyruvate lyase	[c] : chor --> 4hbz + pyr
FTL_1203	YwnE	CLPNS_EC	Cardiolipin Synthase (E.coli)	[c] : (0.04) pg_EC <==> (0.02) clpn_EC + glyc
FTL_1022	HemF	CPPPGO	coproporphyrinogen oxidase	[c] : cpppg3 + (2) h + o2 --> (2) co2 + (2) h2o + pppg9
FTL_1775	HemN	CPPPGOAN	Oxygen Independent coproporphyrinogen-III oxidase	[c] : (2) amet + cpppg3 + (2) fdxo-4:2 + (2) nadph --> (2) co2 + (2) dad-5 + (2) fdxr-4:2 + (2) h + (2) met-L + (2) nadp + pppg9
FTL_1789	GltA	CS	citrate synthase	[c] : accoa + h2o + oaa --> cit + coa + h
FTL_1311	PyrG	CTPS2	CTP synthase (glutamine)	[c] : atp + gln-L + h2o + utp --> adp + ctp + glu-L + (2) h + pi
FTL_0504	Nit3	CTUD	citrulline ureidase	[c] : citr-L + h2o --> co2 + nh3 + orn-L
FTL_1765	CydABCD	CYOR1m	cytochrome-c reductase (menaquinol 7: 1 protons)	(2) ficytcc[c] + mql7[c] --> (2) focytcc[c] + h[e] + h[c] + mqn7[c]
FTL_1174	Cys4	CYSTGL	cystathionine g-lyase	[c] : cysth-L + h2o --> 2obut + cys-L + nh4
FTL_1174	Cys4	CYSTL	cystathionine b-lyase	[c] : cysth-L + h2o --> hcys-L + nh4 + pyr
FTL_1683	CysS	CYSTRS	Cysteinyl-tRNA synthetase	[c] : atp + cys-L + trnacys --> amp + cystrna + ppi

LVS GENE	Protein	Abbreviation	Name	Equation
FTL_1174	Cys4	CYSTS	cystathionine b-synthase	[c] : hcys-L + ser-L --> cysth-L + h2o
FTL_1534	Udk	CYTDK1	cytidine kinase (ATP)	[c] : atp + cytd --> adp + cmp + h
FTL_1534	Udk	CYTDK2	cytidine kinase (GTP)	[c] : cytd + gtp --> cmp + gdp + h
FTL_1534	Udk	CYTDK3	cytidine kinase (ITP)	[c] : cytd + itp --> cmp + h + idp
FTL_1661	NupCec	CYTDt2	cytidine transport in via proton symport	cytd[e] + h[e] --> cytd[c] + h[c]
FTL_1017	Cmk	CYTK1	cytidylate kinase (CMP)	[c] : atp + cmp <==> adp + cdp
FTL_1017	Cmk	CYTK2	cytidylate kinase (dCMP)	[c] : atp + dcmp <==> adp + dcdp
FTL_0102	ClC	Clt	chloride ion transport out via diffusion	cl[e] <==> cl[c]
FTL_0795	Adk	DADK	deoxyadenylate kinase	[c] : atp + damp <==> adp + dadp
FTL_1661	NupCec	DADNt2	deoxyadenosine transport in via proton symport	dad-2[e] + h[e] --> dad-2[c] + h[c]
FTL_1240	AroG	DAHPS	3-deoxy-D-arabino-heptulosonate 7-phosphate synthetase	[c] : e4p + h2o + pep --> 2dda7p + pi
FTL_1834	LysA	DAPDC	diaminopimelate decarboxylase	[c] : 26dap-M + h --> co2 + lys-L
FTL_0229	CdsA	DASYN_EC	CDP-Diacylglycerol synthetase (Ecoli)	[c] : ctp + h + (0.02) pa_EC <==> (0.02) cdpdag_EC + ppi
FTL_0076	RibA	DB4PS	3,4-Dihydroxy-2-butanone-4-phosphate	[c] : ru5p-D --> db4p + for + h
FTL_1275	BioDec	DBTSr	dethiobiotin synthase	[c] : atp + co2 + dann <==> adp + dtbt + (3) h + pi
FTL_0858	YedO	DCYSL	D-cysteine desulfhydrase	[c] : cys-D + h2o --> h + h2s + nh4 + pyr
FTL_1661	NupCec	DCYTt2	deoxycytidine transport in via proton symport	dcyt[e] + h[e] --> dcyt[c] + h[c]
FTL_1740	Ole1	DESAT161	Palmitoyl-CoA desaturase (n-C16:0CoA -> n-C16:1CoA)	[c] : h + nadph + o2 + pmtcoa --> (2) h2o + hdcoa + nadp
FTL_1740	Ole1	DESAT181	stearoyl-CoA desaturase (n-C18:0CoA -> n-C18:1CoA)	[c] : h + nadph + o2 + strcoa --> (2) h2o + nadp + odecoa
FTL_1391	Gmk	DGK1	deoxyguanylate kinase (dGMP:ATP)	[c] : atp + dgmp <==> adp + dgdp
FTL_1503	Dgt	DGTPH	dGTPase	[c] : dgtp + h2o --> dgsn + pppi
FTL_0223	DfrA	DHFOR2	dihydrofolate reductase	[c] : dhf + nadp <==> fol + nadph
FTL_0223	DfrA	DHFR	dihydrofolate reductase	[c] : dhf + h + nadph <==> nadp + thf
FTL_1308	FolC	DHFS	dihydrofolate synthase	[c] : atp + dhpt + glu-L --> adp + dhf + h + pi
FTL_1264	FolB	DHNPA	dihydroneopterin aldolase	[c] : dhnpt --> 2ahhmp + gcald
FTL_0046	PyrD	DHORD1	dihydoorotic acid dehydrogenase	[c] : dhor-S + o2 <==> h2o2 + orot
FTL_0046	PyrD	DHORD2	dihydoorotic acid dehydrogenase (quinone8)	[c] : dhor-S + ubq8 --> orot + ubq8h2
FTL_0033	PucH	DHORTS	dihydroorotase	[c] : dhor-S + h2o <==> cbasp + h
FTL_0078	RibD	DHPPDA2	diaminohydroxyphosphoribosylaminopyrimidine deaminase	[c] : 25dhpp + h + h2o --> 5apru + nh4
FTL_1265	FolP2	DHPS3	dihydropteroate synthase	[c] : 2ahhmd + 4abz --> dhpt + ppi
FTL_1593	AroD	DHQD1	3-dehydroquinate dehydratase	[c] : 3dhq <==> 3dhsk + h2o
FTL_0802	AroB	DHQS	3-dehydroquinate synthase	[c] : 2dda7p --> 3dhq + pi
FTL_0041	DidalaABC	DIDALAabc	D-ala-D-ala Dipeptide transport via ABC system	alaala[e] + atp[c] + h2o[c] --> adp[c] + alaala[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc1	Dipeptide transport via ABC system (ala-asp)	ala-L-asp-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-asp-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc10	Dipeptide transport via ABC system (gly-glu)	atp[c] + gly-glu-L[e] + h2o[c] --> adp[c] + gly-glu-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc11	Dipeptide transport via ABC system (gly-met)	atp[c] + gly-met-L[e] + h2o[c] --> adp[c] + gly-met-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc12	Dipeptide transport via ABC system (met-ala)	atp[c] + h2o[c] + met-L-ala-L[e] --> adp[c] + h[c] + met-L-ala-L[c] + pi[c]
FTL_1648	DppD	DIPEPabc13	Dipeptide transport via ABC system (gly-asp)	atp[c] + gly-asp-L[e] + h2o[c] --> adp[c] + gly-asp-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc14	Dipeptide transport via ABC system (gly-pro-L)	atp[c] + gly-pro-L[e] + h2o[c] --> adp[c] + gly-pro-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc15	Dipeptide transport via ABC system (cgly)	atp[c] + cgly[e] + h2o[c] --> adp[c] + cgly[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc2	Dipeptide transport via ABC system (ala-gln)	ala-L-gln-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-gln-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc3	Dipeptide transport via ABC system (ala-glu)	ala-L-glu-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-glu-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc4	Dipeptide transport via ABC system (ala-gly)	L-alagly[e] + atp[c] + h2o[c] --> L-alagly[c] + adp[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc5	Dipeptide transport via ABC system (ala-his)	ala-L-his-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-his-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc6	Dipeptide transport via ABC system (ala-leu)	ala-L-leu-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-leu-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc7	Dipeptide transport via ABC system (ala-thr)	ala-L-Thr-L[e] + atp[c] + h2o[c] --> adp[c] + ala-L-Thr-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc8	Dipeptide transport via ABC system (gly-asn)	atp[c] + gly-asn-L[e] + h2o[c] --> adp[c] + gly-asn-L[c] + h[c] + pi[c]
FTL_1648	DppD	DIPEPabc9	Dipeptide transport via ABC system (gly-gln)	atp[c] + gly-gln-L[e] + h2o[c] --> adp[c] + gly-gln-L[c] + h[c] + pi[c]
FTL_0546	IspA	DMATT	dimethylallyltranstransferase	[c] : dmpp + ipdp --> grdp + ppi
FTL_1399	KdsB	DMOCT	3-deoxy-manno-octulosonate cytidylyltransferase	[c] : ctp + kdo --> ckdo + ppi
FTL_0327	LytB	DMPPS	1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate reductase (dmpp)	[c] : h + h2mb4p + nadh --> dmpp + h2o + nad
FTL_1638	UbiG	DMQMT	3-Dimethylubiquinonol 3-methyltransferase	[c] : 2omhmbl + amet --> ahcys + h + ubq8h2
FTL_0307	CoaE	DPCOAK	dephospho-CoA kinase	[c] : atp + dpcoa --> adp + coa + h
FTL_1663	DeoC	DRPA	deoxyribose-phosphate aldolase	[c] : 2dr5p --> acald + g3p
FTL_1660	Tmk	DTMPK	dTMP kinase	[c] : atp + dtmp <==> adp + dtdp
FTL_0890	Tdk	DURIK1	deoxyuridine kinase (ATP:Deoxyuridine)	[c] : atp + duri --> adp + dump + h
FTL_1661	NupCec	DURIt2	deoxyuridine transport in via proton symport	duri[e] + h[e] --> duri[c] + h[c]
FTL_0230	Dut	DUTPDP	dUTP diphosphatase	[c] : dutp + h2o --> dump + h + ppi
FTL_0534	Dxr	DXPRI	1-deoxy-D-xylulose-5-phosphate reductoisomerase	[c] : dxyl5p + h + nadph <==> 2me4p + nadp
FTL_1072	Dxs	DXPS	1-deoxy-D-xylulose 5-phosphate synthase	[c] : g3p + h + pyr --> co2 + dxyl5p
FTL_0179	LpxP	EDTXS3	Endotoxin Synthesis (palmitoleoyl ACP)	[c] : hdeACP + kdo2lipid4 --> ACP + kdo2lipid4p
FTL_1527	Eno	ENO	enolase	[c] : 2pg <==> h2o + pep
FTL_0612	Ppx	EPPP	exopolyphosphatase	[c] : h2o + polypi --> (2) h + pi
FTL_1211	SsuA	ETHSabc	ethanesulfonate transport via ABC system	atp[c] + eths[e] + h2o[c] --> adp[c] + eths[c] + h[c] + pi[c]
FTL_0586	FadD	FAO1	Fatty acid oxidation (tetradecanoate)	[c] : atp + (7) coa + (6) fad + (6) h2o + (6) nad + ttdca --> (7) accoa + amp + (6) fadh2 + (6) h + (6) nadh + ppi
FTL_0586	FadD	FAO2	Fatty acid oxidation (n-C16:0)	[c] : atp + (8) coa + (7) fad + (7) h2o + hdca + (7) nad --> (8) accoa + amp + (7) fadh2 + (7) h + (7) nadh + ppi
FTL_0586	FadD	FAO3	Fatty acid oxidation (octadecanoate)	[c] : atp + (9) coa + (8) fad + (8) h2o + (8) nad + ocdca --> (9) accoa + amp + (8) fadh2 + (8) h + (8) nadh + ppi
FTL_0585	FadE	FAO4	fatty acid oxidation (Butanoyl-CoA)	[c] : btcoa + fad + h2o + nad --> aacoa + fadh2 + h + nadh
FTL_1149	FbaA	FBA	fructose-bisphosphate aldolase	[c] : fdp <==> dhap + g3p
FTL_1149	FbaA	FBA2	D-Fructose 1-phosphate D-glyceraldehyde-3-phosphate-lyase	[c] : f1p <==> dhap + glyald
FTL_1701	Fbp1	FBP	fructose-bisphosphatase	[c] : fdp + h2o --> f6p + pi
FTL_0821	HemH	FCLT	Heme B synthesis reaction	[c] : fe2 + ppp9 --> h + pheme
FTL_0127	Fdh1	FDH	formate dehydrogenase	[c] : for + nad --> co2 + nadh
FTL_0133	FeoB	FE2abc	iron (II) transport via ABC system	atp[c] + fe2[e] + h2o[c] --> adp[c] + fe2[c] + h[c] + pi[c]
FTL_0215	YfkO	FLVR	flavin reductase	[c] : h + nadph + ribflv --> nadp + ribflvRD
FTL_1285	Fmt	FMETTRS	Methionyl-tRNA formyltransferase	[c] : 10fthf + mettrna --> fmettrna + thf
FTL_0437	RibFec	FMNAT	FMN adenylyltransferase	[c] : atp + fmn + h --> fad + ppi
FTL_0570	Frd	FRD	fumarate reductase	[c] : fadh2 + fum --> fad + succ
FTL_0570	Frd	FRD2	fumarate reductase	[c] : fum + mql8 --> mqn8 + succ
FTL_0570	Frd	FRD3	fumarate reductase	[c] : 2dmmql8 + fum --> 2dmmq8 + succ
FTL_1492	YdhR	FRUK	fructokinase	[c] : atp + fru --> adp + f6p + h
FTL_1278	FucP	FUCt	L-fucose transport via proton symport	fuc-L[e] + h[e] <==> fuc-L[c] + h[c]
FTL_0525	FumB	FUM	fumarase	[c] : fum + h2o <==> mal-L
FTL_1497	DctA	FUMt6_na	fumarate transport in/out via sodium symport	fum[e] + na1[e] <==> fum[c] + na1[c]
FTL_0605	RffH	G1PTMT	glucose-1-phosphate thymidylyltransferase	[c] : dttp + g1p + h --> dtdpglc + ppi
FTL_1283	HemLec	G1SATi	glutamate-1-semialdehyde aminotransferase	[c] : glu1sa --> 5aop
FTL_0372	GpsA	G3PD2	glycerol-3-phosphate dehydrogenase (NADP)	[c] : glyc3p + nadp <==> dhap + h + nadph
FTL_1756	GlpA	G3PD5	glycerol-3-phosphate dehydrogenase (ubiquinone-8)	[c] : glyc3p + ubq8 --> dhap + ubq8h2
FTL_0443	YcbE	GALCTRt2	galactarate transport in via proton symport	galctr-D[e] + h[e] --> galctr-D[c] + h[c]
FTL_1397	GalK	GALKr	galactokinase	[c] : atp + gal <==> adp + gal1p + h
FTL_1396	GalT	GALT	galactose-1-phosphate uridylyltransferase	[c] : gal1p + h + utp <==> ppi + udpgal
FTL_1395	GalP	GALt2	D-galactose transport in via proton symport	gal[e] + h[e] --> gal[c] + h[c]
FTL_1146	GapA	GAPD	glyceraldehyde-3-phosphate dehydrogenase (NAD)	[c] : g3p + nad + pi <==> 13dpg + h + nadh
FTL_1146	GapA	GAPD_NADP	glyceraldehyde-3-phosphate dehydrogenase (phosphorylating)	[c] : 13dpg + h + nadph --> g3p + nadp + pi
FTL_0397	PurN	GARFT	phosphoribosylglycinamide formyltransferase	[c] : 10fthf + gar <==> fgam + h + thf
FTL_0092	PurT	GART	Phosphoribosylglycinamide formyltransferase 2	[c] : atp + for + gar --> adp + fgam + h + pi
FTL_0483	GlgB	GBEZY	1,4-alpha-glucan branching enzyme	[c] : 14glun --> glycogen
FTL_0454	GlmS	GF6PTA	glutamine-fructose-6-phosphate transaminase	[c] : f6p + gln-L --> gam6p + glu-L

LVS GENE	Protein	Abbreviation	Name	Equation
FTL_0703	GlyA	GHMT2	glycine hydroxymethyltransferase	[c] : ser-L + thf --> gly + h2o + mlthf
FTL_1391	Gmk	GK1	guanylate kinase (GMP:ATP)	[c] : atp + gmp <==> adp + gdp
FTL_0487	GlgP	GLCP	glycogen phosphorylase	[c] : glycogen + pi --> g1p
FTL_0443	YcbE	GLCRt2	glucarate transport in via proton symport	glcr[e] + h[e] --> glcr[c] + h[c]
FTL_0486	GlgA	GLCS1	glycogen synthase (ADPGlc)	[c] : adpglc --> adp + glycogen + h
FTL_1180	PtsN	GLCpts	D-glucose transport via PEP:Pyr PTS	glc-D[e] + pep[c] --> g6p[c] + pyr[c]
FTL_1395	GalP	GLCt2	D-glucose transport in via proton symport	glc-D[e] + h[e] --> glc-D[c] + h[c]
FTL_1899	Gln1	GLNS	glutamine synthetase	[c] : atp + glu-L + nh4 --> adp + gln-L + h + pi
FTL_1617	GlnS	GLNTRS	Glutaminyl-tRNA synthetase	[c] : atp + gln-L + trnagln --> amp + glntrna + ppi
FTL_1233	XasA	GLUABUTt7	4-aminobutyrate/glutamate antiport	4abut[c] + glu-L[e] <==> 4abut[e] + glu-L[c]
FTL_1304	GshA	GLUCYSL	glutamate-cysteine ligase	[c] : atp + cys-L + glu-L --> adp + glucys + h + pi
FTL_1863	GadA	GLUDC	glutamate decarboxylase	[c] : glu-L + h --> 4abut + co2
FTL_0269	GdhA	GLUDy	glutamate dehydrogenase (NADP)	[c] : glu-L + h2o + nadp <==> akg + h + nadph + nh4
FTL_1861	PurF	GLUPRT	glutamine phosphoribosyldiphosphate amidotransferase	[c] : gln-L + h2o + prpp --> glu-L + ppi + pram
FTL_0747	MurI	GLUR	glutamate racemase	[c] : glu-D <==> glu-L
FTL_1722	HemA	GLUTRR	glutamyl-tRNA reductase	[c] : glutrna + h + nadph --> glu1sa + nadp + trnaglu
FTL_0218	GltX	GLUTRS	Glutamyl-tRNA synthetase	[c] : atp + glu-L + trnaglu --> amp + glutrna + ppi
FTL_0863	GltP	GLUt6	L-glutamate transport in/out via proton symporter	glu-L[e] + h[e] <==> glu-L[c] + h[c]
FTL_1510	GlpT	GLY3Pt2	glycerol-3-phosphate transport in via proton symport	glyc3p[e] + h[e] --> glyc3p[c] + h[c]
FTL_1522	KbL	GLYAT	glycine C-acetyltransferase	[c] : accoa + gly <==> 2aobut + coa
FTL_1417	ProPec	GLYBt6	betaine (glycine betaine) transport in/out via proton symport	glyb[e] + h[e] <==> glyb[c] + h[c]
FTL_1755	GlpF	GLYCt5	glycerol transport in/out via diffusion reversible	glyc[c] <==> glyc[e]
FTL_1644	GlpK	GLYK	glycerol kinase	[c] : atp + glyc --> adp + glyc3p + h
FTL_0657	GloB	GLYOX	hydroxyacylglutathione hydrolase	[c] : h2o + lgt-S --> gthrd + h + lac-D
FTL_1071	GuaA	GMPS2	GMP synthase (glutamine-hydrolysing)	[c] : atp + gln-L + h2o + xmp --> amp + glu-L + gmp + (2) h + ppi
FTL_1594	ApaH	GP4GH	Gp4G hydrolase	[c] : gp4g + h2o --> (2) gdp + (2) h
FTL_0546	IspA	GRTT	geranyltranstransferase	[c] : grdp + ipdp --> frdp + ppi
FTL_1248	Gor	GTHRD	glutathione-disulfide reductase	[c] : (2) gthrd + nadp <==> gthox + h + nadph
FTL_0076	RibA	GTPCII	GTP cyclohydrolase II	[c] : gtp + (3) h2o --> 25dhpp + for + (2) h + ppi
FTL_0285	RelA	GTPDPK	GTP diphosphokinase	[c] : atp + gtp --> amp + gdptp + h
FTL_0319	PbuG	GUAt2	guanine transport in via proton symport	gua[e] + h[e] --> gua[c] + h[c]
FTL_0584	YusL	HACD1	3-hydroxyacyl-CoA dehydrogenase (acetoacetyl-CoA)	[c] : aacoa + h + nadh <==> 3hbycoa + nad
FTL_0584	YusL	HACD2	3-hydroxyacyl-CoA dehydrogenase (3-oxohexanoyl-CoA)	[c] : 3ohcoa + h + nadh <==> 3hhcoa + nad
FTL_0584	YusL	HACD3	3-hydroxyacyl-CoA dehydrogenase (3-oxooctanoyl-CoA)	[c] : 3oocoa + h + nadh <==> 3hocoa + nad
FTL_0584	YusL	HACD4	3-hydroxyacyl-CoA dehydrogenase (3-oxodecanoyl-CoA)	[c] : 3odcoa + h + nadh <==> 3hdcoa + nad
FTL_0584	YusL	HACD5	3-hydroxyacyl-CoA dehydrogenase (3-oxododecanoyl-CoA)	[c] : 3oddcoa + h + nadh <==> 3hddcoa + nad
FTL_0584	YusL	HACD6	3-hydroxyacyl-CoA dehydrogenase (3-oxotetradecanoyl-CoA)	[c] : 3otdcoa + h + nadh <==> 3htdcoa + nad
FTL_0584	YusL	HACD7	3-hydroxyacyl-CoA dehydrogenase (3-oxohexadecanoyl-CoA)	[c] : 3ohdcoa + h + nadh <==> 3hhdcoa + nad
FTL_0584	YusL	HACD8	3-hydroxyacyl-CoA dehydrogenase (2-Methylacetoacetyl-CoA)	[c] : 3hmbcoa + nad <==> 2maacoa + h + nadh
FTL_0584	YusL	HACOADr	3-hydroxyacyl-CoA dehydrogenase	[c] : 3hmp + nad --> h + mmalsa + nadh
FTL_0355	UbiA	HBZOPT	4-hydroxybenzoate octaprenyltransferase	[c] : 4hbz + octdp --> 3ophb + ppi
FTL_0856	YadF	HCO3E	carbonate dehydratase (HCO3 equilibration reaction)	[c] : co2 + h2o <==> h + hco3
FTL_0404	Glk	HEX1	hexokinase (D-glucose:ATP)	[c] : atp + glc-D --> adp + g6p + h
FTL_0104	Hxk2	HEX4	hexokinase (D-mannose:ATP)	[c] : atp + man --> adp + h + man6p
FTL_1211	SsuA	HEXSabc	hexanesulfonate transport via ABC system	atp[c] + h2o[c] + hexs[e] --> adp[c] + h[c] + hexs[c] + pi[c]
FTL_0026	YkwC	HIBD	3-hydroxyisobutyrate dehydrogenase	[c] : 3hmp + nad --> 2mop + h + nadh
FTL_0938	Hdc	HISDC	histidine decarboxylase	[c] : his-L --> co2 + hista
FTL_1807	HisS	HISTRS	Histidyl-tRNA synthetase	[c] : atp + his-L + trnahis --> amp + histrna + ppi
FTL_0140	HemCec	HMBS	hydroxymethylbilane synthase	[c] : h2o + (4) ppbng --> hmbil + (4) nh4
FTL_1265	FolP2	HPPK	2-amino-4-hydroxy-6-hydroxymethyldihydropteridine diphosphokinase	[c] : 2ahhmp + atp --> 2ahhmd + amp + h
FTL_0319	PbuG	HXANt2	hypoxanthine transport in via proton symport	h[e] + hxan[e] --> h[c] + hxan[c]
FTL_0588	Icd	ICDHy	isocitrate dehydrogenase (NADP)	[c] : icit + nadp <==> akg + co2 + nadph
FTL_1958	TrpCec	IGPS	indole-3-glycerol-phosphate synthase	[c] : 2cpr5p + h --> 3ig3p + co2 + h2o
FTL_0131	IlvE	ILETA	isoleucine transaminase	[c] : akg + ile-L <==> 3mop + glu-L
FTL_0436	IleS	ILETRS	Isoleucyl-tRNA synthetase	[c] : atp + ile-L + trnaile --> amp + iletrna + ppi
FTL_1929	PurH	IMPC	IMP cyclohydrolase	[c] : h2o + imp <==> fprica
FTL_1478	GuaB	IMPD	IMP dehydrogenase	[c] : h2o + imp + nad --> h + nadh + xmp
FTL_0327	LytB	IPDPS	1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate reductase (ipdp)	[c] : h + h2mb4p + nadh --> h2o + ipdp + nad
FTL_0130	LeuA	IPPS	2-isopropylmalate synthase	[c] : 3mob + accoa + h2o --> 3c3hmp + coa + h
FTL_1211	SsuA	ISTNTabc	Isethionate transport via ABC system	atp[c] + h2o[c] + istnt[e] --> adp[c] + h[c] + istnt[c] + pi[c]
FTL_0548	IxpP	ITPASE	dITP pyrophosphatase	[c] : ditp + h2o --> dimp + ppi
FTL_1141	FabHec	KAS15	b-ketoacyl synthase	[c] : accoa + h + malACP --> actACP + co2 + coa
FTL_1137	FabF	KAS16	3-hydroxy-myristoyl-ACP synthesis	[c] : ddcaACP + (2) h + malACP + nadph --> 3htdACP + ACP + co2 + nadp
FTL_1062	KdoP	KDOPP	3-deoxy-manno-octulosonate-8-phosphatase	[c] : h2o + kdo8p --> kdo + pi
FTL_1535	KdsA	KDOPS	2-dehydro-3-deoxy-phosphooctonate aldolase	[c] : ara5p + h2o + pep --> kdo8p + pi
FTL_1211	SsuA	LCYSTabc	cysteate transport via ABC system	Lcyst[e] + atp[c] + h2o[c] --> Lcyst[c] + adp[c] + h[c] + pi[c]
FTL_0131	IlvE	LEUTAi	leucine transaminase (irreversible)	[c] : 4mop + glu-L --> akg + leu-L
FTL_1212	LeuS	LEUTRS	Leucyl-tRNA synthetase	[c] : atp + leu-L + trnaleu --> amp + leutrna + ppi
FTL_0540	LpxB	LPADSS	Lipid A disaccaride synthase	[c] : lipidX + u23ga --> h + lipidAds + udp
FTL_1362	KamA	LYSAM	lysine 2,3-aminomutase	[c] : lys-L <==> 36dahx
FTL_0476	CadA	LYSDC	lysine decarboxylase	[c] : h + lys-L --> 15dap + co2
FTL_1903	LysS2	LYSTRS	Lysyl-tRNA synthetase	[c] : atp + lys-L + trnalys --> amp + lystrna + ppi
FTL_1951	LysE2	LYSt3	L-lysine transport out via proton antiport	h[e] + lys-L[c] --> h[c] + lys-L[e]
FTL_1703	LysP	LYSt6	L-lysine transport in/out via proton symport	h[e] + lys-L[e] <==> h[c] + lys-L[c]
FTL_1497	DctA	MALt6_na	malate/sodium symporter	mal-L[e] + na1[e] <==> mal-L[c] + na1[c]
FTL_1140	FabD	MCOATA	Malonyl-CoA-ACP transacylase	[c] : ACP + malcoa <==> coa + malACP
FTL_1911	YaaJ	MCSNAH1r	5-Methylcytosine aminohydrolase	[c] : 5mcsn + h + h2o <==> nh4 + thym
FTL_0987	MLdh	MDH	malate dehydrogenase	[c] : mal-L + nad <==> h + nadh + oaa
FTL_0438	YwkA	ME1x	malic enzyme (NAD)	[c] : mal-L + nad --> co2 + nadh + pyr
FTL_0438	YwkA	ME2	malic enzyme (NADP)	[c] : mal-L + nadp --> co2 + nadph + pyr
FTL_0459	Map	MEAMP1(ala-asp)	methionyl aminopeptidase	[c] : ala-L-asp-L + h2o <==> ala-L + asp-L
FTL_0459	Map	MEAMP1(ala-gln)	methionyl aminopeptidase	[c] : ala-L-gln-L + h2o <==> ala-L + gln-L
FTL_0459	Map	MEAMP1(ala-glu)	methionyl aminopeptidase	[c] : ala-L-glu-L + h2o <==> ala-L + glu-L
FTL_0459	Map	MEAMP1(ala-gly)	methionyl aminopeptidase	[c] : L-alagly + h2o <==> ala-L + gly
FTL_0459	Map	MEAMP1(ala-his)	methionyl aminopeptidase	[c] : ala-L-his-L + h2o <==> ala-L + his-L
FTL_0459	Map	MEAMP1(ala-leu)	methionyl aminopeptidase	[c] : ala-L-leu-L + h2o <==> ala-L + leu-L
FTL_0459	Map	MEAMP1(ala-thr)	methionyl aminopeptidase	[c] : ala-L-Thr-L + h2o <==> ala-L + thr-L
FTL_0459	Map	MEAMP1(gly-asn)	methionyl aminopeptidase	[c] : gly-asn-L + h2o <==> asn-L + gly
FTL_0459	Map	MEAMP1(gly-asp)	methionyl aminopeptidase	[c] : gly-asp-L + h2o <==> asp-L + gly
FTL_0459	Map	MEAMP1(gly-gln)	methionyl aminopeptidase	[c] : gly-gln-L + h2o <==> gln-L + gly
FTL_0459	Map	MEAMP1(gly-glu)	methionyl aminopeptidase	[c] : gly-glu-L + h2o <==> glu-L + gly
FTL_0459	Map	MEAMP1(gly-met)	methionyl aminopeptidase	[c] : gly-met-L + h2o <==> gly + met-L
FTL_0459	Map	MEAMP1(gly-pro-L)	methionyl aminopeptidase	[c] : gly-pro-L + h2o <==> gly + pro-L
FTL_0459	Map	MEAMP1(met-ala)	methionyl aminopeptidase	[c] : h2o + met-L-ala-L <==> ala-L + met-L
FTL_0875	YqfY	MECDPDH	2C-methyl-D-erythritol 2,4 cyclodiphosphate dehydratase	[c] : 2mecdp + nadh --> h2mb4p + h2o + nad
FTL_0833	IspF	MECDPS	2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase	[c] : 2p4c2me --> 2mecdp + cmp
FTL_1525	IspD	MEPCT	2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase	[c] : 2me4p + ctp + h --> 4c2me + ppi
FTL_1739	MetK	METAT	methionine adenosyltransferase	[c] : atp + h2o + met-L --> amet + pi + ppi

LVS GENE	Protein	Abbreviation	Name	Equation
FTL_0379	YppQ	METSR-R1	L-methionine R-oxide reductase (trdrd)	[c] : metox-R + trdrd --> h2o + met-L + trdox
FTL_0444	MetS	METTRS	Methionyl-tRNA synthetase	[c] : atp + met-L + trnamet --> amp + mettrna + ppi
FTL_1132	SuhB	MI1PP	myo-inositol 1-phosphatase	[c] : h2o + mi1p-D --> inost + pi
FTL_0547	KdtA	MOAT	3-deoxy-D-manno-octulosonic acid transferase	[c] : ckdo + lipidA --> cmp + h + kdolipid4
FTL_0547	KdtA	MOAT2	3-deoxy-D-manno-octulosonic acid transferase	[c] : ckdo + kdolipid4 --> cmp + h + kdo2lipid4
FTL_0674	PanB	MOHMT	3-methyl-2-oxobutanoate hydroxymethyltransferase	[c] : 3mob + h2o + mlthf --> 2dhp + thf
FTL_1211	SsuA	MOPSabc	MOPS transport via ABC system	atp[c] + h2o[c] + mops[e] --> adp[c] + h[c] + mops[c] + pi[c]
FTL_1211	SsuA	MSO3abc	methanesulfonate transport via ABC system	atp[c] + h2o[c] + mso3[e] --> adp[c] + h[c] + mso3[c] + pi[c]
FTL_0463	Mtn	MTAN	methylthioadenosine nucleosidase	[c] : 5mta + h2o --> 5mtr + ade
FTL_0394	FolD	MTHFC	methenyltetrahydrofolate cyclohydrolase	[c] : h2o + methf <==> 10fthf + h
FTL_0394	FolD	MTHFD	methylenetetrahydrofolate dehydrogenase (NADP)	[c] : mlthf + nadp <==> methf + nadph
FTL_0463	Mtn	MTRK	5-methylthioribose kinase	[c] : 5mtr + atp --> 5mdr1p + adp + h
FTL_0676	Lig	NADDP	NAD diphosphatase	[c] : h2o + nad --> amp + (2) h + nmn
FTL_0626	YfjB	NADK	NAD kinase	[c] : atp + nad --> adp + h + nadp
FTL_0685	NadE	NADS1	NAD synthase (nh4)	[c] : atp + dnad + nh4 --> amp + h + nad + ppi
FTL_0304	YvgP	NAt3	sodium transport out via proton antiport	h[e] + na1[c] --> h[c] + na1[e]
FTL_0378	NhaB	NAt3_1.5	sodium proton antiporter (H:NA is 1.5)	(3) h[e] + (2) na1[c] --> (3) h[c] + (2) na1[e]
FTL_0085	NhaA	NAt3_2	sodium proton antiporter (H:NA is 2)	(2) h[e] + na1[c] --> (2) h[c] + na1[e]
FTL_1310	Ndk	NDPK1	nucleoside-diphosphate kinase (ATP:GDP)	[c] : atp + gdp <==> adp + gtp
FTL_1310	Ndk	NDPK2	nucleoside-diphosphate kinase (ATP:UDP)	[c] : atp + udp <==> adp + utp
FTL_1310	Ndk	NDPK3	nucleoside-diphosphate kinase (ATP:CDP)	[c] : atp + cdp <==> adp + ctp
FTL_1310	Ndk	NDPK4	nucleoside-diphosphate kinase (ATP:dTDP)	[c] : atp + dtdp <==> adp + dttp
FTL_1310	Ndk	NDPK5	nucleoside-diphosphate kinase (ATP:dGDP)	[c] : atp + dgdp <==> adp + dgtp
FTL_1310	Ndk	NDPK6	nucleoside-diphosphate kinase (ATP:dUDP)	[c] : atp + dudp <==> adp + dutp
FTL_1310	Ndk	NDPK7	nucleoside-diphosphate kinase (ATP:dCDP)	[c] : atp + dcdp <==> adp + dctp
FTL_1310	Ndk	NDPK8	nucleoside-diphosphate kinase (ATP:dADP)	[c] : atp + dadp <==> adp + datp
FTL_0889	Ep4	NMNR	nmn hydrolysis	[e] : h2o + nmn --> pi + rnam
FTL_0980	NadD	NNAT	nicotinate-nucleotide adenylyltransferase	[c] : atp + h + nicrnt --> dnad + ppi
FTL_1389	NadCec	NNDPR	nicotinate-nucleotide diphosphorylase (carboxylating)	[c] : (2) h + prpp + quln --> co2 + nicrnt + ppi
FTL_1110	NapA2	NTRARfc	nitrate reductase	[c] : (2) focytcc + (2) h + no3 --> (2) ficytcc + h2o + no2
FTL_0963	P_1.7.2.2_4	NTRIRfc	nitrite reductase	[c] : (6) focytcc + (8) h + no2 --> (6) ficytcc + (2) h2o + nh4
FTL_1041	IspB	OCTDPS	Octaprenyl pyrophosphate synthase	[c] : frdp + (5) ipdp --> octdp + (5) ppi
FTL_0405	UbiE	OMBZLM	2-Octaprenyl-6-methoxy-benzoquinol methylase	[c] : 2ombzl + amet --> 2ommbl + ahcys + h
FTL_0045	PyrF	OMPDC	orotidine-5'-phosphate decarboxylase	[c] : h + orot5p --> co2 + ump
FTL_0726	UbiH	OMPHHX	2-octaprenyl-6-methoxyphenol hydroxylase	[c] : 2omph + (0.5) o2 --> 2ombzl
FTL_0407	UbiB	OPHHX	2-Octaprenylphenol hydroxylase	[c] : 2oph + (0.5) o2 --> 2ohph
FTL_1497	DctA	OROTt2_2	orotate transport via sodium symport	na1[e] + orot[e] <==> na1[c] + orot[c]
FTL_0507	PyrE	ORPT	orotate phosphoribosyltransferase	[c] : orot5p + ppi <==> orot + prpp
FTL_0805	PutAec	P5CD	1-pyrroline-5-carboxylate dehydrogenase	[c] : 1pyr5c + (2) h2o + nad --> glu-L + h + nadh
FTL_0549	ProC	P5CR	pyrroline-5-carboxylate reductase	[c] : 1pyr5c + (2) h + nadph --> nadp + pro-L
FTL_0673	PanCec	PANTS	pantothenate synthase	[c] : ala-B + atp + pant-R --> amp + h + pnto-R + ppi
FTL_1615	MraY	PAPPT3	phospho-N-acetylmuramoyl-pentapeptide-transferase (meso-2,6-diaminopimelate)	[c] : udcpp + ugmda --> uagmda + ump
FTL_1142	PlsX	PASYN_EC	Phosphatidic acid synthase (Ecoli)	[c] : glyc3p + (0.322) hdeACP + (0.208) myrsACP + (0.373) octeACP + (0.982) palmACP + (0.115) tdeACP --> (2) ACP + (0.02) pa_EC
FTL_0710	YxeI	PENCAC	penicillin acylase	[c] : h + h2o + pencil --> 6ampenc + for
FTL_1781	MrsA2	PGAMT	phosphoglucosamine mutase	[c] : gam1p <==> gam6p
FTL_0714	SerA	PGCD	phosphoglycerate dehydrogenase	[c] : 3pg + nad --> 3php + h + nadh
FTL_1476	Pgi	PGI	glucose-6-phosphate isomerase	[c] : g6p <==> f6p
FTL_1147	Pgk	PGK	phosphoglycerate kinase	[c] : 13dpg + adp <==> 3pg + atp
FTL_1569	Gph	PGLYCP	phosphoglycolate phosphatase	[c] : 2pglyc + h2o --> glyclt + pi
FTL_1490	YibO	PGM	phosphoglycerate mutase	[c] : 3pg <==> 2pg
FTL_0484	Pgm2	PGMT	phosphoglucomutase	[c] : g1p <==> g6p
FTL_0231	PgsA	PGSA_EC	Phosphatidylglycerol synthase (Ecoli)	[c] : (0.02) cdpdag_EC + glyc3p <==> cmp + h + (0.02) pgp_EC
FTL_0131	IlvE	PHETA1	phenylalanine transaminase	[c] : akg + phe-L <==> glu-L + phpyr
FTL_1197	PheRS	PHETRS	Phenylalanyl-tRNA synthetase	[c] : atp + phe-L + trnaphe --> amp + phetrna + ppi
FTL_0156	PitA	PIt6	phosphate transport in/out via proton symporter	h[e] + pi[e] <==> h[c] + pi[c]
FTL_0609	CpsG	PMANM	phosphomannomutase	[c] : man1p <==> man6p
FTL_1061	Ppa	PPA	inorganic diphosphatase	[c] : h2o + ppi --> h + (2) pi
FTL_0808	Dfp	PPCDC	phosphopantothenoylcysteine decarboxylase	[c] : 4ppcys + h --> co2 + pan4p
FTL_1616	PckA	PPCK	phosphoenolpyruvate carboxykinase	[c] : atp + oaa --> adp + co2 + pep
FTL_0132	PpdK	PPDK	pyruvate phosphate dikinase	[c] : atp + pi + pyr --> amp + h + pep + ppi
FTL_1664	DeoB	PPM	phosphopentomutase	[c] : r1p <==> r5p
FTL_1664	DeoB	PPM2	phosphopentomutase (deoxyribose)	[c] : 2dr1p <==> 2dr5p
FTL_0808	Dfp	PPNCL2	phosphopantothenate-cysteine ligase	[c] : 4ppan + ctp + cys-L --> 4ppcys + cmp + h + ppi
FTL_1336	PheA	PPNDH	prephenate dehydratase	[c] : h + pphn --> co2 + h2o + phpyr
FTL_1188	HemY	PPPGO	protoporphyrinogen oxidase	[c] : (1.5) o2 + pppg9 --> (3) h2o + ppp9
FTL_0132	PpdK	PPS	phosphoenolpyruvate synthase	[c] : atp + h2o + pyr --> amp + (2) h + pep + pi
FTL_0396	PurD	PRAGS	phosphoribosylglycinamide synthetase	[c] : atp + gly + pram --> adp + gar + h + pi
FTL_0395	PurM	PRAIS	phosphoribosylaminoimidazole synthetase	[c] : atp + fpram --> adp + air + h + pi
FTL_1958	TrpCec	PRAIi	phosphoribosylanthranilate isomerase (irreversible)	[c] : pran --> 2cpr5p
FTL_0396	PurD	PRASCS	phosphoribosylaminoimidazolesuccinocarboxamide synthase	[c] : 5aizc + asp-L + atp <==> 25aics + adp + h + pi
FTL_1860	Ade6	PRFGS	phosphoribosylformylglycinamidine synthase	[c] : atp + fgam + gln-L + h2o --> adp + fpram + glu-L + (2) h + pi
FTL_0805	PutAec	PRO1z	proline oxidase	[c] : fad + pro-L --> 1pyr5c + fadh2 + h
FTL_0650	ProS	PROTRS	Prolyl-tRNA synthetase	[c] : atp + pro-L + trnapro --> amp + ppi + protrna
FTL_1700	PutPec	PROt4	Na+/Proline-L symporter	na1[e] + pro-L[e] --> na1[c] + pro-L[c]
FTL_1417	ProPec	PROt6	L-proline transport in/out via proton symport	h[e] + pro-L[e] <==> h[c] + pro-L[c]
FTL_0949	PrsA	PRPPS	phosphoribosylpyrophosphate synthetase	[c] : atp + r5p <==> amp + h + prpp
FTL_0852	AroA	PSCVT	3-phosphoshikimate 1-carboxyvinyltransferase	[c] : pep + skm5p <==> 3psme + pi
FTL_0450	Psd	PSD_EC	Phosphatidylserine decarboxylase (Ecoli)	[c] : h + (0.02) ps_EC --> co2 + (0.02) pe_EC
FTL_1018	SerC	PSERT	phosphoserine transaminase	[c] : 3php + glu-L --> akg + pser-L
FTL_1427	Ser2	PSP_L	phosphoserine phosphatase (L-serine)	[c] : h2o + pser-L --> pi + ser-L
FTL_0016	Pta	PTA2	Phosphate acetyltransferase	[c] : pi + ppcoa --> coa + ppap
FTL_0016	Pta	PTAr	phosphotransacetylase	[c] : accoa + pi <==> actp + coa
FTL_1296	PotEec	PTRCORNt7	putrescine/ornithine antiporter	orn-L[c] + ptrc[e] <==> orn-L[e] + ptrc[c]
FTL_1296	PotEec	PTRCt2	putrescine transport in via proton symport, reversible	h[e] + ptrc[e] <==> h[c] + ptrc[c]
FTL_0688	Mdr	PURabc1	Puromycin efflux via ABC system	atp[c] + h2o[c] + pur[c] --> adp[c] + h[c] + pi[c] + pur[e]
FTL_1148	Pyka	PYK	pyruvate kinase	[c] : adp + h + pep --> atp + pyr
FTL_1487	Udp	PYNP2	pyrimidine-nucleoside phosphorylase (uracil)	[c] : pi + uri <==> r1p + ura
FTL_1390	NadA	QULNS	quinolinate synthase	[c] : dhap + iasp --> (2) h2o + pi + quln
FTL_0437	RibFec	RBFK	riboflavin kinase	[c] : atp + ribflv --> adp + fmn + h
FTL_1529	PnuC	RNAMt	Nicotinamide riboside transport	rnam[e] --> rnam[c]
FTL_0984	Rnr12	RNDR1	ribonucleoside-diphosphate reductase (ADP)	[c] : adp + trdrd --> dadp + h2o + trdox
FTL_0984	Rnr12	RNDR2	ribonucleoside-diphosphate reductase (GDP)	[c] : gdp + trdrd --> dgdp + h2o + trdox
FTL_0984	Rnr12	RNDR3	ribonucleoside-diphosphate reductase (CDP)	[c] : cdp + trdrd --> dcdp + h2o + trdox
FTL_0984	Rnr12	RNDR4	ribonucleoside-diphosphate reductase (UDP)	[c] : trdrd + udp --> dudp + h2o + trdox
FTL_1432	Rpeec	RPE	ribulose 5-phosphate 3-epimerase	[c] : ru5p-D <==> xu5p-D
FTL_0736	Rpi	RPI	ribose-5-phosphate isomerase	[c] : r5p <==> ru5p-D
FTL_0068	GmhA	S7PI	sedoheptulose 7-phosphate isomerase	[c] : s7p <==> gmh7p
FTL_1034	CysD	SADT2	sulfate adenylyltransferase	[c] : atp + gtp + h2o + so4 --> aps + gdp + pi + ppi

LVS GENE	Protein	Abbreviation	Name	Equation
FTL_1334	SdaB	SERD_L	L-serine deaminase	[c] : ser-L --> nh4 + pyr
FTL_1491	SerS	SERTRS	Seryl-tRNA synthetase	[c] : atp + ser-L + trnaser --> amp + ppi + sertrna
FTL_0024	SdaC	SERt6	L-serine transport in/out via proton symport	h[e] + ser-L[e] <==> h[c] + ser-L[c]
FTL_0801	AroK	SHKK	shikimate kinase	[c] : atp + skm --> adp + h + skm5p
FTL_1499	YbaR	SO4t2	sulfate transport in via proton symport	h[e] + so4[e] --> h[c] + so4[c]
FTL_1622	Blt	SPMDt3	spermidine transport out via proton antiport	h[e] + spmd[c] --> h[c] + spmd[e]
FTL_0500	SpeE	SPMS	spermidine synthase	[c] : ametam + ptrc --> 5mta + h + spmd
FTL_1263	MenE	SUCBZL	o-succinylbenzoate-CoA ligase	[c] : atp + coa + sucbz --> amp + ppi + sbzcoa
FTL_1497	DctA	SUCCt6_na	succinate transporter in/out via sodium symport	na1[e] + succ[e] <==> na1[c] + succ[c]
FTL_0053	Suc2-e	SUCRe	sucrose hydrolyzing enzyme, extracellular	[e] : h2o + sucr --> fru + glc-D
FTL_1211	SsuA	SULAabc	sulfoacetate transport via ABC system	atp[c] + h2o[c] + sula[e] --> adp[c] + h[c] + pi[c] + sula[c]
FTL_1607	YccK	SULR	sulfite reductase (NADPH2)	[c] : (3) h2o + h2s + (3) nadp <==> (4) h + (3) nadph + so3
FTL_1109	TalB	TAL	transaldolase	[c] : g3p + s7p <==> e4p + f6p
FTL_1921	TauB	TAURabc	taurine transport via ABC system	atp[c] + h2o[c] + taur[e] --> adp[c] + h[c] + pi[c] + taur[c]
FTL_1667	LpxK	TDSK	Tetraacyldisaccharide 4'kinase	[c] : atp + lipidAds --> adp + h + lipidA
FTL_1431	TuaA	TEICH45	teichuronic acid (n=45), unlinked, GalNAc-GlcA repeated	[c] : (45) uacgala + (45) udpglcur <==> (45) h + teich-45_BS + (45) udp + (45) ump
FTL_0960	SthA	THD5	NAD transhydrogenase	[c] : nad + nadph --> nadh + nadp
FTL_1308	FolC	THFGLUS	Tetrahydrofolate:L-glutamate gamma-ligase (ADP-forming)	[c] : atp + glu-L + thf <==> adp + h + pi + thfglu
FTL_1661	NupCec	THMDt2	thymidine transport in via proton symport	h[e] + thymd[e] --> h[c] + thymd[c]
FTL_0703	GlyA	THRA	threonine aldolase	[c] : thr-L <==> acald + gly
FTL_1523	Tdh	THRD	L-threonine dehydrogenase (w/ AOBUTDs)	[c] : nad + thr-L --> 2aobut + h + nadh
FTL_1334	SdaB	THRD_L	L-threonine deaminase	[c] : thr-L --> 2obut + nh4
FTL_0498	ThrC	THRS	threonine synthase	[c] : h2o + phom --> pi + thr-L
FTL_1407	ThrS	THRTRS	Threonyl-tRNA synthetase	[c] : atp + thr-L + trnathr --> amp + ppi + thrtrna
FTL_0718	IscS	THZPSN	thiazole phosphate synthesis	[c] : atp + cys-L + dxyl5p + tyr-L --> 4hba + 4mpetz + ala-L + amp + co2 + h + h2o + ppi
FTL_1145	TktA	TKT1	transketolase	[c] : r5p + xu5p-D <==> g3p + s7p
FTL_1145	TktA	TKT2	transketolase	[c] : e4p + xu5p-D <==> f6p + g3p
FTL_0890	Tdk	TMDK1	thymidine kinase (ATP:thymidine)	[c] : atp + thymd --> adp + dtmp + h
FTL_0715	ThyA	TMDS	thymidylate synthase	[c] : dump + mlthf --> dhf + dtmp
FTL_1780	Tpi	TPI	triose-phosphate isomerase	[c] : dhap <==> g3p
FTL_1571	TrxB	TRDR	thioredoxin reductase (NADPH)	[c] : h + nadph + trdox --> nadp + trdrd
FTL_0459	Map	TRIA	membrane alanyl aminopeptidase	[c] : cgly + h2o <==> cys-L + gly
FTL_0306	TrpS	TRPTRS	Tryptophanyl-tRNA synthetase	[c] : atp + trnatrp + trp-L --> amp + ppi + trptrna
FTL_0968	Tys1	TYRTRS	Tyrosyl-tRNA synthetase	[c] : atp + trnatyr + tyr-L --> amp + ppi + tyrtrna
FTL_0058	TyrP	TYRt6	L-tyrosine transport in/out via proton symport	h[e] + tyr-L[e] <==> h[c] + tyr-L[c]
FTL_0490	MurE	UAAGDS	UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimelate synthetase	[c] : 26dap-M + atp + uamag --> adp + h + pi + ugmd
FTL_0596	WecC	UACMAMO	UDP-N-acetyl-D-mannosamine oxidoreductase	[c] : h2o + (2) nad + uacmam --> (3) h + (2) nadh + uacmamu
FTL_0539	LpxA	UAGAAT	UDP-N-acetylglucosamine acyltransferase	[c] : 3htdACP + uacgam <==> ACP + u3aga
FTL_0413	MurAA	UAGCVT	UDP-N-acetylglucosamine 1-carboxyvinyltransferase	[c] : pep + uacgam --> pi + uaccg
FTL_1410	MurG	UAGPT3	UDP-N-acetylglucosamine-N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase	[c] : uacgam + uagmda --> h + uaagmda + udp
FTL_1614	MurD	UAMAGS	UDP-N-acetylmuramoyl-L-alanyl-D-glutamate synthetase	[c] : atp + glu-D + uama --> adp + h + pi + uamag
FTL_0172	MurC	UAMAS	UDP-N-acetylmuramoyl-L-alanine synthetase	[c] : ala-L + atp + uamr --> adp + h + pi + uama
FTL_0412	MurB	UAPGR	UDP-N-acetylenolpyruvoylglucosamine reductase	[c] : h + nadph + uaccg --> nadp + uamr
FTL_1396	GalT	UGLT	UDPglucose--hexose-1-phosphate uridylyltransferase	[c] : gal1p + udpg <==> g1p + udpgal
FTL_0492	MurFec	UGMDDS	UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine synthetase	[c] : alaala + atp + ugmd --> adp + h + pi + ugmda
FTL_1017	Cmk	UMPK	UMP kinase	[c] : atp + ump <==> adp + udp
FTL_1812	HemE	UPPDC1	uroporphyrinogen decarboxylase (uroporphyrinogen III)	[c] : (4) h + uppg3 --> (4) co2 + cpppg3
FTL_1520	Upp	UPPRT	uracil phosphoribosyltransferase	[c] : prpp + ura --> ppi + ump
FTL_1660	Tmk	URIDK2	uridylate kinase (dUMP)	[c] : atp + dump --> adp + dudp
FTL_0226	PyrHec	URIDK3	uridylate kinase (dUMP)	[c] : atp + dump <==> adp + dudp
FTL_1534	Udk	URIK1	uridine kinase (ATP:Uridine)	[c] : atp + uri --> adp + h + ump
FTL_1534	Udk	URIK2	uridine kinase (GTP:Uridine)	[c] : gtp + uri --> gdp + h + ump
FTL_1534	Udk	URIK3	uridine kinase (ITP:Uridine)	[c] : itp + uri --> h + idp + ump
FTL_0131	IlvE	VALTA	valine transaminase	[c] : akg + val-L <==> 3mob + glu-L
FTL_0210	ValS	VALTRS	Valyl-tRNA synthetase	[c] : atp + trnaval + val-L --> amp + ppi + valtrna
FTL_0548	IxpP	XTPASE	XTP pyrophosphatase	[c] : h2o + xtp --> h + ppi + xmp
FTL_1591	AccC	bCBXL	biotin carboxylase	[c] : atp + biotccp + hco3 --> adp + cbtnccp + pi
FTL_1433	ArpI	A5PISO	arabinose-5-phosphate isomerase	[c] : ru5p-D <==> ara5p
FTL_0915	IlvH	ACHBS	2-aceto-2-hydroxybutanoate synthase	[c] : 2obut + h + pyr --> 2ahbut + co2
FTL_0915	IlvH	ACLS	acetolactate synthase (Also catalyzes ACHBS)	[c] : h + (2) pyr --> alac-S + co2
FTL_0916	IlvC	AHAI	acetohydroxy acid isomeroreductase	[c] : alac-S + h + nadph --> 23dhmb + nadp
FTL_0916		ALCD2y	alcohol dehydrogenase (ethanol, NADP)	[c] : etoh + nadp <==> acald + h + nadph
FTL_1488	Cdd	CYTD	cytidine deaminase	[c] : cytd + h + h2o --> nh4 + uri
FTL_1208	Dcd	DCTPD	dCTP deaminase	[c] : dctp + h + h2o --> dutp + nh4
FTL_0127	FdhF	FDH2	formate dehydrogenase (quinone-8: 2 protons)	for[c] + (3) h[c] + ubq8[c] --> co2[c] + (2) h[e] + ubq8h2[c]
FTL_0453	GlmU	G1PACT	glucosamine-1-phosphate N-acetyltransferase	[c] : accoa + gam1p --> acgam1p + coa + h
FTL_1357	GalU	GALU	UTP-glucose-1-phosphate uridylyltransferase	[c] : g1p + h + utp <==> ppi + udpg
FTL_0594	Gcd	GLCDe	Glucose dehydrogenase (ubiquinone-8 as acceptor)	glc-D[e] + h2o[e] + ubq8[c] --> glcn-D[e] + h[e] + ubq8h2[c]
FTL_1284	GshB	GTHS	glutathione synthase	[c] : atp + glucys + gly --> adp + gthrd + h + pi
FTL_1253	FolE	GTPCI	GTP cyclohydrolase I	[c] : gtp + h2o --> ahdt + for + h
FTL_1931	Hpt	GUAPRT	guanine phosphoribosyltransferase	[c] : gua + prpp --> gmp + ppi
FTL_1286	NarGHI	NTR3B	nitrate reductase	(2) h[c] + mql7[c] + no3[c] --> (2) h[e] + h2o[c] + mqn7[c] + no2[c]
FTL_1602	HemB	PPBNGS	porphobilinogen synthase	[c] : (2) 5aop --> h + (2) h2o + ppbng
FTL_1330	CoaD	PTPAT	pantetheine-phosphate adenylyltransferase	[c] : atp + h + pan4p <==> dpcoa + ppi
FTL_0010	GlpE	TSULST	thiosulfate sulfurtransferase	[c] : cyan + tsul --> h + so3 + tcynt
FTL_0537	LpxD	U23GAAT	UDP-3-O-(3-hydroxymyristoyl)glucosamine acyltransferase	[c] : 3htdACP + u3hga --> ACP + h + u23ga
FTL_0453	GlmU	UAGDP	UDP-N-acetylglucosamine diphosphorylase	[c] : acgam1p + h + utp --> ppi + uacgam
FTL_0228	UppS	UDCPDP	undecaprenyl-diphosphatase	[c] : h2o + udcpdp --> h + pi + udcpp
FTL_0228	UppS	UDCPDPS	Undecaprenyl diphosphate synthase	[c] : frdp + (8) ipdp --> (8) ppi + udcpdp
FTL_1906	LpxC	UHGADA	UDP-3-0-acyl N-acetylglucosamine deacetylase	[c] : h2o + u3aga --> ac + u3hga
FTL_0583	fadA	ACACT1r	acetyl-CoA C-acetyltransferase	[c] : (2) accoa <==> aacoa + coa
FTL_0453	glmU	ACGAMT	UDP-N-acetylglucosamine:undecaprenylphosphate N-acetylglucosamine -1-phosphate transferase	[c] : uacgam + udcpp --> ump + unaga
FTL_0585	FadE	ADHEr	acetaldehyde-CoA dehydrogenase	[c] : accoa + (2) h + (2) nadh <==> coa + etoh + (2) nad
FTL_1036	cysC	ADSK	adenylyl-sulfate kinase	[c] : aps + atp --> adp + h + paps
FTL_1433	ArpI	ARABI	arabinose isomerase	[c] : arab-D <==> rbl-D
FTL_1495		CYSabc	L-cysteine transport via ABC system	atp[c] + cys-L[e] + h2o[c] --> adp[c] + cys-L[c] + h[c] + pi[c]
FTL_1834		DAPE	diaminopimelate epimerase	[c] : 26dap-LL <==> 26dap-M
FTL_1149		F6PA	fructose 6-phosphate aldolase	[c] : f6p <==> dha + g3p
FTL_0916	ilvC	KARA2i	ketol-acid reductoisomerase (2-Aceto-2-hydroxybutanoate)	[c] : 2ahbut + h + nadph --> 23dhmp + nadp
FTL_0383	manC	MAN6PI	mannose-6-phosphate isomerase	[c] : man6p <==> f6p
FTL_0394	fold	MTHFR2	5,10-methylenetetrahydrofolate reductase (NADH)	[c] : (2) h + mlthf + nadh --> 5mthf + nad

Supplemental Data S1. B. Multigene-protein-reactions in iRS605

Protein	Abbreviation	Name	Equation	Genes
AccC+AccA+AccB+AccD	ACCOAC	acetyl-CoA carboxylase	[c] : accoa + atp + hco3 --> adp + h + malcoa + pi	FTL_1591 FTL_0295 FTL_1592
SucA+SucB	AKGD	2-oxoglutarate dehydrogenase	[c] : akg + coa + nad --> co2 + nadh + succoa	FTL_1784 FTL_1783
TrpEec, TrpG	ANS1	anthranilate synthase	[c] : chor + gln-L --> anth + glu-L + h + pyr	FTL_1966 FTL_1261
AnsA, AnsB	ASNN	L-asparaginase	[c] : asn-L + h2o --> asp-L + nh4	FTL_0855 FTL_1600
AspB2, AspC	ASPTA1	aspartate transaminase	[c] : akg + asp-L <==> glu-L + oaa	FTL_0789 FTL_0387
Amd4+AgaB	ASPTS	asparaginyl-tRNA synthase (glutamine-hydrolysing)	[c] : adp + asntrna + glu-L + pi --> asptrna + atp + gln-L	FTL_1842 FTL_1841
AtpABCDEFGHI, AtpF1+AtpF0	ATPS4r	ATP synthase (four protons for one ATP)	adp[c] + (4) h[e] + pi[c] <==> atp[c] + (3) h[c] + h2o[c]	FTL_1794 FTL_1797 FTL_1796 FTL_1795 FTL_1798 FTL_1801 FTL_1799
FabGec+FabZ+FabI	C141SN	Fatty acid biosynthesis (n-C14:1)	[c] : actACP + (16) h + (5) malACP + (11) nadph --> (5) ACP + (5) co2 + (6) h2o + (11) nadp + tdeACP	FTL_1139 FTL_0538 FTL_1442
FabGec+FabI+FabZ	C161SN	Fatty acid biosynthesis (n-C16:1)	[c] : actACP + (19) h + (6) malACP + (13) nadph --> (6) ACP + (6) co2 + (7) h2o + hdeACP + (13) nadp	FTL_1139 FTL_1442 FTL_0538
FabGec+FabZ+FabI+FabF	C181SN	Fatty acid biosynthesis (n-C18:1)	[c] : actACP + (22) h + (7) malACP + (15) nadph --> (7) ACP + (7) co2 + (8) h2o + (15) nadp + octeACP	FTL_1139 FTL_0538 FTL_1442 FTL_1137
Car	CBPS	carbamoyl-phosphate synthase (glutamine-hydrolysing)	[c] : (2) atp + gln-L + h2o + hco3 --> (2) adp + cbp + glu-L + (2) h + pi	FTL_0030 FTL_0029
TyrA, AroH	CHORM	chorismate mutase	[c] : chor --> pphn	FTL_0043 FTL_0328
CydCD	CYSabc2	L-cysteine export via ABC system	atp[c] + cys-L[c] + h2o[c] --> adp[c] + cys-L[e] + h[c] + pi[c]	FTL_1496 FTL_1495
CydA	CYTBD	cytochrome oxidase bd (ubiquinol-8: 2 protons)	(2) h[c] + (0.5) o2[c] + ubq8h2[c] --> (2) h[e] + h2o[c] + ubq8[c]	FTL_0189 FTL_0188
CyoA	CYTBO3	cytochrome oxidase bo3 (ubiquinol-8: 2.5 protons)	(2.5) h[c] + (0.5) o2[c] + ubq8h2[c] --> (2.5) h[e] + h2o[c] + ubq8[c]	FTL_0191 FTL_0194 FTL_0193 FTL_0192
DeoD	DURIPP	purine-nucleoside phosphatase (deoxyuridine)	[c] : duri + pi <==> 2dr1p + ura	FTL_1460 FTL_1461
Def	FMETDF	formylmethionine deformylase	[c] : fmet + h2o --> for + met-L	FTL_0473 FTL_0074
GcvH+GcvP1	GCCa	glycine-cleavage complex	[c] : gly + h + lpro --> alpro + co2	FTL_1409 FTL_0478 FTL_0480 FTL_0479
GcvT, GcvH	GCCb	glycine cleavage complex	[c] : alpro + thf --> dhlpro + mlthf + nh4	FTL_0477 FTL_1409 FTL_0478
Amd4+AgaB	GLUH	glutaminyl-tRNA synthase (glutamine-hydrolysing);	[c] : atp + gln-L + glutrna --> adp + glntrna + glu-L + pi	FTL_1842 FTL_1841
GcvT+GcvH+GcvP1	GLYCL	Glycine Cleavage System	[c] : gly + nad + thf --> co2 + mlthf + nadh + nh4	FTL_0477 FTL_1409 FTL_0478 FTL_0480 FTL_0479
GlyS+GlyQ	GLYTRS	Glycyl-tRNA synthetase	[c] : atp + gly + trnagly --> amp + glytrna + ppi	FTL_1350 FTL_0489
ProW+ProV	GLYt6	glycine transport in/out via proton symport	gly[e] + h[e] <==> gly[c] + h[c]	FTL_0145 FTL_0146
GlpQ	GPDDA1	Glycerophosphodiester phosphodiesterase (sn-Glycero-3-phosphocholine)	[c] : g3pc + h2o --> chol + glyc3p + h	FTL_1511 FTL_0829
GlpQ	GPDDA2	Glycerophosphodiester phosphodiesterase (Glycerophosphoethanolamine)	[c] : g3pe + h2o --> etha + glyc3p + h	FTL_1511 FTL_0829
GlpQ	GPDDA4	Glycerophosphodiester phosphodiesterase (Glycerophosphoglycerol)	[c] : g3pg + h2o --> glyc + glyc3p + h	FTL_1511 FTL_0829
BsaA	GSHPO	glutathione peroxidase	[c] : (2) gthrd + h2o2 --> gthox + (2) h2o	FTL_1383
CydCD	GTHRDabc	Glutathione export via ABC system	atp[c] + gthrd[c] + h2o[c] --> adp[c] + gthrd[e] + h[c] + pi[c]	FTL_1496 FTL_1495
KdpABC	Kabc	potassium transport via ABC system	atp[c] + h2o[c] + k[e] --> adp[c] + h[c] + k[c] + pi[c]	FTL_1882 FTL_1880
TrkA, TrkA	Kt6	potassium transport in/out via proton symport	h[e] + k[e] <==> h[c] + k[c]	
YfdH, WbtG, WbtD	MANGLTF	Mannose Glycosyltransferases	[c] : qdpman + mannan <==> qdp + h + mannan(n+1)	FTL_1611 FTL_0599 FTL_0595
MetN+MetQ	METDabc	D-methionine transport via ABC system	atp[c] + h2o[c] + met-D[e] --> adp[c] + h[c] + met-D[c] + pi[c]	FTL_0838 FTL_0837
MsrA	METSR-S1	L-methionine-S-oxide reductase (trdrd)	[c] : metox + trdrd --> h2o + met-L + trdox	FTL_1960 FTL_1093
MsrA	METSR-S2	L-methionine S-oxide reductase (H2O2)	[c] : h2o2 + met-L --> h2o + metox	FTL_1960 FTL_1093
MetN+MetQ	METabc	L-methionine transport via ABC system	atp[c] + h2o[c] + met-L[e] --> adp[c] + h[c] + met-L[c] + pi[c]	FTL_0838 FTL_0837
Nadhd5	NADH12	NADH dehydrogenase (ubiquinone-8)	[c] : h + nadh + ubq8 --> nad + ubq8h2	FTL_1822 FTL_1827 FTL_1819 FTL_1829 FTL_1828 FTL_1825 FTL_1818
Nuo	NADH6	NADH dehydrogenase (ubiquinone-8 & 3.5 protons)	(4.5) h[c] + nadh[c] + ubq8[c] --> (3.5) h[e] + nad[c] + ubq8h2[c]	FTL_1830 FTL_1817 FTL_1820 FTL_1824
AceFec+AceEec+LpdA	PDH	pyruvate dehydrogenase	[c] : coa + nad + pyr --> accoa + co2 + nadh	FTL_0310 FTL_0311
RluC, RluD	PSUDS	pseudouridylate synthase	[c] : r5p + ura --> h2o + psd5p	FTL_1804 FTL_0699
PotH+PotF+PotG+PotI	PTRCabc	putrescine transport via ABC system	atp[c] + h2o[c] + ptrc[e] --> adp[c] + h[c] + pi[c] + ptrc[c]	FTL_0680 FTL_1582 FTL_0681 FTL_0679
DeoD	PUNP1	purine-nucleoside phosphorylase (Adenosine)	[c] : adn + pi <==> ade + r1p	FTL_1460 FTL_1461
DeoD	PUNP2	purine-nucleoside phosphorylase (Deoxyadenosine)	[c] : dad-2 + pi <==> 2dr1p + ade	FTL_1460 FTL_1461
DeoD	PUNP3	purine-nucleoside phosphorylase (Guanosine)	[c] : gsn + pi <==> gua + r1p	FTL_1460 FTL_1461
DeoD	PUNP4	purine-nucleoside phosphorylase (Deoxyguanosine)	[c] : dgsn + pi <==> 2dr1p + gua	FTL_1460 FTL_1461
DeoD	PUNP5	purine-nucleoside phosphorylase (Inosine)	[c] : ins + pi <==> hxan + r1p	FTL_1460 FTL_1461
DeoD	PUNP6	purine-nucleoside phosphorylase (Deoxyinosine)	[c] : din + pi <==> 2dr1p + hxan	FTL_1460 FTL_1461
DeoD	PUNP7	purine-nucleoside phosphorylase (Xanthosine)	[c] : pi + xtsn <==> r1p + xan	FTL_1460 FTL_1461
DeoD	PUNP8	purine-nucleoside phosphorylase (nebularine)	[c] : h + nebari + pi <==> purine + r1p	FTL_1460 FTL_1461
RibEH	RBFSa	riboflavin synthase	[c] : 4r5au + db4p --> dmlz + (2) h2o + pi	FTL_0075 FTL_0077
RibEH	RBFSb	riboflavin synthase	[c] : (2) dmlz --> 4r5au + ribflv	FTL_0075 FTL_0077
DeoD	RIOR	N-Ribosylnicotinamide:orthophosphate ribosyltransferase	[c] : pi + rnam <==> h + ncam + r1p	FTL_1460 FTL_1461
AroEec	SHK3D	shikimate dehydrogenase	[c] : 3dhsk + h + nadph <==> nadp + skm	FTL_0481 FTL_0173
SodC, SodB	SOD	superoxide dismutase	[c] : (2) h + (2) o2- --> h2o2 + o2	FTL_0380 FTL_1791
GabD2+GabD	SSALy	succinate-semialdehyde dehydrogenase (NADP)	[c] : h2o + nadp + sucsal --> (2) h + nadph + succ	
SdhD+SdhC+SdhB+SdhA	SUCD1i	succinate dehydrogenase	[c] : fad + succ --> fadh2 + fum	FTL_1787 FTL_1788 FTL_1785 FTL_1786
SdhD+SdhC+SdhB+SdhA	SUCD4	succinate dehyrdogenase	[c] : fadh2 + ubq8 <==> fad + ubq8h2	FTL_1787 FTL_1788 FTL_1785 FTL_1786
SucC	SUCOAS	succinyl-CoA synthetase (ADP-forming)	[c] : atp + coa + succ <==> adp + pi + succoa	FTL_1554 FTL_1553
RffG, RfbB	TDPGDH	dTDPglucose 4,6-dehydratase	[c] : dtdpglc --> dtdpddg + h2o	FTL_0606 FTL_0592
TrpA	TRPS1	tryptophan synthase (indoleglycerol phosphate)	[c] : 3ig3p + ser-L --> g3p + h2o + trp-L	FTL_0098 FTL_0099
TrpA	TRPS2	tryptophan synthase (indole)	[c] : indole + ser-L --> h2o + trp-L	FTL_0098 FTL_0099
TrpA	TRPS3	tryptophan synthase (indoleglycerol phosphate)	[c] : 3ig3p --> g3p + indole	FTL_0098 FTL_0099
YtcB, GalE	UDPG4E	UDPglucose 4-epimerase	[c] : udpq <==> udpgal	FTL_0597 FTL_1430
Deg1, Pus4	YUMPS	yUMP synthetase	[c] : r5p + ura <==> h2o + psd5p	FTL_1068 FTL_0555
ZntA, YceA, MtsB	ZN2abc2	zinc transport in via ABC system	atp[c] + h2o[c] + zn2[e] --> adp[c] + h[c] + pi[c] + zn2[c]	FTL_1935 FTL_1934 FTL_1936
PNTK	PNTK	pantothenate kinase	[c] : atp + pnto-R --> 4ppan + adp + h	FTL_1665 FTL_0671
If2+EfG+If3+Rf3+Eftu2+Rf1+RpS+RpL+Rf2+LepA	PROTSYN_Eco	Protein synthesis, E. coli	[c] : (103) alatrna + (59) argtrna + (48) asntrna + (48) asptrna + (18) cystrna + (53) glntrna + (53) glutrna + (53) glytrna + (2000) gtp + (2000) h2o + (19) histrna + (58) iletrna + (90) leutrna + (69) lystrna + (31) mettrna + (37) phetrna + (44) protrna + (43) sertrna + (51) thrtrna + (11) trptrna + (28) tyrtrna + (85) valtrna --> (2000) gdp + (3001) h + (2000) pi + protein_Eco + (103) trnaala + (59) trnaarg + (48) trnaasn + (48) trnaasp + (18) trnacys + (53) trnagln + (53) trnaglu + (53) trnagly + (19) trnahis + (58) trnaile + (90) trnaleu + (69) trnalys + (31) trnamet + (37) trnaphe + (44) trnapro + (43) trnaser + (51) trnathr + (11) trnatrp + (28) trnatyr + (85) trnaval	FTL_1809 FTL_0234 FTL_1659 FTL_1751 FTL_1721 FTL_0259 FTL_1025 FTL_0070 FTL_0245 FTL_0253 FTL_1538 FTL_1912 FTL_0260 FTL_0250 FTL_0233 FTL_0242 FTL_0235 FTL_0224 FTL_1738 FTL_0248 FTL_0262 FTL_0255 FTL_1453 FTL_0247 FTL_1303 FTL_0950 FTL_1143 FTL_1745 FTL_1452 FTL_1746 FTL_1748 FTL_0239 FTL_1747 FTL_1735 FTL_1187 FTL_0252 FTL_0238 FTL_0244 FTL_0251 FTL_1404 FTL_1026 FTL_0243

Supplemental Data S1 C: Gene-ProteIn-Reaction associations in the final version of the reconstruction iRS605

-Reactions includng biomass formation reaction that have no annotated gene information yet but are needed in silico for growth

RXN	NAME	EQN	REFERENCE	ADDITIONAL COMMENTS
AGMHE	ADP-D-glycero-D-manno-heptose epimerase	[c] : adphep-D,D --> adphep-L,D	Essential for Lipopolysaccharide Biosynthesis / Recycling	Required for Biomass Formation
AGMT	agmatinase	[c] : agm + h2o --> ptrc + urea	Essential for Arginine and Proline Metabolism	Required for Biomass Formation
ARAB-Dt	D-arabinose reversible transport	arab-D[e] <==> arab-D[c]	This study; transport needed for growth	
ASP2DC	aspartate 2-decarboxylase	[c] : asp-L + h --> ala-L + co2	Essential for Cofactor and Prosthetic Group Biosynthesis	
AST	Arginine succinyltransferase	[c] : arg-L + succoa --> coa + h + sucarg	Essential for Arginine and Proline Metabolism	
BPNT	3',5'-bisphosphate nucleotidase	[c] : h2o + pap --> amp + pi	Essential for Cysteine Metabolism	
CO2t	CO2 transport out via diffusion	co2[e] <==> co2[c]	Essential for transport	
DAGK_EC	Diacylglycerol kinase	[c] : (0.02) 12dgr_EC + atp --> adp + h + (0.02) pa_EC	Lipids. 1986 Oct;21(10):669-71.	Required for Biomass Formation
DHAPT	Dihydroxyacetone phosphotransferase	[c] : dha + pep --> dhap + pyr		
DKMPPD	2,3-diketo-5-methylthio-1-phosphopentane degradation reaction	[c] : dkmpp + h2o + o2 --> 2kmb + for + (2) h + pi	Essential for Arginine and Proline Metabolism	Required for Biomass Formation
EDTXS1	Endotoxin Synthesis (lauroyl transferase)	[c] : ddcaACP + kdo2lipid4 --> ACP + kdo2lipid4L	Microbiology. 2007 Sep;153(Pt 9):3141-53; Ann N Y Acad Sci. 2007, Gunn JS, Ernst RK	Required for Biomass Formation
EDTXS2	Endotoxin Synthesis (myristoyl transferase)	[c] : kdo2lipid4L + myrsACP --> ACP + lipa	Ann N Y Acad Sci. 2007, Gunn JS, Ernst RK	Required for Biomass Formation
FRUt2	D-fructose transport in via proton symport	fru[e] + h[e] --> fru[c] + h[c]	This study; transport needed for growth	
GLYCTO2	Glycolate oxidase	[c] : glyclt + ubq8 --> glx + ubq8h2	Essential for ubiquinone metabolism	Required for Biomass Formation
H2Ot5	H2O transport via diffusion	h2o[e] <==> h2o[c]	transport needed	
HISt6	L-histidine transport in via proton symport	h[e] + his-L[e] <==> h[c] + his-L[c]	Appl Microbiol. 1965 Mar;13:232-5.	Required for Biomass Formation
ILEt6	L-isoeucine transport in/out via proton symport	h[e] + ile-L[e] <==> h[c] + ile-L[c]	Appl Microbiol. 1965 Mar;13:232-5.	Required for Biomass Formation
LEUt6	L-leucine transport in/out via proton symport	h[e] + leu-L[e] <==> h[c] + leu-L[c]	Appl Microbiol. 1965 Mar;13:232-5.	Required for Biomass Formation
LPSSYN_EC	Lipopolysaccharide synthesis (Ecoli)	[c] : (3) adphep-L,D + (2) cdpea + (3) ckdo + lipa + (2) udpg --> (3) adp + (2) cdp + (3) cmp + (10) h + lps_EC + (2) udp	Ann N Y Acad Sci. 2007, Gunn JS, Ernst RK	Required for Biomass Formation
MALS	malate synthase	[c] : accoa + glx + h2o --> coa + h + mal-L	Anaplerotic Reactions	Required for Biomass Formation
MDRPD	5-Methylthio-5-deoxy-D-ribulose 1-phosphate dehydratase	[c] : 5mdru1p --> dkmpp + h2o	Essential for Arginine and Proline Metabolism	Required for Biomass Formation
NADPPPS	NADP phosphatase	[c] : h2o + nadp --> nad + pi	Cofactor and Prosthetic Group Biosynthesis	
NAt7	sodium transport in/out via proton antiport (one H+)	h[e] + na1[c] <==> h[c] + na1[e]	transport needed	
NH4t	ammonium transport via diffusion	nh4[e] <==> nh4[c]	Appl Microbiol. 1968 Jun;16(6):855-61	
NNATr	nicotinate-nucleotide adenylyltransferase	[c] : atp + h + nicrnt <==> dnad + ppi	Structure. 2008 Feb;16(2):196-209.	Required for Biomass Formation
NTD11	5'-nucleotidase (IMP)	[c] : h2o + imp --> ins + pi	Structure. 2008 Feb;16(2):196-209.	
NTD2	5'-nucleotidase (UMP)	[c] : h2o + ump --> pi + uri	Structure. 2008 Feb;16(2):196-209.	
NTD5	5'-nucleotidase (dTMP)	[c] : dtmp + h2o --> pi + thymd	Structure. 2008 Feb;16(2):196-209.	
NTD6	5'-nucleotidase (dAMP)	[c] : damp + h2o --> dad-2 + pi	Structure. 2008 Feb;16(2):196-209.	
NTD8	5'-nucleotidase (dGMP)	[c] : dgmp + h2o --> dgsn + pi	Structure. 2008 Feb;16(2):196-209.	
O2t	O2 transport in via diffusion	o2[e] <==> o2[c]	transport needed	Required for Biomass Formation
PAPSR	phosphoadenylyl-sulfate reductase (thioredoxin)	[c] : paps + trdrd --> (2) h + pap + so3 + trdox	Essential for Cysteine Metabolism	
PASYN_EC2	Phosphatidic acid synthase (Ecoli)	[c] : glyc3p + (0.14) hdeACP + (0.04) myrsACP + octeACP + (0.72) palmACP + (0.1) tdeACP--> (2) ACP + (0.02) pa_EC	Lipids. 1986 Oct;21(10):669-71.	
PGL	6-phosphogluconolactonase	[c] : 6pgl + h2o --> 6pgc + h	Pentose Phosphate Pathway	
PGPP_EC	Phosphatidylglycerol phosphate phosphatase (Ecoli)	[c] : h2o + (0.02) pgp_EC --> (0.02) pg_EC + pi	Lipids. 1986 Oct;21(10):669-71.	Required for Biomass Formation
PMDPHT	pyrimidine phosphatase	[c] : 5aprbu + h2o --> 4r5au + pi	Cofactor and Prosthetic Group Biosynthesis	Required for Biomass Formation
PPC	phosphoenolpyruvate carboxylase	[c] : co2 + h2o + pep --> h + oaa + pi	Anaplerotic Reactions	
PPTGS	Peptidoglycan subunit synthesis	[c] : uaagmda --> h + peptido_EC + udcpdp	Microbiology. 2007 Sep;153(Pt 9):3141-53	Required for Biomass Formation
RNTR4	ribonucleoside-triphosphate reductase (UTP)	[c] : trdrd + utp --> dutp + h2o + trdox	Nucleotide Salvage Pathway	Required for Biomass Formation
SDPDS	succinyl-diaminopimelate desuccinylase	[c] : h2o + sl26da --> 26dap-LL + succ	Essential for Threonine and Lysine Metabolism	Required for Biomass Formation
SDPTA	succinyldiaminopimelate transaminase	[c] : akg + sl26da <==> glu-L + sl2a6o	Essential for Threonine and Lysine Metabolism	
THDPS	tetrahydropicolinate succinylase	[c] : h2o + succoa + thdp --> coa + sl2a6o		Required for Biomass Formation
THRt6	L-threonine transport in/out via proton symporter	h[e] + thr-L[e] <==> h[c] + thr-L[c]	Appl Microbiol. 1965 Mar;13:232-5.	Required for Biomass Formation
UNK3	2-keto-4-methylthiobutyrate transamination	[c] : 2kmb + glu-L --> akg + met-L	Essential for Arginine and Proline Metabolism	Required for Biomass Formation
USHD	UDP-sugar hydrolase	[c] : h2o + u23ga --> (2) h + lipidX + ump	Lipopolysaccharide Biosynthesis / Recycling	Required for Biomass Formation
VALt6	L-valine transport in/out via proton symport	h[e] + val-L[e] <==> h[c] + val-L[c]	Appl Microbiol. 1965 Mar;13:232-5.	Required for Biomass Formation
ACS	acetyl-CoA synthetase	[c] : ac + atp + coa --> accoa + amp + ppi	Essential for Pyruvate Metabolism	probable pseudogene
ASPK	aspartate kinase	[c] : asp-L + atp <==> 4pasp + adp	Essential for Threonine and Lysine Metabolism	probable pseudogene
CBL1abc	Cob(1)alamin transport via ABC system	atp[c] + cbl1[e] + h2o[c] --> adp[c] + cbl1[c] + h[c] + pi[c]	transport needed	probable pseudogene
DPR	2-dehydropantoate 2-reductase	[c] : 2dhp + h + nadph --> nadp + pant-R	Cofactor and Prosthetic Group Biosynthesis	probable pseudogene
HSK	homoserine kinase	[c] : atp + hom-L --> adp + h + phom	Essential for Threonine and Lysine Metabolism	probable pseudogene
NTPP1	Nucleoside triphosphate pyrophosphorylase (dgtp)	[c] : dgtp + h2o --> dgmp + h + ppi	Structure. 2008 Feb;16(2):196-209.	probable pseudogene
NTPP2	Nucleoside triphosphate pyrophosphorylase (gtp)	[c] : gtp + h2o --> gmp + h + ppi	Structure. 2008 Feb;16(2):196-209.	probable pseudogene
NIabc	nickel transport via ABC system	atp[c] + h2o[c] + ni2[e] --> adp[c] + h[c] + ni2[c] + pi[c]	hypothetical protein	probable pseudogene
FT_Biomx_DM	Biomass Formation	0.05) 5mthf + (0.00005) accoa + (0.012208) ala-L + (0.001) amp + (0.002283) arg-L + (0.010908) asn-L + (0.014961) asp-L + (95.0) atp + (0.000006) coa + (0.126) ctp + (0.00031) cys-L + (0.0247) datp + (0.0254) dctp + (0.0254) dgtp + (0.0247) dttp + (0.00005) fad + (0.003829) gln-L + (0.004897) glu-L + (0.0256) gly + (0.154) glycogen + (0.203) gtp + (45.5608) h2o + (0.001611) his-L + (0.002764) ile-L + (0.004003) leu-L + (0.0084) lps_EC + (0.009342) lys-L + (0.001843) met-L + (0.00215) nad + (0.00005) nadh + (0.00013) nadp + (0.0004) nadph + (0.001935) pe_EC + (0.0276) peptido_EC + (0.000464) pg_EC + (0.002951) phe-L + (0.005615) pro-L + (0.000052) ps_EC + (0.035) ptrc + (0.007613) ser-L + (0.007) spmd + (0.000003) succoa + (0.006822) thr-L + (0.00192) trp-L + (0.00069) tyr-L + (0.003) udpg + (0.136) utp + (0.005443) val-L --> (95) adp + (95) h + (95) pi + (0.7302) ppi	Biomass Reaction	Required for Biomass Formation

Supplemental Data S1 D:

Metabolite Names, formula and Charges associated with the model database iRS605

METABOLITE ABBR	NAME	NEUTRAL FORMULA	CHARGE	KeggID
10fthf	10-Formyltetrahydrofolate	C20H23N7O7	-2	C00234
12ppd-S	(S)-Propane-1,2-diol	C3H8O2	0	C02917
13dpg	3-Phospho-D-glyceroyl phosphate	C3H8O10P2	-4	C00236
15dap	1,5-Diaminopentane	C5H14N2	2	C01672
1pyr5c	1-Pyrroline-5-carboxylate	C5H7NO2	-1	C03912
23camp	2',3'-Cyclic AMP	C10H12N5O6P	-1	C02353
23ccmp	2',3'-Cyclic CMP	C9H12N3O7P	-1	C02354
23cgmp	2',3'-Cyclic GMP	C10H12N5O7P	-1	C06194
23cump	2',3'-Cyclic UMP	C9H11N2O8P	-1	C02355
23ddhb	2,3-Dihydro-2,3-dihydroxybenzoate	C7H8O4	-1	C04171
23dhb	2,3-Dihydroxybenzoate	C7H6O4	-1	C00196
23dhba	(2,3-Dihydroxybenzoyl)adenylate	C17H18N5O10P	-1	C04030
23dhdp	2,3-Dihydrodipicolinate	C7H7NO4	-2	C03340
23dhmb	(R)-2,3-Dihydroxy-3-methylbutanoate	C5H10O4	-1	C04272
23dhmp	(R)-2,3-Dihydroxy-3-methylpentanoate	C6H12O4	-1	C06007
23doguln	2,3-Dioxo-L-gulonate	C6H8O7	-1	C04575
24dhhed	2,4-Dihydroxyhept-2-enedioate	C7H10O6	-2	
25aics	(S)-2-[5-Amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamido]succinate	C13H19N4O12P	-4	C04823
25dhpp	2,5-Diamino-6-hydroxy-4-(5'-phosphoribosylamino)-pyrimidine	C9H16N5O8P	-2	C01304
25dkglcn	2,5-diketo-D-gluconate	C6H8O7	-1	C02780
26dap-LL	LL-2,6-Diaminoheptanedioate	C7H14N2O4	0	C00666
26dap-M	meso-2,6-Diaminoheptanedioate	C7H14N2O4	0	C00680
2aeppn	(2-Aminoethyl)phosphonate	C2H8NO3P	-1	C03557
2ahbut	(S)-2-Aceto-2-hydroxybutanoate	C6H10O4	-1	C06006
2ahhmd	2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine diphosphate	C7H11N5O8P2	-3	C04807
2ahhmp	2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine	C7H9N5O2	0	C01300
2aobut	L-2-Amino-3-oxobutanoate	C4H7NO3	0	C03508
2cpr5p	1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose 5-phosphate	C12H16NO9P	-3	C01302
2dda7p	2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate	C7H13O10P	-3	C04691
2ddg6p	2-Dehydro-3-deoxy-D-gluconate 6-phosphate	C6H11O9P	-3	C04442
2ddglcn	2-Dehydro-3-deoxy-D-gluconate	C6H10O6	-1	C00204
2dh3dgal	2-Dehydro-3-deoxy-D-galactonate	C6H10O6	-1	C01216
2dh3dgal6p	2-Dehydro-3-deoxy-D-galactonate 6-phosphate	C6H11O9P	-3	C01286
2dhglcn	2-Dehydro-D-gluconate	C6H10O7	-1	C00629
2dhguln	2-Dehydro-L-gulonate	C6H10O7	-1	
2dhp	2-Dehydropantoate	C6H10O4	-1	C00966
2dmmq8	2-Demethylmenaquinone 8	C50H70O2	0	C05818
2dmmql8	2-Demethylmenaquinol 8	C50H72O2	0	
2dr1p	2-Deoxy-D-ribose 1-phosphate	C5H11O7P	-2	C00672
2dr5p	2-Deoxy-D-ribose 5-phosphate	C5H11O7P	-2	C00673
2h3opp	2-Hydroxy-3-oxopropanoate	C3H4O4	-1	C01146
2hh24dd	2-Hydroxyhepta-2,4-dienedioate	C7H8O5	-2	C05600
2ins	2-Inososе	C6H10O6	0	C00691
2ippm	2-Isopropylmaleate	C7H10O4	-2	C02631
2kmb	2-keto-4-methylthiobutyrate	C5H8O3S	-1	C01180
2mahmp	2-Methyl-4-amino-5-hydroxymethylpyrimidine diphosphate	C6H11N3O7P2	-3	C04752
2mcacn	cis-2-Methylaconitate	C7H8O6	-3	C04225
2mcit	2-Hydroxybutane-1,2,3-tricarboxylate	C7H10O7	-3	C02225
2me4p	2-C-methyl-D-erythritol 4-phosphate	C5H13O7P	-2	C11434
2mecdp	2-C-methyl-D-erythritol 2,4-cyclodiphosphate	C5H12O9P2	-2	C11453
2mop	2-Methyl-3-oxopropanoate	C4H6O3	-1	C00349
2obut	2-Oxobutanoate	C4H6O3	-1	C00109
2oh3d	2-Oxohept-3-ene-1,7-dioate	C7H8O5	-2	C03063
2ohph	2-Octaprenyl-6-hydroxyphenol	C46H70O2	0	C05811
2ombzl	2-Octaprenyl-6-methoxy-1,4-benzoquinol	C47H72O3	0	
2omhmbl	2-Octaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinol	C48H74O4	0	
2ommbl	2-Octaprenyl-3-methyl-6-methoxy- 1,4-benzoquinol	C48H74O3	0	
2omph	2-Octaprenyl-6-methoxyphenol	C47H72O2	0	C05812
2oph	2-Octaprenylphenol	C46H70O	0	C05810
2p4c2me	2-phospho-4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol	C14H26N3O17P3	-4	C11436
2pg	D-Glycerate 2-phosphate	C3H7O7P	-3	C00631
2pglyc	2-Phosphoglycolate	C2H5O6P	-3	C00988
2shchc	2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate	C11H12O6	-2	C05817
34dhpha	3,4-Dihydroxyphenylacetate	C8H8O4	-1	C01161
34hpp	3-(4-Hydroxyphenyl)pyruvate	C9H8O4	-1	C01179
36dahx	(3S)-3,6-Diaminohexanoate	C6H14N2O2	1	C01142
3amp	3'-AMP	C10H14N5O7P	-2	C01367
3c2hmp	3-Carboxy-2-hydroxy-4-methylpentanoate	C7H12O5	-2	C04411
3c3hmp	3-Carboxy-3-hydroxy-4-methylpentanoate	C7H12O5	-2	C02504
3c4mop	3-Carboxy-4-methyl-2-oxopentanoate	C7H10O5	-2	C04236
3cmp	3'-CMP	C9H14N3O8P	-2	C05822
3dgulnp	3-keto-L-gulonate-6-phosphate	C6H11O10P	-3	
3dhguln	3-Dehydro-L-gulonate	C6H10O7	-1	C00618
3dhq	3-Dehydroquinate	C7H10O6	-1	C00944
3dhsk	3-Dehydroshikimate	C7H8O5	-1	C02637
3gmp	Guanosine 3'-phosphate	C10H14N5O8P	-2	C06193
3hmp	3-Hydroxy-2-methylpropanoate	C4H8O3	-1	C01188
3htdACP	(3R)-3-Hydroxytetradecanoyl-[acyl-carrier protein]	C14H27O2X	0	C04688
3ig3p	C'-(3-Indolyl)-glycerol 3-phosphate	C11H14NO6P	-2	C03506
3mob	3-Methyl-2-oxobutanoate	C5H8O3	-1	C00141
3mop	(S)-3-Methyl-2-oxopentanoate	C6H10O3	-1	C00671
3ophb	3-Octaprenyl-4-hydroxybenzoate	C47H70O3	-1	C05809
3pg	3-Phospho-D-glycerate	C3H7O7P	-3	C00197
3php	3-Phosphohydroxypyruvate	C3H5O7P	-3	C03232
3psme	5-O-(1-Carboxyvinyl)-3-phosphoshikimate	C10H13O10P	-4	C01269
3ump	3'-UMP	C9H13N2O9P	-2	C01368
4abut	4-Aminobutanoate	C4H9NO2	0	C00334
4abutn	4-Aminobutanal		1	C00555
4abz	4-Aminobenzoate	C7H7NO2	-1	C00568
4adcho	4-amino-4-deoxychorismate	C10H11NO5	-1	C11355
4ahmmp	4-Amino-5-hydroxymethyl-2-methylpyrimidine	C6H9N3O	0	C01279
4ampm	4-Amino-2-methyl-5-phosphomethylpyrimidine	C6H10N3O4P	-2	C04556
4c2me	4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol	C14H25N3O14P2	-2	C11435
4hba	4-Hydroxy-benzyl alcohol	C7H8O2	0	
4hbz	4-Hydroxybenzoate	C7H6O3	-1	C00156
4hphac	4-Hydroxyphenylacetate	C8H8O3	-1	C00642
4hthr	4-Hydroxy-L-threonine	C4H9NO4	0	C06056
4izp	4-Imidazolone-5-propanoate	C6H8N2O3	-1	C03680
4mhetz	4-Methyl-5-(2-hydroxyethyl)-thiazole		0	C04294
4mop	4-Methyl-2-oxopentanoate	C6H10O3	-1	C00233
4mpetz	4-Methyl-5-(2-phosphoethyl)-thiazole	C6H10NO4PS	-2	C04327
4pasp	4-Phospho-L-aspartate	C4H8NO7P	-2	C03082
4per	4-Phospho-D-erythronate	C4H9O8P	-3	C03393
4ppan	D-4'-Phosphopantothenate	C9H18NO8P	-3	C03492
4ppcys	N-((R)-4-Phosphopantothenoyl)-L-cysteine	C12H23N2O9PS	-3	C04352
4r5au	4-(1-D-Ribitylamino)-5-aminouracil	C9H16N4O6	0	C04732
5aizc	5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate	C9H14N3O9P	-3	C04751
5aop	5-Amino-4-oxopentanoate	C5H9NO3	0	C00430

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5aprbu	5-Amino-6-(5'-phosphoribitylamino)uracil	C9H17N4O9P	-2	C04454
5apru	5-Amino-6-(5'-phosphoribosylamino)uracil	C9H15N4O9P	-2	C01268
5caiz	5-phosphoribosyl-5-carboxyaminoimidazole	C9H14N3O9P	-3	C04751
5cmhm	5-Carboxymethyl-2-hydroxymuconate	C8H8O7	-3	
5cmhmsa	5-Carboxymethyl-2-hydroxymuconate semialdehyde	C8H8O6	-2	
5cohe	5-Carboxy-2-oxohept-3-enedioate	C8H8O7	-3	
5d4dglcr	5-Dehydro-4-deoxy-D-glucarate	C6H8O7	-2	C00679
5dglcn	5-Dehydro-D-gluconate	C6H10O7	-1	C01062
5drib	5'-deoxyribose	C5H10O4	0	
5mdr1p	5-Methylthio-5-deoxy-D-ribose 1-phosphate	C6H13O7PS	-2	C04188
5mdru1p	5-Methylthio-5-deoxy-D-ribulose 1-phosphate	C6H13O7PS	-2	C04582
5mta	5-Methylthioadenosine	C11H15N5O3S	0	C00170
5mthf	5-Methyltetrahydrofolate	C20H25N7O6	-1	C00440
5mthglu	5-Methyltetrahydropteroyltri-L-glutamate	C25H36N8O12	-2	C04489
5mtr	5-Methylthio-D-ribose	C6H12O4S	0	C03089
5prdmbz	N1-(5-Phospho-alpha-D-ribosyl)-5,6-dimethylbenzimidazole	C14H19N2O7P	-2	C04778
6pgc	6-Phospho-D-gluconate	C6H13O10P	-3	C00345
6pgg	6-Phospho-beta-D-glucosyl-(1,4)-D-glucose	C12H23O14P	-2	C04534
6pgl	6-phospho-D-glucono-1,5-lactone	C6H11O9P	-2	C01236
6pthp	6-Pyruvoyl-5,6,7,8-tetrahydropterin	C9H11N5O3	0	C03684
8aonn	8-Amino-7-oxononanoate	C9H17NO3	0	C01092
ACP	acyl carrier protein	HX	0	C00229
L-alagly	L-alanylglycine	C5H10N2O3	0	
N1aspmd	N1-Acetylspermidine	C9H21N3O	2	C00612
N8aspmd	N8-Acetylspermidine	C9H21N3O	2	C01029
ac	Acetate	C2H4O2	-1	C00033
acACP	Acetyl-ACP	C2H3OX	0	C03939
acald	Acetaldehyde	C2H4O	0	C00084
accoa	Acetyl-CoA	C23H38N7O17P3S	-4	C00024
acg5p	N-Acetyl-L-glutamyl 5-phosphate	C7H12NO8P	-3	C04133
acg5sa	N-Acetyl-L-glutamate 5-semialdehyde	C7H11NO4	-1	C01250
acgam	N-Acetyl-D-glucosamine	C8H15NO6	0	C00140
acgam1p	N-Acetyl-D-glucosamine 1-phosphate	C8H16NO9P	-2	C04256
acgam6p	N-Acetyl-D-glucosamine 6-phosphate	C8H16NO9P	-2	C00357
acglu	N-Acetyl-L-glutamate	C7H11NO5	-2	C00624
acmana	N-Acetyl-D-mannosamine	C8H15NO6	0	C00645
acmanap	N-Acetyl-D-mannosamine 6-phosphate	C8H16NO9P	-2	C04257
acnam	N-Acetylneuraminate	C11H19NO9	-1	C00270
acon-C	cis-Aconitate	C6H6O6	-3	C00417
acorn	N2-Acetyl-L-ornithine	C7H14N2O3	0	C00437
acser	O-Acetyl-L-serine	C5H9NO4	0	C00979
actACP	Acetoacetyl-ACP	C4H5O2X	0	C05744
actp	Acetyl phosphate	C2H5O5P	-2	C00227
adcoba	Adenosyl cobinamide	C58H87CoN16O11	1	C06508
adcobap	Adenosyl cobinamide phosphate	C58H88CoN16O14P	-1	C06509
adcobdam	Adenosyl cobyrinate diamide	C55H76CoN11O15	-4	C06506
adcobhex	adenosyl-cobyric acid	C55H80CoN15O11	0	C06507
ade	Adenine	C5H5N5	0	C00147
adgcoba	Adenosine-GDP-cobinamide	C68H100CoN21O21P2	-1	C06510
adn	Adenosine	C10H13N5O4	0	C00212
adp	ADP	C10H15N5O10P2	-3	C00008
adpglc	ADPglucose	C16H25N5O15P2	-2	C00498
adphep-D,D	ADP-D-glycero-D-manno-heptose	C17H27N5O16P2	-2	C06397
adphep-L,D	ADP-L-glycero-D-manno-heptose	C17H27N5O16P2	-2	C06398
adprib	ADPribose	C15H23N5O14P2	-2	C00301
agm	Agmatine	C5H14N4	2	C00179
ahcys	S-Adenosyl-L-homocysteine	C14H20N6O5S	0	C00021
ahdt	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate	C9H16N5O13P3	-4	C04895
aicar	5-Amino-1-(5-Phospho-D-ribosyl)imidazole-4-carboxamide	C9H15N4O8P	-2	C04677
air	5-amino-1-(5-phospho-D-ribosyl)imidazole	C8H14N3O7P	-2	C03373
akg	2-Oxoglutarate	C5H6O5	-2	C00026
ala-B	beta-Alanine	C3H7NO2	0	C00099
ala-D	D-Alanine	C3H7NO2	0	C00133
ala-L	L-Alanine	C3H7NO2	0	C00041
ala-L-Thr-L	ala-L-Thr-L	C7H14N2O4	0	
ala-L-asp-L	ala-L-asp-L	C7H12N2O5	-1	
ala-L-gln-L	Ala-Gln	C8H15N3O4	0	
ala-L-glu-D	ala-L-glu-D	C8H14N2O5	-1	
ala-L-glu-D-dap	L-Ala-γ-D-Glu-diaminopimelate	C15H26N4O8	-1	
ala-L-glu-L	ala-L-glu-L	C8H14N2O5	-1	
ala-L-his-L	Ala-His	C9H14N4O3	0	
ala-L-leu-L	Ala-Leu	C9H18N2O3	0	
alaala	D-Alanyl-D-alanine	C6H12N2O3	0	C00993
alac-S	(S)-2-Acetolactate	C5H8O4	-1	C06010
alatrna	L-Alanyl-tRNA(Ala)	C3H6NO2X	1	C00886
alltn	Allantoin		0	C01551
alltt	Allantoate	C4H8N4O4	-1	C00499
amet	S-Adenosyl-L-methionine	C15H23N6O5S	1	C00019
ametam	S-Adenosylmethioninamine	C14H23N6O3S	2	C01137
amob	S-Adenosyl-4-methylthio-2-oxobutanoate	C15H20N5O6S	0	C04425
amopbut-L	2-Amino-3-oxo-4-phosphonooxybutyrate	C4H8NO7P	-2	C07335
amp	AMP	C10H14N5O7P	-2	C00020
ampcln	ampicillin	C16H19N3O4S	-1	
anth	Anthranilate	C7H7NO2	-1	C00108
aopp	3-Amino-2-oxopropyl phosphate	C3H8NO5P	-1	
ap4a	P1,P4-Bis(5'-adenosyl) tetraphosphate		-4	C01260
ap5a	P1,P5-Bis(5'-adenosyl) pentaphosphate	C20H29N10O22P5	-5	C04058
apoACP	apoprotein [acyl carrier protein]	RHO	0	C03688
applp	D-1-Aminopropan-2-ol O-phosphate	C3H10NO4P	-1	
aps	Adenosine 5'-phosphosulfate	C10H14N5O10PS	-2	C00224
ara5p	D-Arabinose 5-phosphate	C5H11O8P	-2	C01112
arab-L	L-Arabinose		0	C00259
arg-L	L-Arginine	C6H14N4O2	1	C00062
argsuc	N(omega)-(L-Arginino)succinate	C10H18N4O6	-1	C03406
argtrna	L-Arginyl-tRNA(Arg)	C6H13N4O2X	2	C02163
ascb	L-Ascorbate	C6H8O6	0	C00072
ascb6p	L-ascorbate-6-phosphate	C6H9O9P	-2	
asn-L	L-Asparagine	C4H8N2O3	0	C00152
asntrna	L-Asparaginyl-tRNA(Asn)	C4H7N2O3X	1	C03402
asp-D	D-Aspartate	C4H7NO4	-1	C00402
asp-L	L-Aspartate	C4H7NO4	-1	C00049
aspsa	L-Aspartate 4-semialdehyde	C4H7NO3	0	C00441
asptrna	L-Aspartyl-tRNA(Asp)	C4H6NO4X	0	C02984
atp	ATP	C10H16N5O13P3	-4	C00002
bbtcoa	gamma-butyrobetainyl-CoA	C28H50N8O17P3S	-3	
btn	Biotin	C10H16N2O3S	-1	C00120
btnso	d-biotin d-sulfoxide	C10H16N2O4S	-1	
cam	chloramphenicol	C11H12CL2N2O5	0	
camp	cAMP	C10H12N5O6P	-1	C00575
cbasp	N-Carbamoyl-L-aspartate	C5H8N2O5	-2	C00438
cbi	Cobinamide	C48H75CoN11O8	0	C05774

METABOLITE ABBR	NAME	NEUTRAL FORMULA	CHARGE	KeggID
cbl1	Cob(I)alamin	C62H93CoN13O14P	0	C00853
cbp	Carbamoyl phosphate	CH4NO5P	-2	C00169
cdp	CDP	C9H15N3O11P2	-3	C00112
cdpabe	CDP-abequose	C15H25N3O14P2	-2	
cdpdddg	CDP-4-dehydro-3,6-dideoxy-D-glucose	C15H23N3O14P2	-2	
cdpddg	CDP-4-dehydro-6-deoxy-D-glucose	C15H23N3O15P2	-2	
cdpglc	CDPglucose	C15H25N3O16P2	-2	
cell	Cellulose	C6H10O5	0	C00760
cellb	cellobiose	C12H22O11	0	C00185
cftxm	cefotaxime	C16H17N5O7S2	-1	
cgly	Cys-Gly	C5H10N2O3S	0	C01419
chit6p	chitobiose-6-phosphate	C16H29N2O14P	-2	
chitob	Chitobiose	C16H28N2O11	0	C01674
chor	Chorismate	C10H10O6	-2	C00251
cit	Citrate	C6H8O7	-3	C00158
citr-L	L-Citrulline	C6H13N3O3	0	C00327
ckdo	CMP-3-deoxy-D-manno-octulosonate	C17H26N3O15P	-2	C04121
cl	Chloride	Cl	-1	C00115
cmp	CMP	C9H14N3O8P	-2	C00055
co1dam	Cob(I)yrinate a,c diamide	C45H64CoN6O12	-4	C06505
co2	CO2	CO2	0	C00011
co2dam	Cob(II)yrinate a,c diamide	C45H64CoN6O12	-3	C06504
coa	Coenzyme A	C21H36N7O16P3S	-4	C00010
cobalt2	Co2+	Co	2	C00175
cobamcoa	Cobamide coenzyme	C72H105CoN18O17P	2	C00194
cobya	Cobyrinate	C45H58N4O14Co	-6	
codhpre6	Cobalt-dihydro-precorrin 6	C44H55CoN4O16	-7	C11543
copre2	cobalt-precorrin 2	C42H46N4O16Co	-8	C11538
copre3	cobalt-precorrin 3	C43H48N4O16Co	-8	C11539
copre4	cobalt-precorrin 4	C44H50N4O16Co	-7	C11540
copre5	cobalt-precorrin 5	C45H52N4O16Co	-7	C11541
copre6	Cobalt-precorrin 6	C44H53CoN4O16	-7	C11542
copre8	Cobalt-precorrin 8	C45H59CoN4O14	-6	C11545
cpfxn	ciprofloxacin	C17H18FN3O3	-1	
cpppg3	Coproporphyrinogen III	C36H44N4O8	-4	C03263
crn	L-Carnitine		0	C00318
crncoa	Carnitinyl-CoA	C28H50N8O18P3S	-3	
csn	Cytosine		0	C00380
ctbt	crotonobetaine	C7H14NO2	0	C04114
ctbtcoa	crotonobetainyl-CoA	C28H48N8O17P3S	-3	
ctp	CTP	C9H16N3O14P3	-4	C00063
cu1	Copper +1	Cu	1	
cu2	Cu2+	Cu	2	C00070
cyan	cyanide	HCN	0	C01326
cys-D	D-Cysteine		0	C00793
cys-L	L-Cysteine	C3H7NO2S	0	C00097
cysth-L	L-Cystathionine	C7H14N2O4S	0	C02291
cystrna	L-Cysteinyl-tRNA(Cys)	C3H6NO2SX	1	C03125
cytd	Cytidine		0	C00475
d5kg	2-Deoxy-5-keto-D-gluconic acid	C6H10O6	-1	
d5kgp	2-Deoxy-5-keto-D-gluconic acid 6-phosphate	C6H11O9P	-3	
dad-2	Deoxyadenosine		0	C00559
dad-5	5'-Deoxyadenosine	C10H13N5O3	0	C05198
dadp	dADP	C10H15N5O9P2	-3	C00206
damp	dAMP	C10H14N5O6P	-2	C00360
dann	7,8-Diaminononanoate	C9H20N2O2	1	C01037
datp	dATP	C10H16N5O12P3	-4	C00131
db4p	3,4-dihydroxy-2-butanone 4-phosphate	C4H9O6P	-2	
dcamp	N6-(1,2-Dicarboxyethyl)-AMP	C14H18N5O11P	-4	C03794
dcdp	dCDP	C9H15N3O10P2	-3	C00705
dcmp	dCMP	C9H14N3O7P	-2	C00239
dctp	dCTP	C9H16N3O13P3	-4	C00458
dcyt	Deoxycytidine		0	C00881
ddca	dodecanoate (C12:0)	C12H24O2	-1	C02679
ddcaACP	Dodecanoyl-ACP (n-C12:0ACP)	C12H23OX	0	
dgdp	dGDP	C10H15N5O10P2	-3	C00361
dgmp	dGMP	C10H14N5O7P	-2	C00362
dgsn	Deoxyguanosine	C10H13N5O4	0	C00330
dgtp	dGTP	C10H16N5O13P3	-4	C00286
dha	Dihydroxyacetone		0	C00184
dhap	Dihydroxyacetone phosphate	C3H7O6P	-2	C00111
dhf	7,8-Dihydrofolate	C19H21N7O6	-2	C00415
dhna	1,4-Dihydroxy-2-naphthoate	C11H8O4	-1	C03657
dhnpt	2-Amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine		0	C04874
dhor-S	(S)-Dihydroorotate	C5H6N2O4	-1	C00337
dhpmp	Dihydroneopterin monophosphate	C9H14N5O7P	-2	C05925
dhpt	Dihydropteroate	C14H14N6O3	-1	C00921
dhptd	4,5-dihydroxy-2,3-pentanedione	C5H8O4	0	C11838
din	Deoxyinosine		0	C05512
dkdglcn	2,5-Diketo-3-deoxy-D-gluconate	C6H8O6	-1	
dkdi	D-2,3-Diketo 4-deoxy-epi-inositol	C6H8O5	0	
dkmpp	2,3-diketo5-methylthio-1-phosphopentane	C6H11O6PS	-2	
dmbzid	5,6-Dimethylbenzimidazole	C9H10N2	0	C03114
dmlz	6,7-Dimethyl-8-(1-D-ribityl)lumazine	C13H18N4O6	0	C04332
dmpp	Dimethylallyl diphosphate	C5H12O7P2	-3	C00235
dms	Dimethyl sulfide	C2H6S	0	C00580
dmso	Dimethyl sulfoxide	C2H6OS	0	C11143
dnad	Deamino-NAD+	C21H27N6O15P2	-2	C00857
dpcoa	Dephospho-CoA	C21H35N7O13P2S	-2	C00882
drib	Deoxyribose	C5H10O4	0	C01801
dt5hsu	4-Deoxy-L-threo-5-hexosulose uronate	C6H8O6	-1	
dtbt	Dethiobiotin	C10H18N2O3	-1	C01909
dtdp	dTDP	C10H16N2O11P2	-3	C00363
dtdp4aaddg	dTDP-4-acetamido-4,6-dideoxy-D-galactose	C18H29N3O15P2	-2	
dtdp4addg	dTDP-4-amino-4,6-dideoxy-D-glucose	C16H27N3O14P2	-1	C04268
dtdpddg	dTDP-4-dehydro-6-deoxy-D-glucose	C16H24N2O15P2	-2	C00687
dtdpddm	dTDP-4-dehydro-6-deoxy-L-mannose	C16H24N2O15P2	-2	C00688
dtdpglc	dTDPglucose	C16H26N2O16P2	-2	C00842
dtdprmn	dTDP-6-deoxy-L-mannose	C16H26N2O15P2	-2	C03319
dtmp	dTMP	C10H15N2O8P	-2	C00364
dttp	dTTP	C10H17N2O14P3	-4	C00459
dudp	dUDP	C9H14N2O11P2	-3	C01346
dump	dUMP	C9H13N2O8P	-2	C00365
duri	Deoxyuridine		0	C00526
dutp	dUTP	C9H15N2O14P3	-4	C00460
dxyl	1-deoxy-D-xylulose	C5H10O4	0	C06257
dxyl5p	1-deoxy-D-xylulose 5-phosphate	C5H11O7P	-2	C11437
e4p	D-Erythrose 4-phosphate	C4H9O7P	-2	C00279
eca_EC	Enterobacterial common antigen polysaccharide (Ecoli)	C24H37N3O15	-1	
eig3p	D-erythro-1-(Imidazol-4-yl)glycerol 3-phosphate	C6H11N2O6P	-2	C04666

METABOLITE ABBR	NAME	NEUTRAL FORMULA	CHARGE	KeggID
enter	Enterochelin	C30H27N3O15	0	C05821
etha	Ethanolamine	C2H7NO	1	C00189
etoh	Ethanol		0	C00469
f1p	D-Fructose 1-phosphate	C6H13O9P	-2	C02976
f6p	D-Fructose 6-phosphate	C6H13O9P	-2	C00085
fad	FAD	C27H33N9O15P2	-2	C00016
fadh2	FADH2	C27H35N9O15P2	-2	C01352
fald	Formaldehyde		0	C00067
fc1p	L-Fuculose 1-phosphate	C6H13O8P	-2	C01099
fcl-L	L-fuculose	C6H12O5	0	C01721
fdp	D-Fructose 1,6-bisphosphate	C6H14O12P2	-4	C00354
fe2	Fe2+	Fe	2	C00023
ferrich	Ferrichrome	C24H38FeN9O11	0	C06228
fgam	N2-Formyl-N1-(5-phospho-D-ribosyl)glycinamide	C8H15N2O9P	-2	C04376
fglut-S	S-Formylglutathione	C11H17N3O7S	-1	C01031
fldox	flavodoxin (oxidized)	X	0	
fldrd	flavodoxin (reduced)	XH2	0	
flqn	fluoroquinolone deriv	C25H29FN4O4	-1	
fmet	N-Formyl-L-methionine	C6H11NO3S	-1	C03145
fmettrna	N-Formylmethionyl-tRNA	C6H10NO3SX	1	C03294
fmn	flavin mononucleotide	C17H21N4O9P	-2	C00061
for	Formate	CH2O2	-1	C00058
forglu	N-Formimidoyl-L-glutamate	C6H10N2O4	-1	C00439
fpram	2-(Formamido)-N1-(5-phospho-D-ribosyl)acetamidine	C8H16N3O8P	-2	C04640
fprica	5-Formamido-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide	C10H15N4O9P	-2	C04734
frdp	Farnesyl diphosphate	C15H28O7P2	-3	C00448
frmd	Formamide	CH3NO	0	C00488
fru	D-Fructose		0	C00095
fruur	D-Fructuronate	C6H10O7	-1	C00905
fuc-L	L-Fucose	C6H12O5	0	C01019
fum	Fumarate	C4H4O4	-2	C00122
g1p	D-Glucose 1-phosphate	C6H13O9P	-2	C00103
g3p	Glyceraldehyde 3-phosphate	C3H7O6P	-2	C00661
g3pe	sn-Glycero-3-phosphoethanolamine	C5H14NO6P	0	C01233
g3pg	Glycerophosphoglycerol	C6H15O8P	-1	C03274
g3ps	Glycerophosphoserine	C6H14NO8P	-1	
g6p	D-Glucose 6-phosphate	C6H13O9P	-2	C00092
gal	D-Galactose		0	C00124
gal1p	alpha-D-Galactose 1-phosphate	C6H13O9P	-2	C00446
galctn-D	D-Galactonate	C6H12O7	-1	C00880
galctr-D	D-Galactarate	C6H10O8	-2	C00879
galt	Galactitol	C6H14O6	0	C01697
galt1p	Galactitol 1-phosphate	C6H15O9P	-2	C06311
gam	D-Glucosamine	C6H13NO5	1	C00329
gam1p	D-Glucosamine 1-phosphate	C6H14NO8P	-1	C06156
gam6p	D-Glucosamine 6-phosphate	C6H14NO8P	-1	C00352
gar	N1-(5-Phospho-D-ribosyl)glycinamide	C7H15N2O8P	-1	C03838
gbbtn	gamma-butyrobetaine	C7H16NO2	0	C01181
gcald	Glycolaldehyde	C2H4O2	0	C00266
gdp	GDP	C10H15N5O11P2	-3	C00035
gdpddm	GDP-4-dehydro-6-deoxy-D-mannose	C16H23N5O15P2	-2	C01222
gdpdp	Guanosine 3',5'-bis(diphosphate)	C10H17N5O17P4	-6	C01228
gdpfuc	GDP-L-fucose	C16H25N5O15P2	-2	C00325
gdpman	GDP-D-mannose	C16H25N5O16P2	-2	C00096
gdpofuc	GDP-4-oxo-L-fucose	C16H23N5O15P2	-2	C05389
gdptp	Guanosine 3'-diphosphate 5'-triphosphate	C10H18N5O20P5	-7	C04494
glc-D	D-Glucose	C6H12O6	0	C00031
glcn-D	D-Gluconate	C6H12O7	-1	C00257
glcr	D-Glucarate	C6H10O8	-2	C00818
glcur	D-Glucuronate	C6H10O7	-1	C00191
gln-L	L-Glutamine	C5H10N2O3	0	C00064
glntrna	L-Glutaminyl-tRNA(Gln)	C5H9N2O3X	1	C02282
glu-D	D-Glutamate	C5H9NO4	-1	C00217
glu-L	L-Glutamate	C5H9NO4	-1	C00025
glu1sa	L-Glutamate 1-semialdehyde	C5H9NO3	0	C03741
glu5p	L-Glutamate 5-phosphate	C5H10NO7P	-2	C03287
glu5sa	L-Glutamate 5-semialdehyde	C5H9NO3	0	C01165
glucys	gamma-L-Glutamyl-L-cysteine	C8H14N2O5S	-1	C00669
glutrna	L-Glutamyl-tRNA(Glu)	C5H8NO4X	0	C02987
glx	Glyoxylate	C2H2O3	-1	C00048
gly	Glycine	C2H5NO2	0	C00037
gly-asn-L	gly-asn-L	C6H11N3O4	0	
gly-asp-L	gly-asp-L	C6H10N2O5	-1	
gly-gln-L	Gly-Gln	C7H13N3O4	0	
gly-glu-L	gly-glu-L	C7H12N2O5	-1	
gly-met-L	Gly-Met	C7H14N2O3S	0	
gly-pro-L	gly-pro-L	C7H12N2O3	0	
glyb	Glycine betaine	C5H11NO2	0	C00719
glyc	Glycerol	C3H8O3	0	C00116
glyc-R	(R)-Glycerate	C3H6O4	-1	C00258
glyc3p	sn-Glycerol 3-phosphate	C3H9O6P	-2	C00093
glyclt	Glycolate	C2H4O3	-1	C00160
glycogen	glycogen	C6H10O5	0	C00182
glytrna	Glycyl-tRNA(Gly)	C2H4NO2X	1	C02412
gmh17bp	D-Glycero-D-manno-heptose 1,7-bisphosphate	C7H16O13P2	-4	C11472
gmh1p	D-Glycero-D-manno-heptose 1-phosphate	C7H15O10P	-2	C07838
gmh7p	D-Glycero-D-manno-heptose 7-phosphate	C7H15O10P	-2	C07836
gmp	GMP	C10H14N5O8P	-2	C00144
gp4g	P1,P4-Bis(5'-guanosyl) tetraphosphate		-4	C01261
grdp	Geranyl diphosphate	C10H20O7P2	-3	C00341
gsn	Guanosine		0	C00387
gthox	Oxidized glutathione	C20H32N6O12S2	-2	C00127
gthrd	Reduced glutathione	C10H17N3O6S	-1	C00051
gtp	GTP	C10H16N5O14P3	-4	C00044
gtspmd	Glutathionylspermidine	C17H34N6O5S	2	C05730
gua	Guanine	C5H5N5O	0	C00242
h	H+	H	1	C00080
h2	H2	H2	0	C00282
h2mb4p	1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate	C5H12O8P2	-3	C11811
h2o	H2O	H2O	0	C00001
h2o2	Hydrogen peroxide	H2O2	0	C00027
h2s	Hydrogen sulfide	H2S	-1	C00283
hco3	Bicarbonate	CH2O3	-1	C00288
hcys-L	L-Homocysteine	C4H9NO2S	0	C00155
hdca	hexadecanoate (n-C16:0)	C16H32O2	-1	C00249
hdcea	hexadecenoate (n-C16:1)	C16H30O2	-1	
hdeACP	Hexadecenoyl-ACP (n-C16:1ACP)	C16H29OX	0	
hemeO	Heme O	C49H58FeN4O5	-2	
his-L	L-Histidine	C6H9N3O2	0	C00135
hisp	L-Histidinol phosphate	C6H12N3O4P	-1	C01100
histd	L-Histidinol	C6H11N3O	1	C00860

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histrna	L-Histidyl-tRNA(His)	C6H8N3O2X	1	C02988
hmbil	Hydroxymethylbilane	C40H46N4O17	-8	C01024
hmfurn	4-hydroxy-5-methyl-3(2H)-furanone	C5H6O3	0	
hom-L	L-Homoserine	C4H9NO3	0	C00263
hpyr	Hydroxypyruvate	C3H4O4	-1	C00168
hxan	Hypoxanthine	C5H4N4O	0	C00262
iasp	Iminoaspartate	C4H5NO4	-2	C05840
ichor	Isochorismate	C10H10O6	-2	C00885
icit	Isocitrate	C6H8O7	-3	C00311
idon-L	L-Idonate	C6H12O7	-1	C00770
idp	IDP	C10H14N4O11P2	-3	C00104
ile-L	L-Isoleucine	C6H13NO2	0	C00407
iletrna	L-Isoleucyl-tRNA(Ile)	C6H12NO2X	1	C03127
imacp	3-(Imidazol-4-yl)-2-oxopropyl phosphate	C6H9N2O5P	-1	C01267
imp	IMP	C10H13N4O8P	-2	C00130
indole	Indole	C8H7N	0	C00463
inost	myo-Inositol		0	C00137
ins	Inosine		0	C00294
ipdp	Isopentenyl diphosphate	C5H12O7P2	-3	C00129
itp	ITP	C10H15N4O14P3	-4	C00081
k	K+	K	1	C00238
kdo	3-Deoxy-D-manno-2-octulosonate	C8H14O8	-1	C01187
kdo2lipid4	KDO(2)-lipid IV(A)	C84H154N2O37P2	-6	C06025
kdo2lipid4L	KDO(2)-lipid IV(A) with laurate	C96H176N2O38P2	-6	C06251
kdo8p	3-Deoxy-D-manno-octulosonate 8-phosphate	C8H15O11P	-3	C04478
kdolipid4	KDO-lipid IV(A)		-5	C06024
lac-D	D-Lactate	C3H6O3	-1	C00256
lac-L	L-Lactate	C3H6O3	-1	C00186
lald-L	L-Lactaldehyde		0	C00424
leu-L	L-Leucine	C6H13NO2	0	C00123
leutrna	L-Leucyl-tRNA(Leu)	C6H12NO2X	1	C02047
lgt-S	(R)-S-Lactoylglutathione	C13H21N3O8S	-1	C03451
lipa	KDO(2)-lipid (A)	C110H202N2O39P2	-6	C06026
lipidA	2,3-Bis(3-hydroxytetradecanoyl)-D-glucosaminyl-1,6-beta-D-2,3-bis -(3-hydroxytetradecanoyl)-beta-D-glucosaminyl 1-phosphate	C68H129N2O2OP2	-4	C04932
lipidAds	Lipid A Disaccharide	C68H129N2O20P	-2	C04932
lipidX	2,3-Bis(3-hydroxytetradecanoyl)-beta-D-glucosaminyl 1-phosphate	C34H66NO12P	-2	C04824
llx	L-Lyxose	C5H10O5	0	
lys-L	L-Lysine	C6H14N2O2	1	C00047
lystrna	L-Lysine-tRNA (Lys)	C6H13N2O2X	2	C01931
mal-L	L-Malate	C4H6O5	-2	C00149
malACP	Malonyl-[acyl-carrier protein]	C3H3O3X	-1	C01209
malcoa	Malonyl-CoA	C24H38N7O19P3S	-5	C00083
malt	Maltose		0	C00208
malthp	Maltoheptaose	C42H72O36	0	
malthx	Maltohexaose	C36H62O31	0	C01936
maltpt	Maltopentaose	C30H52O26	0	
malttr	Maltotriose	C18H32O16	0	C01835
maltttr	Maltotetraose	C24H42O21	0	C02052
man	D-Mannose		0	C00159
man1p	D-Mannose 1-phosphate	C6H13O9P	-2	C03812
man6p	D-Mannose 6-phosphate	C6H13O9P	-2	C00275
mana	D-Mannonate	C6H12O7	-1	C00514
melib	Mellibiose		0	C05402
met-D	D-Methionine	C5H11NO2S	0	C00855
met-L	L-Methionine	C5H11NO2S	0	C00073
met-L-ala-L	met-L-ala-L	C8H16N2O3S	0	
methf	5,10-Methenyltetrahydrofolate	C20H22N7O6	-1	C00445
metox	L-Methionine S-oxide	C5H11NO3S	0	C02989
metox-R	L-methionine R-oxide	C5H11NO3S	0	
mettrna	L-Methionyl-tRNA (Met)	C5H10NO2SX	1	C02430
mg2	Mg	Mg	2	C00305
mi1p-D	1D-myo-Inositol 1-phosphate		-2	C01177
micit	Methylisocitrate	C7H10O7	-3	C04593
mlthf	5,10-Methylenetetrahydrofolate	C20H23N7O6	-2	C00143
mnl	D-Mannitol		0	C00392
mnl1p	D-Mannitol 1-phosphate	C6H15O9P	-2	C00644
mql8	Menaquinol 8	C51H74O2	0	C05819
mqn8	Menaquinone 8	C51H72O2	0	C00828
msa	Malonate semialdehyde	C3H4O3	-1	C00222
mthgxl	Methylglyoxal	C3H4O2	0	C00546
mtrp-N	N-methyltryptophan	C12H14N2O2	0	C02983
myrsACP	Myristoyl-ACP (n-C14:0ACP)	C14H27OX	0	
n2o	Nitrous oxide		0	C00887
na1	Sodium	Na	1	C01330
nac	Nicotinate	C6H5NO2	-1	C00253
nad	Nicotinamide adenine dinucleotide	C21H28N7O14P2	-1	C00003
nadh	Nicotinamide adenine dinucleotide - reduced	C21H29N7O14P2	-2	C00004
nadp	Nicotinamide adenine dinucleotide phosphate	C21H29N7O17P3	-3	C00006
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	C21H30N7O17P3	-4	C00005
ncam	Nicotinamide	C6H6N2O	0	C00153
nglut-S	S-Nitrosoglutathione	C10H15O7N4S	-2	
nh4	Ammonium	H4N	1	C01342
ni2	Ni2+	Ni	2	C00291
nicrnt	Nicotinate D-ribonucleotide	C11H15NO9P	-2	C01185
nmn	NMN		-1	C00455
no	Nitric oxide		0	C00533
no2	Nitrite	HNO2	-1	C00088
no3	Nitrate	HNO3	-1	C00244
o2	O2	O2	0	C00007
o2-	Superoxide	O2	-1	C00704
oaa	Oxaloacetate	C4H4O5	-2	C00036
ocdACP	Octadecanoyl-ACP (n-C18:0ACP)	C18H35OX	0	
ocdca	octadecanoate (n-C18:0)	C18H36O2	-1	C01530
ocdcea	octadecenoate (n-C18:1)	C18H34O2	-1	
ocdcte	Octadecatetraenoic acid (n-C18:4)	C18H28O2	-1	
ocdcteACP	Octadecatetraenoyl-ACP (n-C18:4ACP)		0	
ocdcya	octadecdienoate (n-C18:2)	C18H32O2	-1	
ocdcyaACP	Octadecynoyl-ACP (n-C18:2ACP)	C18H31OX	0	
octdp	all-trans-Octaprenyl diphosphate	C40H68O7P2	-3	C04146
octeACP	Octadecenoyl-ACP (n-C18:1ACP)	C18H33OX	0	
ohpb	2-Oxo-3-hydroxy-4-phosphobutanoate		-3	C06054
orn-L	L-Ornithine	C5H12N2O2	1	C00077
orot	Orotate	C5H4N2O4	-1	C00295
orot5p	Orotidine 5'-phosphate	C10H13N2O11P	-3	C01103
oxur	Oxalureate	C3H4N2O4	-1	
pald	phosphonoacetaldehyde	C2H5O4P	-2	
palmACP	Palmitoyl-ACP (n-C16:0ACP)	C16H31OX	0	
pan4p	Pantetheine 4'-phosphate	C11H23N2O7PS	-2	C01134
pant-R	(R)-Pantoate	C6H12O4	-1	C00522
pap	Adenosine 3',5'-bisphosphate	C10H15N5O10P2	-4	C00054

METABOLITE ABBR	NAME	NEUTRAL FORMULA	CHARGE	KeggID
paps	3'-Phosphoadenylyl sulfate	C10H15N5O13P2S	-4	C00053
pdx5p	Pyridoxine 5'-phosphate	C8H12NO6P	-2	C00627
peng	Penicillin G	C16H18N2O4S	-1	C05551
pep	Phosphoenolpyruvate	C3H5O6P	-3	C00074
phe-L	L-Phenylalanine	C9H11NO2	0	C00079
pheme	Protoheme	C34H32FeN4O4	-1	C00032
phetrna	L-Phenylalanyl-tRNA(Phe)	C9H10NO2X	1	C03511
phom	O-Phospho-L-homoserine	C4H10NO6P	-2	C01102
phpyr	Phenylpyruvate	C9H8O3	-1	C00166
phthr	O-Phospho-4-hydroxy-L-threonine	C4H10NO7P	-2	C06055
pi	Phosphate	H3O4P	-2	C00009
pime	Pimelate	C7H12O4	-2	C02656
pmcoa	Pimeloyl-CoA	C28H46N7O19P3S	-5	C01063
pnto-R	(R)-Pantothenate	C9H17NO5	-1	C00864
polypi	Polyphosphate	HO3P	0	C00890
ppa	Propionate	C3H6O2	-1	C00163
ppal	Propanal	C3H6O	0	C00479
ppap	Propanoyl phosphate	C3H7O5P	-2	C02876
ppbng	Porphobilinogen	C10H14N2O4	-1	C00931
ppcoa	Propanoyl-CoA	C24H40N7O17P3S	-4	C00100
pphn	Prephenate	C10H10O6	-2	C00254
ppi	Diphosphate	H4O7P2	-3	C00013
ppoh	Propanol	C3H8O	0	
ppp9	Protoporphyrin	C34H34N4O4	-2	C02191
pppg9	Protoporphyrinogen IX	C34H40N4O4	-2	C01079
pppi	Inorganic triphosphate	H5O10P3	-4	C03279
pppn	Phenylpropanoate	C9H10O2	-1	C05629
pram	5-Phospho-beta-D-ribosylamine	C5H12NO7P	-1	C03090
pran	N-(5-Phospho-D-ribosyl)anthranilate	C12H16NO9P	-3	C04302
prbamp	1-(5-Phosphoribosyl)-AMP	C15H23N5O14P2	-4	C02741
prbatp	1-(5-Phosphoribosyl)-ATP	C15H25N5O20P4	-6	C02739
prfp	1-(5-Phosphoribosyl)-5-[(5-phosphoribosylamino)methylideneamino]imidazole-4-carboxamide	C15H25N5O15P2	-3	C04896
prlp	5-[(5-phospho-1-deoxyribulos-1-ylamino)methylideneamino]-1-	C15H25N5O15P2	-3	C04916
pro-L	L-Proline	C5H9NO2	0	C00148
protrna	L-Prolyl-tRNA(Pro)	C5H8NO2X	1	C02702
prpp	5-Phospho-alpha-D-ribose 1-diphosphate	C5H13O14P3	-5	C00119
psd5p	Pseudouridine 5'-phosphate	C9H13N2O9P	-2	C01168
pser-L	O-Phospho-L-serine	C3H8NO6P	-2	C01005
ptrc	Putrescine	C4H12N2	2	C00134
pyam5p	Pyridoxamine 5'-phosphate	C8H13N2O5P	-2	C00647
pydam	Pyridoxamine	C8H12N2O2	0	C00534
pydx	Pyridoxal		0	C00250
pydx5p	Pyridoxal 5'-phosphate	C8H10NO6P	-3	C00018
pydxn	Pyridoxine		0	C00314
pyr	Pyruvate	C3H4O3	-1	C00022
quln	Quinolinate	C7H5NO4	-2	C03722
r1p	alpha-D-Ribose 1-phosphate	C5H11O8P	-2	C00442
r5p	alpha-D-Ribose 5-phosphate	C5H11O8P	-2	C00117
rbl-L	L-Ribulose	C5H10O5	0	C00508
rdmbzi	N1-(alpha-D-ribosyl)-5,6-dimethylbenzimidazole	C14H18N2O4	0	C05775
rhcys	S-Ribosyl-L-homocysteine	C9H17NO6S	0	C03539
rib-D	D-Ribose	C5H10O5	0	C00121
ribflv	Riboflavin	C17H20N4O6	0	C00255
rml	L-Rhamnulose	C6H12O5	0	C00861
rml1p	L-Rhamnulose 1-phosphate	C6H13O8P	-2	C01131
rmn	L-Rhamnose	C6H12O5	0	C00507
rnam	N-Ribosylnicotinamide	C11H15N2O5	1	C03150
ru5p-D	D-Ribulose 5-phosphate	C5H11O8P	-2	C00199
ru5p-L	L-Ribulose 5-phosphate	C5H11O8P	-2	C01101
s7p	Sedoheptulose 7-phosphate	C7H15O10P	-2	C00281
sbt-D	D-Sorbitol		0	C00794
sbt6p	D-Sorbitol 6-phosphate	C6H15O9P	-2	C01096
sbzcoa	O-Succinylbenzoyl-CoA	C32H44N7O20P3S	-5	C03160
seln	Selenide	H2Se	-1	C01528
selnp	Selenophosphate	H3O3PSe	-1	C05172
ser-D	D-Serine	C3H7NO3	0	C00740
ser-L	L-Serine	C3H7NO3	0	C00065
seramp	L-seryl-AMP	C13H19N6O9P	0	C05820
sertrna	L-Seryl-tRNA(Ser)	C3H6NO3X	1	C02553
shcl	dihydrosirohydrochlorin	C42H48N4O16	-7	C02463
sheme	Siroheme	C42H46FeN4O16	-8	C00748
skm	Shikimate	C7H10O5	-1	C00493
skm5p	Shikimate 5-phosphate	C7H11O8P	-3	C03175
sl26da	N-Succinyl-LL-2,6-diaminoheptanedioate	C11H18N2O7	-2	C04421
sl2a6o	N-Succinyl-2-L-amino-6-oxoheptanedioate	C11H15NO8	-3	C04462
slcys	S-Sulfo-L-cysteine	C3H7NO5S2	-1	C05824
so3	Sulfite	H2O3S	-2	C00094
so4	Sulfate	H2O4S	-2	C00059
spmd	Spermidine	C7H19N3	3	C00315
srch	sirohydrochlorin	C42H46N4O16	-8	C05778
ssaltpp	Succinate semialdehyde-thiamin diphosphate anion	C16H24N4O10P2S	-2	C05816
sucarg	N2-Succinyl-L-arginine	C10H18N4O5	-1	C03296
sucbz	o-Succinylbenzoate	C11H10O5	-2	C02730
succ	Succinate	C4H6O4	-2	C00042
succoa	Succinyl-CoA	C25H40N7O19P3S	-5	C00091
sucglu	N2-Succinyl-L-glutamate	C9H13NO7	-3	C05931
sucgsa	N2-Succinyl-L-glutamate 5-semialdehyde	C9H13NO6	-2	C05932
suchms	O-Succinyl-L-homoserine	C8H13NO6	-1	C01118
sucorn	N2-Succinyl-L-ornithine	C9H16N2O5	-1	C03415
sucsal	Succinic semialdehyde	C4H6O3	-1	C00232
tag6p-D	D-Tagatose 6-phosphate		-2	C01097
tagdp-D	D-Tagatose 1,6-biphosphate	C6H14O12P2	-4	C03785
tartr-D	D-Tartrate	C4H6O6	-2	C02107
tartr-L	L-tartarate	C4H6O6	-2	C00898
tcb	tricarballylate	C6H8O6	-3	
tcynt	Thiocyanate	CHNS	-1	C01755
thdp	2,3,4,5-Tetrahydrodipicolinate	C7H9NO4	-2	C03972
thf	5,6,7,8-Tetrahydrofolate	C19H23N7O6	-2	C00101
thglu	Tetrahydropteroyltri-L-glutamate	C24H34N8O12	-2	C04144
thm	Thiamin		1	C00378
thmmp	Thiamin monophosphate	C12H18N4O4PS	-1	C01081
thmpp	Thiamine diphosphate	C12H19N4O7P2S	-2	C00068
thr-L	L-Threonine	C4H9NO3	0	C00188
thrp	L-Threonine O-3-phosphate	C4H10NO6P	-2	C12147
thrtrna	L-Threonyl-tRNA(Thr)	C4H8NO3X	1	C02992
thym	Thymine		0	C00178
thymd	Thymidine	C10H14N2O5	0	C00214
tma	Trimethylamine	C3H9N	1	C00565
tmao	Trimethylamine N-oxide	C3H9NO	0	C01104
trdca	Tridecanoate	C13H26O2	-1	
trdox	Oxidized thioredoxin	X	0	C00343

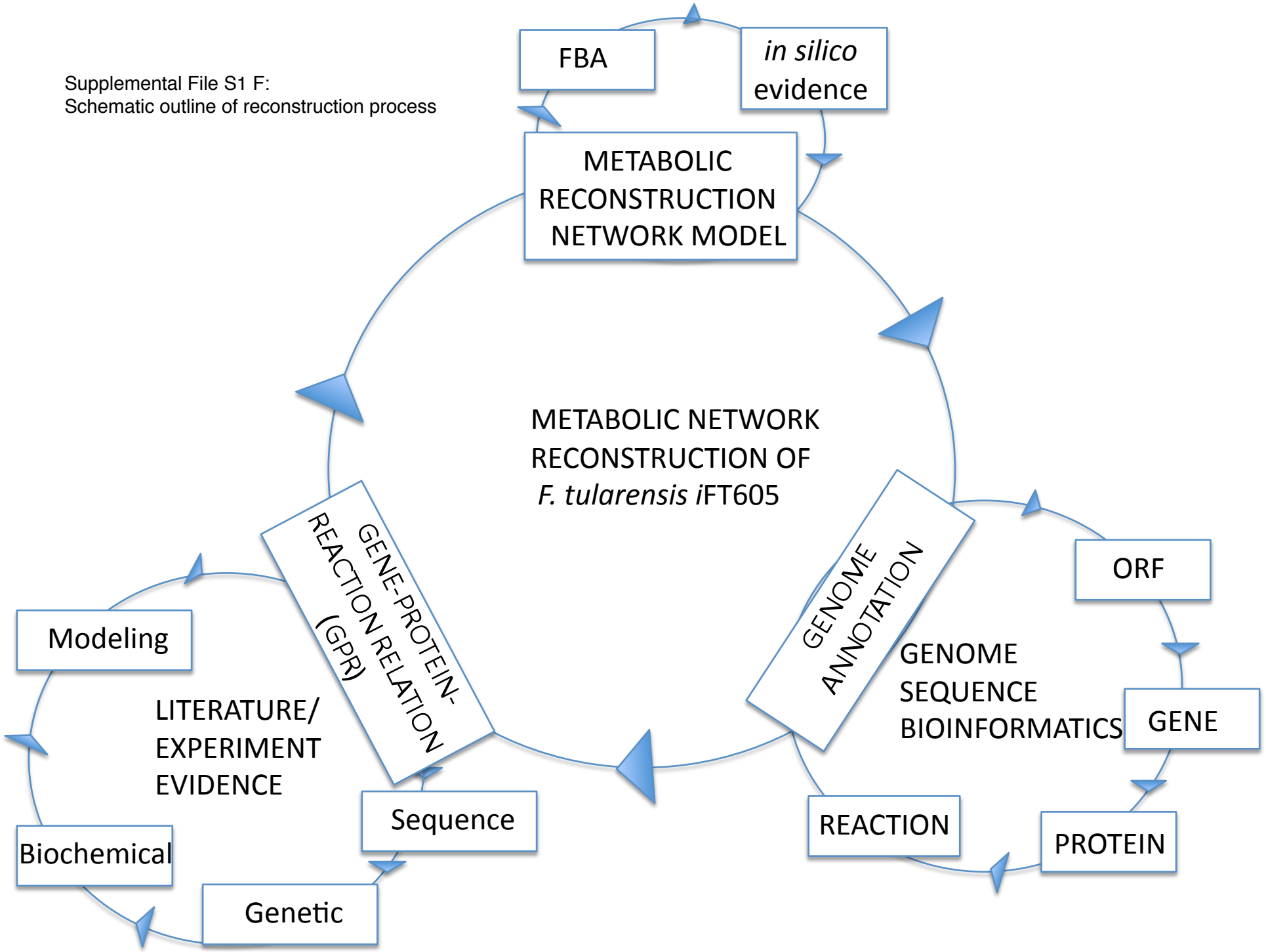
METABOLITE ABBR	NAME	NEUTRAL FORMULA	CHARGE	KeggID
trdrd	Reduced thioredoxin	XH2	0	C00342
tre	Trehalose	C12H22O11	0	C01083
tre6p	alpha,alpha'-Trehalose 6-phosphate	C12H23O14P	-2	C00689
trnaala	tRNA(Ala)	HOX	0	C01635
trnaarg	tRNA(Arg)	HOX	0	C01636
trnaasn	tRNA(Asn)	HOX	0	C01637
trnaasp	tRNA(Asp)	HOX	0	C01638
trnacys	tRNA(Cys)	HOX	0	C01639
trnagln	tRNA(Gln)	HOX	0	C01640
trnaglu	tRNA (Glu)	HOX	0	C01641
trnagly	tRNA(Gly)	HOX	0	C01642
trnahis	tRNA(His)	HOX	0	C01643
trnaile	tRNA(Ile)	HOX	0	C01644
trnaleu	tRNA(Leu)	HOX	0	C01645
trnalys	tRNA(Lys)	HOX	0	C01646
trnamet	tRNA(Met)	HOX	0	C01647
trnaphe	tRNA(Phe)	HOX	0	C01648
trnapro	tRNA(Pro)	HOX	0	C01649
trnaser	tRNA(Ser)	HOX	0	C01650
trnathr	tRNA(Thr)	HOX	0	C01651
trnatrp	tRNA(Trp)	HOX	0	C01652
trnatyr	tRNA(Tyr)	HOX	0	C00787
trnaval	tRNA(Val)	HOX	0	C01653
trp-L	L-Tryptophan	C11H12N2O2	0	C00078
trptrna	L-Tryptophanyl-tRNA(Trp)	C11H11N2O2X	1	C03512
tsul	Thiosulfate	H2O3S2	-2	C00320
ttdca	tetradecanoate (C14:0)	C14H28O2	-1	
tton	Trithionate	H2O6S3	-2	C01861
ttton	tetrathionate	H2O6S4	-2	C02084
tyr-L	L-Tyrosine	C9H11NO3	0	C00082
tyrtrna	L-Tyrosyl-tRNA(Tyr)	C9H10NO3X	1	C02839
u23ga	UDP-2,3-bis(3-hydroxytetradecanoyl)glucosamine	C43H77N3O20P2	-2	C04652
u3aga	UDP-3-O-(3-hydroxytetradecanoyl)-N-acetylglucosamine	C31H53N3O19P2	-2	C04738
u3hga	UDP-3-O-(3-hydroxytetradecanoyl)-D-glucosamine	C29H51N3O18P2	-1	C06022
uaagmda	Undecaprenyl-diphospho-N-acetylmuramoyl-(N-acetylglucosamine) -L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine	C95H156N8O28P2	-4	C05898
uaccg	UDP-N-acetyl-3-O-(1-carboxyvinyl)-D-glucosamine	C20H29N3O19P2	-3	C04631
uacgam	UDP-N-acetyl-D-glucosamine	C17H27N3O17P2	-2	C00043
uacmam	UDP-N-acetyl-D-mannosamine	C17H27N3O17P2	-2	C01170
uacmamu	UDP-N-acetyl-D-mannosaminouronate	C17H25N3O18P2	-3	C06240
uagmda	Undecaprenyl-diphospho-N-acetylmuramoyl-L-alanyl-D-glutamyl -meso-2,6-diaminopimeloyl-D-alanyl-D-alanine	C87H143N7O23P2	-4	C05897
uama	UDP-N-acetylmuramoyl-L-alanine	C23H36N4O20P2	-3	C01212
uamag	UDP-N-acetylmuramoyl-L-alanyl-D-glutamate	C28H43N5O23P2	-4	C00692
uamr	UDP-N-acetylmuramate	C20H31N3O19P2	-3	C01050
ubq8	Ubiquinone-8	C49H74O4	0	C00399
ubq8h2	Ubiquinol-8	C49H76O4	0	
udcpdp	Undecaprenyl diphosphate	C55H92O7P2	-3	C03543
udcpg	Undecaprenyl diphosphate galactose	C61H102O12P2	-2	
udcpgr	Undecaprenyl diphosphate galactose-rhamnose	C67H112O16P2	-2	
udcpgrm	π	C73H122O21P2	-2	
udcpo4	Undecaprenyl diphosphate galactose-rhamnose-mannose-abequose	C79H132O24P2	-2	
udcpo5	Undecaprenyl diphosphate galactose-rhamnose-mannose-abequose-acetyl	C81H134O25P2	-2	
udcpp	Undecaprenyl phosphate	C55H91O4P	-2	C00348
udp	UDP	C9H14N2O12P2	-3	C00015
udpara	Undecaprenyl-phosphate-4-amino-4-deoxy-L-arabinose	C60H100NO7P	0	
udpara4n	UDP-4-amino-4-deoxy-L-arabinose	C14H23N3O15P2	-1	
udpg	UDPglucose	C15H24N2O17P2	-2	C00029
udpgal	UDPgalactose	C15H24N2O17P2	-2	C00052
udpgalfur	UDP-D-galacto-1,4-furanose	C15H24N2O17P2	-2	C03733
udpglcur	UDP-D-glucuronate	C15H22N2O18P2	-3	C00167
udpkp	UDP-4-keto-pyranose	C14H21N2O16P2	-2	
ugmd	UDP-N-acetylmuramoyl-L-alanyl-D-gamma-glutamyl-meso-2,6-diaminopimelate	C35H55N7O26P2	-4	C04877
ugmda	UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine	C41H65N9O28P2	-4	C04882
ump	UMP	C9H13N2O9P	-2	C00105
unaga	Undecaprenyl diphospho N-acetyl-glucosamine	C63H105NO12P2	-2	
unagamu	Undecaprenyl-diphospho-N-acetylglucosamine-N-acetylmannosaminuronate	C71H116N2O18P2	-3	
unagamuf	Undecaprenyl-diphospho N-acetylglucosamine-N-acetylmannosaminuronate -N-acetamido-4,6-dideoxy-D-galactose	C79H129N3O22P2	-3	
uppg3	Uroporphyrinogen III	C40H44N4O16	-8	C01051
ura	Uracil	C4H4N2O2	0	C00106
urcan	Urocanate	C6H6N2O2	-1	C00785
urdglyc	(-)-Ureidoglycolate	C3H6N2O4	-1	C00603
urea	Urea		0	C00086
uri	Uridine		0	C00299
utp	UTP	C9H15N2O15P3	-4	C00075
val-L	L-Valine	C5H11NO2	0	C00183
valtrna	L-Valyl-tRNA(Val)	C5H10NO2X	1	C02554
xan	Xanthine		0	C00385
xmp	Xanthosine 5'-phosphate	C10H13N4O9P	-2	C00655
xtp	XTP	C10H15N4O15P3	-4	C00700
xtsn	Xanthosine		0	C01762
xu5p-D	D-Xylulose 5-phosphate	C5H11O8P	-2	C00231
xu5p-L	L-Xylulose 5-phosphate	C5H11O8P	-2	C03291
xyl-D	D-Xylose		0	C00181
xylu-D	D-Xylulose		0	C00310
xylu-L	L-Xylulose	C5H10O5	0	C00312

Supplemental Data S1 E:

Constraints represented as exchange reactions in the models for metabolites that are exchanged with extracellular media; upper bounds and lower bounds are specified based on appropriate media composition

Abbreviation	Equation	LB	UB
EX_arg-L(e)	[e] : arg-L <==>	-0.87	0
EX_asp-L(e)	[e] : asp-L <==>	-1.14	0
EX_cys-L(e)	[e] : cys-L <==>	-0.63	0
EX_his-L(e)	[e] : his-L <==>	-0.49	0
EX_ile-L(e)	[e] : ile-L <==>	-1.16	0
EX_leu-L(e)	[e] : leu-L <==>	-0.58	0
EX_lys-L(e)	[e] : lys-L <==>	-1.04	0
EX_met-L(e)	[e] : met-L <==>	-0.51	0
EX_o2(e)	[e] : o2 <==>	-2	0
EX_pro-L(e)	[e] : pro-L <==>	-6.61	0
EX_ser-L(e)	[e] : ser-L <==>	-1.45	0
EX_spmd(e)	[e] : spmd <==>	-0.04	0
EX_thr-L(e)	[e] : thr-L <==>	-0.64	0
EX_tyr-L(e)	[e] : tyr-L <==>	-0.42	0
EX_val-L(e)	[e] : val-L <==>	-1.3	0
EX_4abut(e)	[e] : 4abut <==>	0	Infinity
EX_acald(e)	[e] : acald <==>	0	Infinity
EX_acgam(e)	[e] : acgam <==>	0	Infinity
EX_adn(e)	[e] : adn <==>	0	Infinity
EX_ala-L-asp-L(e)	[e] : ala-L-asp-L <==>	0	Infinity
EX_ala-L-gln-L(e)	[e] : ala-L-gln-L <==>	0	Infinity
EX_ala-L-glu-L(e)	[e] : ala-L-glu-L <==>	0	Infinity
EX_ala-L-gly(e)	[e] : L-alagly <==>	0	Infinity
EX_ala-L-his-L(e)	[e] : ala-L-his-L <==>	0	Infinity
EX_ala-L-leu-L(e)	[e] : ala-L-leu-L <==>	0	Infinity
EX_ala-L-Thr-L(e)	[e] : ala-L-Thr-L <==>	0	Infinity
EX_alaala(e)	[e] : alaala <==>	0	Infinity
EX_bilea(e)	[e] : bilea <==>	0	Infinity
EX_buts(e)	[e] : buts <==>	0	Infinity
EX_cbl1(e)	[e] : cbl1 <==>	0	Infinity
EX_cgly(e)	[e] : cgly <==>	0	Infinity
EX_chol(e)	[e] : chol <==>	0	Infinity
EX_cytd(e)	[e] : cytd <==>	0	Infinity
EX_dad-2(e)	[e] : dad-2 <==>	0	Infinity
EX_dcyt(e)	[e] : dcyt <==>	0	Infinity
EX_duri(e)	[e] : duri <==>	0	Infinity
EX_eths(e)	[e] : eths <==>	0	Infinity
EX_fmn(e)	[e] : fmn <==>	0	Infinity
EX_fru(e)	[e] : fru <==>	0	Infinity
EX_fuc-L(e)	[e] : fuc-L <==>	0	Infinity
EX_fum(e)	[e] : fum <==>	0	Infinity
EX_gal(e)	[e] : gal <==>	0	Infinity
EX_galctr-D(e)	[e] : galctr-D <==>	0	Infinity
EX_glcn-D(e)	[e] : glcn-D <==>	0	Infinity
EX_glcr(e)	[e] : glcr <==>	0	Infinity
EX_glu-L(e)	[e] : glu-L <==>	0	Infinity
EX_gly(e)	[e] : gly <==>	0	Infinity
EX_gly-asn-L(e)	[e] : gly-asn-L <==>	0	Infinity
EX_gly-asp-L(e)	[e] : gly-asp-L <==>	0	Infinity
EX_gly-gln-L(e)	[e] : gly-gln-L <==>	0	Infinity
EX_gly-glu-L(e)	[e] : gly-glu-L <==>	0	Infinity
EX_gly-met-L(e)	[e] : gly-met-L <==>	0	Infinity
EX_gly-pro-L(e)	[e] : gly-pro-L <==>	0	Infinity
EX_glyb(e)	[e] : glyb <==>	0	Infinity
EX_glyc(e)	[e] : glyc <==>	0	Infinity
EX_glyc3p(e)	[e] : glyc3p <==>	0	Infinity
EX_gthox(e)	[e] : gthox <==>	0	Infinity
EX_gthrd(e)	[e] : gthrd <==>	0	Infinity
EX_gua(e)	[e] : gua <==>	0	Infinity
EX_h2o2(e)	[e] : h2o2 <==>	0	Infinity
EX_hexs(e)	[e] : hexs <==>	0	Infinity
EX_hxan(e)	[e] : hxan <==>	0	Infinity
EX_istnt(e)	[e] : istnt <==>	0	Infinity
EX_Lcyst(e)	[e] : Lcyst <==>	0	Infinity
EX_mal-L(e)	[e] : mal-L <==>	0	Infinity
EX_met-D(e)	[e] : met-D <==>	0	Infinity
EX_met-L-ala-L(e)	[e] : met-L-ala-L <==>	0	Infinity
EX_mops(e)	[e] : mops <==>	0	Infinity
EX_mso3(e)	[e] : mso3 <==>	0	Infinity
EX_ni2(e)	[e] : ni2 <==>	0	Infinity
EX_nmn(e)	[e] : nmn <==>	0	Infinity
EX_orn-L(e)	[e] : orn-L <==>	0	Infinity
EX_orot(e)	[e] : orot <==>	0	Infinity
EX_ptrc(e)	[e] : ptrc <==>	0	Infinity
EX_pur(e)	[e] : pur <==>	0	Infinity
EX_ribflv(e)	[e] : ribflv <==>	0	Infinity
EX_rnam(e)	[e] : rnam <==>	0	Infinity
EX_succ(e)	[e] : succ <==>	0	Infinity
EX_sucr(e)	[e] : sucr <==>	0	Infinity
EX_sula(e)	[e] : sula <==>	0	Infinity
EX_taur(e)	[e] : taur <==>	0	Infinity
EX_thymd(e)	[e] : thymd <==>	0	Infinity
EX_urea(e)	[e] : urea <==>	0	Infinity
EX_zn2(e)	[e] : zn2 <==>	0	Infinity
EX_cl(e)	[e] : cl <==>	-650	Infinity
EX_co2(e)	[e] : co2 <==>	0	Infinity
EX_fe2(e)	[e] : fe2 <==>	-0.01	Infinity
EX_glc(e)	[e] : glc-D <==>	-8.44	Infinity
EX_h(e)	[e] : h <==>	Infinity	Infinity
EX_h2o(e)	[e] : h2o <==>	Infinity	Infinity
EX_k(e)	[e] : k <==>	-4	Infinity
EX_na1(e)	[e] : na1 <==>	-650	Infinity
EX_nh4(e)	[e] : nh4 <==>	-1000	Infinity
EX_pi(e)	[e] : pi <==>	-4	Infinity
EX_so4(e)	[e] : so4 <==>	-100	Infinity

Supplemental File S1 F:
Schematic outline of reconstruction process



Supplemental Data S2. Dead end metabolites or gaps in iRS605

1. 15dap - 1,5-Diaminopentane
2. 1ag3p - 1-Acyl-sn-glycerol 3-phosphate
3. 2mop - 2-Methyl-3-oxopropanoate
4. 2ohph - 2-Octaprenyl-6-hydroxyphenol
5. 2ommbl - 2-Octaprenyl-3-methyl-6-methoxy- 1,4-benzoquinol
6. 34hpp - 3-(4-Hydroxyphenyl)pyruvate
7. 36dahx - (3S)-3,6-Diaminohexanoate
8. 3c3hmp - 3-Carboxy-3-hydroxy-4-methylpentanoate
9. 3hbycoa - (S)-3-Hydroxybutyryl-CoA
10. 3hdcoa - (S)-3-Hydroxydecanoyl-CoA
11. 3hddcoa - (S)-3-Hydroxydodecanoyl-CoA
12. 3hhcoa - (S)-3-Hydroxyhexanoyl-CoA
13. 3hhdcoa - (S)-3-Hydroxyhexadecanoyl-CoA
14. 3hocoa - (S)-3-Hydroxyoctanoyl-CoA
15. 3htdcoa - (S)-3-Hydroxytetradecanoyl-CoA
16. 3ophb - 3-Octaprenyl-4-hydroxybenzoate
17. 4hba - 4-Hydroxy-benzyl alcohol
18. 4mpetz - 4-Methyl-5-(2-phosphoethyl)-thiazole
19. 4mzym - 4alpha-Methylzymosterol
20. 5mthf - 5-Methyltetrahydrofolate
21. 6ampenc - 6-Aminopenicillanate
22. 6pgc - 6-Phospho-D-gluconate
23. Lcyst - L-Cysteate
24. acamoxm - N-Acetyl-L-2-amino-6-oxopimelate
25. acoa - Acyl-CoA
26. amob - S-Adenosyl-4-methylthio-2-oxobutanoate
27. ara4n-lipa - L-ara4N modified KDO2 Lipid A
28. bilea - Bile acid
29. btn - Biotin
30. buts - butanesulfonate
31. cbl1 - Cob(I)alamin
32. cbtnccp - Carboxybiotin-carboxyl-carrier protein
33. cer2'_24 - Ceramide-2' (Sphinganine:n-C24:0OH)
34. cer2'_26 - Ceramide-2' (Sphinganine:n-C26:0OH)
35. cer3_24 - Ceramide-3 (Phytosphingosine:n-C24:0OH)
36. cer3_26 - Ceramide-3 (Phytosphingosine:n-C26:0OH)
37. cholp - Choline phosphate
38. cl - Chloride
39. clpn_EC - Cardiolipin (Ecoli)
40. dad-5 - 5'-Deoxyadenosine
41. datp - dATP
42. dcyt - Deoxycytidine
43. dhlpro - Dihydrolipolprotein
44. dhpmp - Dihydroneopterin monophosphate
45. dimp - dIMP
46. dtdpddg - dTDP-4-dehydro-6-deoxy-D-glucose
47. etha - Ethanolamine
48. eths - ethanesulfonate
49. fdxr-4:2 - ferrodoxin (reduced form 4:2)
50. fmettrna - N-Formylmethionyl-tRNA
51. fol - Folate
52. fuc-L - L-Fucose
53. galctr-D - D-Galactarate
54. gdptp - Guanosine 3'-diphosphate 5'-triphosphate
55. glcr - D-Glucarate
56. glyald - D-Glyceraldehyde
57. glyb - Glycine betaine
58. hdcoa - Hexadecenoyl-CoA (n-C16:1CoA)
59. hexs - hexanesulfonate
60. hista - Histamine
61. hmbil - Hydroxymethylbilane
62. idp - IDP
63. inost - myo-Inositol
64. istnt - Isethionate
65. kdo2lipid4p - KDO(2)-lipid IV(A) with palmitoleoyl
66. lps_EC - lipopolysaccharide (Ecoli)
67. mannan(n+1) - mannan(n+1)
68. met-D - D-Methionine
69. mmalsa - (S)-Methylmalonate semialdehyde
70. mops - MOPS
71. mso3 - Methanesulfonate
72. ncam - Nicotinamide
73. nh3 - Ammonia
74. ni2 - Ni2+
75. nmn - NMN
76. odecoa - Octadecenoyl-CoA (n-C18:1CoA)
77. pamglyc - Palmitoylglycerone phosphate
78. pencilca - Penicilloic acid
79. peptido_EC - Peptidoglycan subunit of E.coli
80. pheme - Protoheme
81. ppap - Propanoyl phosphate
82. pppi - Inorganic triphosphate
83. protein_Eco - Protein, Escherichia coli
84. ps - Phosphatidylserine
85. purine - Purine
86. rhcys - S-Ribosyl-L-homocysteine
87. ribflvRD - Reduced riboflavin
88. sbzcoa - O-Succinylbenzoyl-CoA
89. sula - Sulfoacetate
90. taur - Taurine
91. tcynt - Thiocyanate
92. teich-45_BS - teichuronic acid (GlcA + GalNac, 45 repeating unit)
93. thfglu - Tetrahydrofolyl-[Glu](2)
94. thglu - Tetrahydropteroyltri-L-glutamate
95. thym - Thymine
96. trnaasn - tRNA(Asn)
97. uacmamu - UDP-N-acetyl-D-mannosaminouronate
98. unaga - Undecaprenyl diphospho N-acetyl-glucosamine
99. vralc - 3,4-Dimethoxybenzyl alcohol
100. xan - Xanthine
101. zn2 - Zinc
102. zymst - Zymosterol

Supplemental Data File S3:

Media composition: Chamberlain media components defined in mg/ml in vitro and as uptake rates or exchange fluxes in silico. Host cell environments for simulations were defined as exchange fluxes in vivo.

Chemical	MEDIA COMPOSITION CONCENTRATION /UPTAKE RATE		
	Chamberlain	in silico	in vivo
	mg/ml	mmol/gDW/hr	mmol/gDW/hr
L-Arginine	0.4	0.781609195	1
L-Valine	0.4	1.162393162	1
L-Isoleucine	0.4	1.038167939	1
L-Serine	0.4	1.295238095	1
L-Lysine HCl	0.4	0.931506849	1
Spermine diP	0.04	0.034170854	1
L-Proline	2	5.913043478	1
KH2PO4	1	2.5	1
K2HPO4	1	1.954022989	1
D-Glucose	4	7.555555556	1
L-Histidine	0.2	0.438709677	1
L-Tyrosine	0.2	0.375690608	1
L-Threonine	0.2	0.571428571	1
L-Methionine	0.2	0.456375839	1
L-Leucine	0.2	0.519083969	1
L-Cysteine HCl	0.2	0.561983471	1
L- Aspartic Acid	0.4	1.022556391	1
Sodium Chloride	100	582.1917808	1
Thiamine-HCl	0.004	0.004035608	1
MgSO4.7H2O	0.135	0.186206897	1
D-Ca-Pantothenate	0.002	0.001427072	1
FeSO4.7H2O	0.002	0.002446043	1
N-Acetyl-D-glucosamine	0	0	1
Adenosine	0	0	1
Deoxyadenosine	0	0	1
Deoxycytidine	0	0	1
fructose	0	0	1
fucose-L	0	0	1
galactose	0	0	1
D-Galactarate	0	0	1
D-Gluconate	0	0	1
D-Glucarate	0	0	1
glutamate-L	0	0	1
hypoxanthine	0	0	1
putrescine	0	0	1
thymidine	0	0	1
ala-ala	0	0	∞
bile acids	0	0	∞
choline	0	0	∞
cl	0	0	∞
flavin mononucleotide	0	0	∞
glutathione (Ox)	0	0	∞
h	0	0	∞
h2o	0	0	∞
k	0	0	∞
Lcyst	0	0	∞
na+	0	0	∞
o2	0	0	∞
Orotate	0	0	∞
Pi	0	0	∞
pur	0	0	∞
Riboflavin	0	0	∞
so4	0	0	∞
sucrose	0	0	∞
Sulfoacetate	0	0	∞
taurine	0	0	∞
zn2	0	0	∞

Supplemental Data File S4. Condition- independent lethal genes

GENE	RXN
1. FTL_0045	OMPDC
2. FTL_0058	TYRt6
3. FTL_0068	S7PI
4. FTL_0075	RBFSa, RBFSb
5. FTL_0076	GTPCII, DB4PS
6. FTL_0077	RBFSa, RBFSb
7. FTL_0078	APRAUR, DHPPDA2
8. FTL_0098	TRPS1, TRPS3, TRPS2
9. FTL_0099	TRPS1, TRPS3, TRPS2
10. FTL_0131	VALTA, PHETA1, LEUTAi, ILETA
11. FTL_0156	PIt6
12. FTL_0172	UAMAS
13. FTL_0223	DHFR, DHFOR2
14. FTL_0228	UDCPDPS, UDCPDP
15. FTL_0229	DASYN_EC
16. FTL_0231	PGSA_EC
17. FTL_0295	ACCOAC
18. FTL_0307	DPCOAK
19. FTL_0377	CHORS
20. FTL_0395	PRAIS
21. FTL_0396	PRASCS, PRAGS
22. FTL_0399	AIRC2, AIRC1
23. FTL_0412	UAPGR
24. FTL_0413	UAGCVT
25. FTL_0437	FMNAT, RBFK
26. FTL_0450	PSD_EC
27. FTL_0453	UAGDP, G1PACT
28. FTL_0463	MTRK, MTAN, AHCYSNS
29. FTL_0486	GLCS1
30. FTL_0490	UAAGDS
31. FTL_0492	UGMDDS
32. FTL_0494	ASADi, ASAD
33. FTL_0499	ADMDC
34. FTL_0500	SPMS
35. FTL_0507	ORPT
36. FTL_0537	U23GAAT
37. FTL_0538	C161SN, C141SN, C181SN
38. FTL_0539	UAGAAT
39. FTL_0540	LPADSS
40. FTL_0547	MOAT, MOAT2
41. FTL_0600	ASNS1
42. FTL_0626	NADK
43. FTL_0672	ASP1DC
44. FTL_0673	PANTS
45. FTL_0674	MOHMT
46. FTL_0685	NADS1
47. FTL_0747	GLUR
48. FTL_0777	AKP1
49. FTL_0795	ADNK1, DADK, ADK1
50. FTL_0801	SHKK
51. FTL_0802	DHQS
52. FTL_0808	PPNCL2, PPCDC
53. FTL_0837	METabc, METDabc
54. FTL_0838	METabc, METDabc
55. FTL_0852	PSCVT
56. FTL_0856	HCO3E
57. FTL_0949	PRPPS
58. FTL_0984	RNDR2, RNDR4, RNDR1, RNDR3
59. FTL_1017	CYTK2, CYTK1, UMPK
60. FTL_1061	PPA
61. FTL_1062	KDOPP
62. FTL_1071	GMPS2
63. FTL_1137	KAS16, ACMAT1, C181SN
64. FTL_1139	C161SN, C141SN, C181SN
65. FTL_1140	MCOATA
66. FTL_1141	ACOATA, KAS15
67. FTL_1145	TKT1, TKT2
68. FTL_1240	DAHPS
69. FTL_1253	GTPCI
70. FTL_1261	ANPRT
71. FTL_1262	ADCL, ADCS
72. FTL_1264	DHNPA
73. FTL_1265	HPPK, DHPS3
74. FTL_1308	THFGLUS, DHFS
75. FTL_1309	ACCOAC
76. FTL_1310	NDPK1, NDPK3, NDPK6, NDPK8, NDPK7, NDPK4, NDPK5, NDPK2
77. FTL_1311	CTPS2
78. FTL_1330	PTPAT
79. FTL_1336	PPNDH
80. FTL_1388	ASPO1, ASPO7, ASPO6
81. FTL_1389	NNDPR
82. FTL_1390	QULNS
83. FTL_1391	DGK1, GK1
84. FTL_1399	DMOCT
85. FTL_1410	UAGPT3
86. FTL_1433	A5PISO
87. FTL_1442	C161SN, C140SN, C141SN, C120SN, C160SN, C181SN
88. FTL_1478	IMPD
89. FTL_1535	KDOPS
90. FTL_1571	TRDR
91. FTL_1591	bCBXL, ACCOAC
92. FTL_1592	ACCOAC
93. FTL_1593	DHQD1
94. FTL_1614	UAMAGS
95. FTL_1615	PAPPT3
96. FTL_1660	DTMPK, URIDK2
97. FTL_1667	TDSK
98. FTL_1739	METAT
99. FTL_1781	PGAMT
100. FTL_1850	ADSL2r, ADSL1r
101. FTL_1860	PRFGS
102. FTL_1861	GLUPRT
103. FTL_1899	GLNS
104. FTL_1906	UHGADA
105. FTL_1929	IMPC, AICART
106. FTL_1958	IGPS, PRAIi

Supplemental Data S5. *In silico F. tularensis* Reactome present in the proteomic data set of Lenco (2009) in Chamberlain media with glucose

PROTEIN	GENE LOCI	RXN	EQUATION
Ade6	FTL_1860	PRFGS	[c] : atp + fgam + gln-L + h2o --> adp + fpram + glu-L + (2) h + pi
Adk	FTL_0795	ADK1	[c] : amp + atp <==> (2) adp
Adk	FTL_0795	ADK1	[c] : amp + atp <==> (2) adp
AroA	FTL_0852	PSCVT	[c] : pep + skm5p <==> 3psme + pi
AroB	FTL_0802	DHQS	[c] : 2dda7p --> 3dhq + pi
AroC	FTL_0377	CHORS	[c] : 3psme --> chor + pi
AroD	#N/A	DHQD1	[c] : 3dhq <==> 3dhsk + h2o
AroG	FTL_1240	DAHPS	[c] : e4p + h2o + pep --> 2dda7p + pi
AroK	FTL_0801	SHKK	[c] : atp + skm --> adp + h + skm5p
ArpI	FTL_1433	A5PISO	[c] : ru5p-D <==> ara5p
Cmk	FTL_1017	CYTK1	[c] : atp + cmp <==> adp + cdp
Cmk	FTL_1017	CYTK1	[c] : atp + cmp <==> adp + cdp
CoaD	FTL_1330	PTPAT	[c] : atp + h + pan4p <==> dpcoa + ppi
Dfp	FTL_0808	PPNCL2	[c] : 4ppan + ctp + cys-L --> 4ppcys + cmp + h + ppi
Dfp	FTL_0808	PPNCL2	[c] : 4ppan + ctp + cys-L --> 4ppcys + cmp + h + ppi
DfrA	FTL_0223	DHFR	[c] : dhf + h + nadph <==> nadp + thf
FabD	FTL_1140	MCOATA	[c] : ACP + malcoa <==> coa + malACP
FabF	FTL_1137	KAS16	[c] : ddcaACP + (2) h + malACP + nadph --> 3htdACP + ACP + co2 + nadp
FabI	FTL_1442	C120SN	[c] : actACP + (14) h + (4) malACP + (10) nadph --> (4) ACP + (4) co2 + ddcaACP + (5) h2o + (10) nadp
FabI	FTL_1442	C120SN	[c] : actACP + (14) h + (4) malACP + (10) nadph --> (4) ACP + (4) co2 + ddcaACP + (5) h2o + (10) nadp
FabI	FTL_1442	C120SN	[c] : actACP + (14) h + (4) malACP + (10) nadph --> (4) ACP + (4) co2 + ddcaACP + (5) h2o + (10) nadp
FolB	#N/A	DHNPA	[c] : dhnpt --> 2ahhmp + gcald
FolC	FTL_1308	DHFS	[c] : atp + dhpt + glu-L --> adp + dhf + h + pi
FolE	FTL_1253	GTPCI	[c] : gtp + h2o --> ahdt + for + h
FolP2	FTL_1265	HPPK	[c] : 2ahhmp + atp --> 2ahhmd + amp + h
FolP2	FTL_1265	HPPK	[c] : 2ahhmp + atp --> 2ahhmd + amp + h
GlgA	FTL_0486	GLCS1	[c] : adpglc --> adp + glycogen + h
GlmS	FTL_0454	GF6PTA	[c] : f6p + gln-L --> gam6p + glu-L
GlmU	FTL_0453	UAGDP	[c] : acgam1p + h + utp --> ppi + uacgam
GlmU	FTL_0453	UAGDP	[c] : acgam1p + h + utp --> ppi + uacgam
Gln1	FTL_1899	GLNS	[c] : atp + glu-L + nh4 --> adp + gln-L + h + pi
GmhA	FTL_0068	S7PI	[c] : s7p <==> gmh7p
Gmk	FTL_1391	GK1	[c] : atp + gmp <==> adp + gdp
GuaA	FTL_1071	GMPS2	[c] : atp + gln-L + h2o + xmp --> amp + glu-L + gmp + (2) h + ppi
GuaB	FTL_1478	IMPD	[c] : h2o + imp + nad --> h + nadh + xmp
KdoP	FTL_1062	KDOPP	[c] : h2o + kdo8p --> kdo + pi
KdsA	FTL_1535	KDOPS	[c] : ara5p + h2o + pep --> kdo8p + pi
KdsB	FTL_1399	DMOCT	[c] : ctp + kdo --> ckdo + ppi
KdtA	FTL_0547	MOAT2	[c] : ckdo + kdolipid4 --> cmp + h + kdo2lipid4
KdtA	FTL_0547	MOAT2	[c] : ckdo + kdolipid4 --> cmp + h + kdo2lipid4
LpxB	FTL_0540	LPADSS	[c] : lipidX + u23ga --> h + lipidAds + udp
LpxC	FTL_1906	UHGADA	[c] : h2o + u3aga --> ac + u3hga
LpxD	FTL_0537	U23GAAT	[c] : 3htdACP + u3hga --> ACP + h + u23ga
LpxK	FTL_1667	TDSK	[c] : atp + lipidAds --> adp + h + lipidA
MetK	FTL_1739	METAT	[c] : atp + h2o + met-L --> amet + pi + ppi
MraY	FTL_1615	PAPPT3	[c] : udcpp + ugmda --> uagmda + ump
Mtn	FTL_0463	MTRK	[c] : 5mtr + atp --> 5mdr1p + adp + h
Mtn	FTL_0463	MTRK	[c] : 5mtr + atp --> 5mdr1p + adp + h
MurB	FTL_0412	UAPGR	[c] : h + nadph + uaccg --> nadp + uamr
MurD	FTL_1614	UAMAGS	[c] : atp + glu-D + uama --> adp + h + pi + uamag
MurE	FTL_0490	UAAGDS	[c] : 26dap-M + atp + uamag --> adp + h + pi + ugmd
MurFec	FTL_0492	UGMDDS	[c] : alaala + atp + ugmd --> adp + h + pi + ugmda
MurG	FTL_1410	UAGPT3	[c] : uacgam + uagmda --> h + uaagmda + udp
NadA	FTL_1390	QULNS	[c] : dhap + iasp --> (2) h2o + pi + quln
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
Ndk	FTL_1310	NDPK8	[c] : atp + dadp <==> adp + datp
PabABC	FTL_1262	ADCL	[c] : 4adcho --> 4abz + h + pyr
PabABC	FTL_1262	ADCL	[c] : 4adcho --> 4abz + h + pyr
PanB	FTL_0674	MOHMT	[c] : 3mob + h2o + mlthf --> 2dhp + thf
PanCec	FTL_0673	PANTS	[c] : ala-B + atp + pant-R --> amp + h + pnto-R + ppi
PheA	FTL_1336	PPNDH	[c] : h + pphn --> co2 + h2o + phpyr
Ppa	FTL_1061	PPA	[c] : h2o + ppi --> h + (2) pi
PrsA	FTL_0949	PRPPS	[c] : atp + r5p <==> amp + h + prpp
Psd	FTL_0450	PSD_EC	[c] : h + (0.02) ps_EC --> co2 + (0.02) pe_EC
PurB	FTL_1850	ADSL2r	[c] : 25aics <==> aicar + fum
PurB	FTL_1850	ADSL2r	[c] : 25aics <==> aicar + fum
PurD	FTL_0396	PRASCS	[c] : 5aizc + asp-L + atp <==> 25aics + adp + h + pi
PurD	FTL_0396	PRASCS	[c] : 5aizc + asp-L + atp <==> 25aics + adp + h + pi
PurF	FTL_1861	GLUPRT	[c] : gln-L + h2o + prpp --> glu-L + ppi + pram
PurH	FTL_1929	AICART	[c] : 10fthf + aicar <==> fprica + thf
PurM	FTL_0395	PRAIS	[c] : atp + fpram --> adp + air + h + pi
PyrF	FTL_0045	OMPDC	[c] : h + orot5p --> co2 + ump
PyrG	FTL_1311	CTPS2	[c] : atp + gln-L + h2o + utp --> adp + ctp + glu-L + (2) h + pi
RibA	FTL_0076	GTPCII	[c] : gtp + (3) h2o --> 25dhpp + for + (2) h + ppi
RibA	FTL_0076	GTPCII	[c] : gtp + (3) h2o --> 25dhpp + for + (2) h + ppi
RibD	FTL_0078	DHPPDA2	[c] : 25dhpp + h + h2o --> 5apru + nh4
RibD	FTL_0078	DHPPDA2	[c] : 25dhpp + h + h2o --> 5apru + nh4
RibFec	FTL_0437	FMNAT	[c] : atp + fmn + h --> fad + ppi
Rnr12	FTL_0984	RNDR3	[c] : cdp + trdrd --> dcdp + h2o + trdox
Rnr12	FTL_0984	RNDR3	[c] : cdp + trdrd --> dcdp + h2o + trdox
Rnr12	FTL_0984	RNDR3	[c] : cdp + trdrd --> dcdp + h2o + trdox
Tmk	FTL_1660	DTMPK	[c] : atp + dtmp <==> adp + dtdp
TrpCec	FTL_1958	PRAIi	[c] : pran --> 2cpr5p
TrpCec	FTL_1958	PRAIi	[c] : pran --> 2cpr5p
TrxB	FTL_1571	TRDR	[c] : h + nadph + trdox --> nadp + trdrd
UppS	FTL_0228	UDCPDP	[c] : h2o + udcpdp --> h + pi + udcpp
WbtH	FTL_0600	ASNS1	[c] : asp-L + atp + gln-L + h2o --> amp + asn-L + glu-L + h + ppi

Supplemental Data S5. *In silico F. tularensis* Reactome present in the transcriptomic data set of Deng (2006) in Chamberlain media with glucose

PROTEIN	GENE LOCI	RXN	EQUATION
Ade6	FTL_1860	PRFGS	[c] : atp + fgam + gln-L + h2o --> adp + fpram + glu-L + (2) h + pi
Adk	FTL_0795	ADK1	[c] : amp + atp <==> (2) adp
AroB	FTL_0802	DHQS	[c] : 2dda7p --> 3dhq + pi
AroK	FTL_0801	SHKK	[c] : atp + skm --> adp + h + skm5p
CoaE	FTL_0307	DPCOAK	[c] : atp + dpcoa --> adp + coa + h
Dfp	FTL_0808	PPNCL2	[c] : 4ppan + ctp + cys-L --> 4ppcys + cmp + h + ppi
Dfp	FTL_0808	PPNCL2	[c] : 4ppan + ctp + cys-L --> 4ppcys + cmp + h + ppi
DidalaABC		DIDALAabc	alaala[e] + atp[c] + h2o[c] --> adp[c] + alaala[c] + h[c] + pi[c]
FabD	FTL_1140	MCOATA	[c] : ACP + malcoa <==> coa + malACP
FabF	FTL_1137	KAS16	[c] : ddcaACP + (2) h + malACP + nadph --> 3htdACP + ACP + co2 + nadp
GlyA	FTL_0703	ALATA_L	[c] : akg + ala-L <==> glu-L + pyr
GmhA	FTL_0068	S7PI	[c] : s7p <==> gmh7p
Gmk	FTL_1391	GK1	[c] : atp + gmp <==> adp + gdp
GuaA	FTL_1071	GMPS2	[c] : atp + gln-L + h2o + xmp --> amp + glu-L + gmp + (2) h + ppi
GuaB	FTL_1478	IMPD	[c] : h2o + imp + nad --> h + nadh + xmp
KdoP	FTL_1062	KDOPP	[c] : h2o + kdo8p --> kdo + pi
KdsB	FTL_1399	DMOCT	[c] : ctp + kdo --> ckdo + ppi
KdtA	FTL_0547	MOAT2	[c] : ckdo + kdolipid4 --> cmp + h + kdo2lipid4
KdtA	FTL_0547	MOAT2	[c] : ckdo + kdolipid4 --> cmp + h + kdo2lipid4
LpxA	FTL_0539	UAGAAT	[c] : 3htdACP + uacgam <==> ACP + u3aga
LpxB	FTL_0540	LPADSS	[c] : lipidX + u23ga --> h + lipidAds + udp
LpxD	FTL_0537	U23GAAT	[c] : 3htdACP + u3hga --> ACP + h + u23ga
MurAA	FTL_0413	UAGCVT	[c] : pep + uacgam --> pi + uaccg
MurB	FTL_0412	UAPGR	[c] : h + nadph + uaccg --> nadp + uamr
NadA	FTL_1390	QULNS	[c] : dhap + iasp --> (2) h2o + pi + quln
NadCec	FTL_1389	NNDPR	[c] : (2) h + prpp + quln --> co2 + nicrnt + ppi
NadE		NADS1	[c] : atp + dnad + nh4 --> amp + h + nad + ppi
PanB	FTL_0674	MOHMT	[c] : 3mob + h2o + mlthf --> 2dhp + thf
PanCec	FTL_0673	PANTS	[c] : ala-B + atp + pant-R --> amp + h + pnto-R + ppi
PanD		ASP1DC	[c] : asp-L + h --> ala-B + co2
PurF	FTL_1861	GLUPRT	[c] : gln-L + h2o + prpp --> glu-L + ppi + pram
PyrF	FTL_0045	OMPDC	[c] : h + orot5p --> co2 + ump
RibA	FTL_0076	GTPCII	[c] : gtp + (3) h2o --> 25dhpp + for + (2) h + ppi
RibA	FTL_0076	GTPCII	[c] : gtp + (3) h2o --> 25dhpp + for + (2) h + ppi
RibD	FTL_0078	DHPPDA2	[c] : 25dhpp + h + h2o --> 5apru + nh4
RibD	FTL_0078	DHPPDA2	[c] : 25dhpp + h + h2o --> 5apru + nh4
TrpCec	FTL_1958	PRAIi	[c] : pran --> 2cpr5p
TrpCec	FTL_1958	PRAIi	[c] : pran --> 2cpr5p
TyrP		TYRt6	h[e] + tyr-L[e] <==> h[c] + tyr-L[c]
WbtH	FTL_0600	ASNS1	[c] : asp-L + atp + gln-L + h2o --> amp + asn-L + glu-L + h + ppi
YfjB	FTL_0626	NADK	[c] : atp + nad --> adp + h + nadp

Supplemental Data S6: Selected metabolic gene set chosen for gene expression or mRNA transcript level detection in F. tularensis extracted from macrophages post infection using GEXP

Gene #	Gene Name
FTL_1789	citrate synthase
FTL_1149	fructose-1,6-bisphosphate aldolase
FTL_1476	glucose-6-phosphate isomerase
FTL_1284	glutathione synthetase
FTL_0438	NAD-dependent malic enzyme
FTL_1887	3-isopropylmalate dehydrogenase
FTL_0766	gamma-glutamyltranspeptidase
FTL_1296	amino acid antiporter;
FTL_1863	glutamate decarboxylase
FTL_1701	GlpX protein
FTL_1148	pyruvate kinase
FTL_0588	isocitrate dehydrogenase
FTL_0294	DNA mismatch repair protein MutS
FTL_0404	glucose kinase
FTL_0001	chromosomal replication initiator protein DnaA
FTL_1616	phosphoenolpyruvate carboxykinase
FTL_0583	3-ketoacyl-CoA thiolase
FTL_1146	glyceraldehyde-3-phosphate dehydrogenase
FTL_0585	acyl-CoA dehydrogenase
FTL_1147	phosphogylcerate kinase
FTL_0586	long chain fatty acid CoA ligase
FTL_0273	glutamate/gamma-aminobutyrate anti-porter
FTL_0501	putative arginine decarboxylase
FTL_1504	peroxidase/catalase
FTL_0484	phosphoglucomutase
FTL_1233	amino acid antiporter;
FTL_1304	glutamate--cysteine ligase
FTL_0132	phosphoenolpyruvate synthase/pyruvate phosphate dikinase
FTL_0472	DNA polymerase III alpha subunit
FTL_1383	glutathione peroxidase
FTL_0648	aminotransferase
FTL_0649	aspartate/tyrosine/aromatic aminotransferase family protein
FTL_1428	ABC transporter, ATP-binding and membrane protein
FTL_1782	adenine phosphoribosyltransferase
FTL_1823	NADH dehydrogenase I, H subunit
FTL_0328	chorismate mutase

Gene #	Gene Name
FTL_0191	cytochrome o ubiquinol oxidase subunit II
FTL_1765	cytochrome oxidase bd-II, subunit II
FTL_1861	amidophosphoribosyltransferase
FTL_0377	chorismate synthase
FTL_0788	glutamine amidotransferases class-II family protein;
FTL_1899	glutamine synthetase
FTL_0131	branched-chain amino acid aminotransferase protein (class IV)
FTL_0195	protoheme IX farnesyltransferase
FTL_1795	ATP synthase beta chain
FTL_1495	ABC transporter, ATP-binding and membrane protein
FTL_0624	ABC transporter, membrane protein
FTL_1788	succinate dehydrogenase, cytochrome b556
FTL_0409	purine/pyrimidine phosphoribosyl transferase family protein
FTL_0405	menaquinone biosynthesis methyltransferase
FTL_1966	anthranilate synthase component I [
FTL_1797	ATP synthase alpha chain
FTL_0801	shikimate kinase
FTL_1261	anthranilate synthase component II
FTL_0356	hypothetical protein
FTL_1791	superoxide dismutase [Fe]
FTL_1492	Fructokinase
FTL_1966	anthranilate synthase component I
FTL_0028	aspartate carbamoyltransferase
FTL_0328	chorismate mutase II
FTL_1309	Acetyl-CoA carboxylase beta subunit
FTL_1272	biotin synthase
FTL0805	bifunctional proline dehydrogenase,pyrroline-5-carboxylate dehydrogenase
FTL_1146	Glyceraldehyde-3-phosphate dehydrogenase
FTL_1570	Phospholipase D family protein.
FTL_0043	chorismate mutase I
FTT1498	acetyl-coenzyme A carboxylase carboxyl transferase subunit alpha
FTL_0478	glycine cleavage system H protein
FTL_1336	prephenate dehydratase
FTL_0158	acid phosphatase (precursor)
FTL_1527	Enolase (2-phosphoglycerate dehydratase)
FTL_1504	Peroxidase/catalase
FTL_0269	NAD(P)-specific glutamate dehydrogenase

Supplemental Data S7: Primer Sequences used to measure Gene expression or mRNA transcript levels of the chosen metabolic gene set described using GEXP

Gene Name	LEFT PRIMER	RIGHT PRIMER
FTL_1789	AGGTGACACTATAGAATACACGAGCAAAATGCTTCAAC	GTACGACTCACTATAGGGAGTCCCCATAATGCGGTAATG
FTL_1149	AGGTGACACTATAGAATACTGAATTTGATCCACGCAAG	GTACGACTCACTATAGGGAAATTTTGCTCGCCATACCAG
FTL_1476	AGGTGACACTATAGAATACCATTAATTGTTGATGGGCA	GTACGACTCACTATAGGGATTTACCAGAGAATCCACGCC
FTL_1284	AGGTGACACTATAGAATAGCGATAATCGTGGCAATCTT	GTACGACTCACTATAGGGAGCAAACATCACGCCTTCTTT
FTL_0438	AGGTGACACTATAGAATAATAGCTGGTGTGAAAACGGC	GTACGACTCACTATAGGGAATACCGCAACCAGCACTACC
FTL_1887	AGGTGACACTATAGAATAAGCCTTCTGGAGGTTCTGCT	GTACGACTCACTATAGGGATCGCATTTGCAATATCCTCA
FTL_0766	AGGTGACACTATAGAATATGCAGCTGTAGCTGTTGGTT	GTACGACTCACTATAGGGATTTCGCTGGAGCTTTTTCAC
FTL_1296	AGGTGACACTATAGAATATTCTTTTGGATACTTGGGGC	GTACGACTCACTATAGGGAAACCATGCCACCATAAAACC
FTL_1863	AGGTGACACTATAGAATACTGCGGAAATAGAGTCTCGC	GTACGACTCACTATAGGGAGCGCTTTCATTTTATCTCGC
FTL_1701	AGGTGACACTATAGAATAAGCCAGATGGGTAGAGGTGA	GTACGACTCACTATAGGGACACCAGCACCAACTTTTTCA
FTL_1148	AGGTGACACTATAGAATAACCTTGTAATGGTAGCGCGT	GTACGACTCACTATAGGGATTCAGCACGAGTTGGTGAAG
FTL_0588	AGGTGACACTATAGAATAGAAAATGGCGCTTTTGATGT	GTACGACTCACTATAGGGAGCCTTTTTCGACTTGATGCT
FTL_0294	AGGTGACACTATAGAATAACCTTCTTTGATGACGCCAC	GTACGACTCACTATAGGGATCTGCGTTACTCCCTTGAGC
FTL_0404	AGGTGACACTATAGAATAAATCTGCCATGGATGGTTTC	GTACGACTCACTATAGGGACCAGCACCAACTACAGCACA
FTL_0001	AGGTGACACTATAGAATAGCCTATCCATGTGGAGCAAA	GTACGACTCACTATAGGGAGGTCCAGCTGTGATAACCTCA
FTL_1616	AGGTGACACTATAGAATATTTGATACGCGGATCGTCTT	GTACGACTCACTATAGGGATGCTGTCAGTGTTGATGCTG
FTL_0583	AGGTGACACTATAGAATATAAATGAAGCTTTTGCGGCT	GTACGACTCACTATAGGGATGCACCCATACCAGTACCAA
FTL_1146	AGGTGACACTATAGAATACGAAAAATGACTTCCGTCGT	GTACGACTCACTATAGGGACAGCTTTCATCGCAGCATTA
FTL_0585	AGGTGACACTATAGAATAAGTGGTGGTTTCACTGCTCC	GTACGACTCACTATAGGGAGAGGTTCGCCTGTGTCCTTA
FTL_1147	AGGTGACACTATAGAATAGAAAATGCCCAAGCAATCAT	GTACGACTCACTATAGGGATCACCACCACCAGCTACTGA
FTL_0586	AGGTGACACTATAGAATAAAAACCGGATGATATCGCAG	GTACGACTCACTATAGGGAATCAGTATTTGAAACGCGCC
FTL_0273	AGGTGACACTATAGAATAGAAAAAGCGGGTGTGTTAGC	GTACGACTCACTATAGGGATCATTCCGAATACTGCACCA
FTL_0501	AGGTGACACTATAGAATAAAAAATACTCAGCAAGCGTGG	GTACGACTCACTATAGGGAGCGCTTAACATCCCCTGATA
FTL_1504	AGGTGACACTATAGAATATCCAGCAGGGCTAAGTGTTT	GTACGACTCACTATAGGGAATTGCAGGCGGTCATACATT
FTL_0484	AGGTGACACTATAGAATAATGGCAGCAGCTAATGGTTT	GTACGACTCACTATAGGGACCCTTTCCTTAGCTGCATCA
FTL_1233	AGGTGACACTATAGAATAAGCAGCCGATGATCATTTTT	GTACGACTCACTATAGGGATTCCCACCAGGGATATGAAA
FTL_1304	AGGTGACACTATAGAATACAAGTCCCGCACAAAAAGAT	GTACGACTCACTATAGGGAGGCTCAAATGGATCGACATC
FTL_0132	AGGTGACACTATAGAATAGCCCTCTTGGTTCAGCTCTA	GTACGACTCACTATAGGGATACTTGGCCCCTCTCAAATG
FTL_0472	AGGTGACACTATAGAATAGGTTCATTGGTGGCGTATTC	GTACGACTCACTATAGGGATAAATGTTGTCCCCGGTGTT
FTL_1383	AGGTGACACTATAGAATATGCGAGTAAGTGCGGTTTTA	GTACGACTCACTATAGGGATATCTTACGACGGTCTCGCC
FTL_0484	AGGTGACACTATAGAATAGTGCGGTGTCTGGTCCTTAT	GTACGACTCACTATAGGGACCCCTCAGCTAAGGCTAATTG
FTL_0648	AGGTGACACTATAGAATAAAGGTGTAACAATCGCCCC	GTACGACTCACTATAGGGAAAATTTTGTGACTCCGGCAT
FTL_0649	AGGTGACACTATAGAATAACTGCAGGTGCTCAAGAAGG	GTACGACTCACTATAGGGATATACCAAGCCTTTGGCGTT
FTL_1428	AGGTGACACTATAGAATAGAAATGTCTTAAAATGGCGCA	GTACGACTCACTATAGGGACAGCAAGAGCAACACCAAAG
FTL_1782	AGGTGACACTATAGAATATGCAGATCCACAAGGACTCA	GTACGACTCACTATAGGGACAAATACCACCGCTTTGAGC
FTL_1823	AGGTGACACTATAGAATAATTTGGCGCATTAAGAGCTG	GTACGACTCACTATAGGGATTTTGCTCCACGCAAGTAAA
FTL_0328	AGGTGACACTATAGAATATGGTCTGGTTGATGTCCCTT	GTACGACTCACTATAGGGAGGGCGATACTCAGCATTAGC
FTL_0191	AGGTGACACTATAGAATATGGAATCCGATGGGTGTTAT	GTACGACTCACTATAGGGAACGCGAAAGCTATTGGAAAC
FTL_1765	AGGTGACACTATAGAATAGTTTTGCACTAGGGATGGGA	GTACGACTCACTATAGGGATATCAGCAGCACCCAAGCTA
FTL_1861	AGGTGACACTATAGAATAGCTGCAGGGATTGCAACTAT	GTACGACTCACTATAGGGATAATCAGCATGACCAGGACG
FTL_0377	AGGTGACACTATAGAATATCAAAATTCACCACTCAGCG	GTACGACTCACTATAGGGACACGTACATGCGCCATAAAA
FTL_0788	AGGTGACACTATAGAATATTCACTCATCACAAGGAGCG	GTACGACTCACTATAGGGATCTGCGTTACTCCCTTGAGC
FTL_0294	AGGTGACACTATAGAATAACCTTCTTTGATGACGCCAC	GTACGACTCACTATAGGGAAGACCAGCACCATTCCAGTC
FTL_1899	AGGTGACACTATAGAATAGAAGTTATGCCAGGGCAATG	GTACGACTCACTATAGGGAGGTCCAGCTGTGATAACCTCA
FTL_0001	AGGTGACACTATAGAATAGCCTATCCATGTGGAGCAAA	GTACGACTCACTATAGGGATCGTGCCTAGAGGAGTCGTT
FTL_0131	AGGTGACACTATAGAATAATTAGAATTCATCCGCGCTC	GTACGACTCACTATAGGGAATACCGCCTAAAACTGTCGC
FTL_0195	AGGTGACACTATAGAATACGTACGCAAAATCGTCCTTT	GTACGACTCACTATAGGGACAGCTTTCATCGCAGCATTA
FTL_1146	AGGTGACACTATAGAATACGAAAAATGACTTCCGTCGT	GTACGACTCACTATAGGGACACCGCCAAATAAACCAACT
FTL_1795	AGGTGACACTATAGAATATCTGTTCCAGTTGGACATGG	GTACGACTCACTATAGGGATCACGCACAACACCTTTAGC
FTL_0472	AGGTGACACTATAGAATAGGTTCATTGGTGGCGTATTC	GTACGACTCACTATAGGGATAATGCAATAGAAGCTGCGG
FTL_1495	AGGTGACACTATAGAATATTGGTTTAGGCGCTGAATCT	GTACGACTCACTATAGGGAGCCTAATAAAAATGCCGCAA
FTL_0624	AGGTGACACTATAGAATAGGCAGTATGGGAGATGGAGT	GTACGACTCACTATAGGGACAGCCATAAGTAACACCCCC
FTL_1788	AGGTGACACTATAGAATACGTGGTTGCGATGAACTATG	GTACGACTCACTATAGGGATCTGCGTAGCCCTTTTATGC
FTL_0409	AGGTGACACTATAGAATATTTATTGGCCGGTGAGATTT	GTACGACTCACTATAGGGATTTGCCTACTTCAAGCATCG
FTL_0405	AGGTGACACTATAGAATAGTGCCTTGGGAAGAAAAACA	GTACGACTCACTATAGGGAATGCGGAACACATGATGCTA
FTL_1966	AGGTGACACTATAGAATACCGCCATAAACACCTCTTGT	GTACGACTCACTATAGGGACACCGACACGTGAAACAGAG
FTL_1797	AGGTGACACTATAGAATACCTGGACGTGAAGCTTATCC	GTACGACTCACTATAGGGATGCTCAATTGTTGCCTCAAG
FTL_0801	AGGTGACACTATAGAATAATTGGTCCAGTTGGTGCTG	GTACGACTCACTATAGGGAGTCACCCGGATGAGCTTAAA
FTL_1261	AGGTGACACTATAGAATATGAGCAAAAGCCATAATTTCA	GTACGACTCACTATAGGGATGCTCGGGTAAAACTAGGAAA
FTL_0356	AGGTGACACTATAGAATATCTCTTAGCAACTCAAACAGCA	GTACGACTCACTATAGGGATGCTCGGGTAAAACTAGGAAA
FTL_1791	AGGTGACACTATAGAATAACTAACCAAGCCCAACCAGA	GTACGACTCACTATAGGGAAAGCAGCATTGATCGAGACA
FTL_1492	AGGTGACACTATAGAATAATCATATCGCGTGGCAATTT	GTACGACTCACTATAGGGATTGTCTTATGCATTACGCCG
FTL_1966	AGGTGACACTATAGAATACCGCCATAAACACCTCTTGT	GTACGACTCACTATAGGGATGGATGCTTTGCATGCTTAT
FTL_0028	AGGTGACACTATAGAATAGTGAGTGAACCGTACGACCA	GTACGACTCACTATAGGGATGGTGAAAATGAACATCCCA
FTL_0328	AGGTGACACTATAGAATATGGTCTGGTTGATGTCCCTT	GTACGACTCACTATAGGGATTTTGCTCCACGCAAGTAAA
FTL_1309	AGGTGACACTATAGAATAGCTGCTGCAACTACAGGAAA	GTACGACTCACTATAGGGAGCAAATGTATCGCCTGTTGA
FTL_1272	AGGTGACACTATAGAATAACAACTACCTGCTGCTCCAAA	GTACGACTCACTATAGGGAAGGCGTGCTTGTGGAAATAG
FTL_1261	AGGTGACACTATAGAATATAATCTCGGAGAGTTTGCCA	GTACGACTCACTATAGGGACACCCGGATGAGCTTAAAAA
FTL_0294	AGGTGACACTATAGAATAAATGGTTGTTGGGGGATTCT	GTACGACTCACTATAGGGAAAGATCTTGTCGCTCTGCGT
FTL0805	AGGTGACACTATAGAATAGTGCTCTGGTTAAGAGCCCA	GTACGACTCACTATAGGGATAACCTGCTCAGGAAGCGAT
FTL_1146	AGGTGACACTATAGAATATCCTCAGCGCAGATGATAAA	GTACGACTCACTATAGGGAGCACGACGGAAGTCATTTTT
FTL_1570	AGGTGACACTATAGAATAATGACCAAGGAAATCAAGCG	GTACGACTCACTATAGGGAGGCTTTTGTAAATTCATCCCA
FTL_0043	AGGTGACACTATAGAATAGGAATGCAACTGAACAAGAGC	GTACGACTCACTATAGGGATAGCTTGGGTCCTGAGGAAT
FTT1498	AGGTGACACTATAGAATAATGCATCCAGAAGGGTATCG	GTACGACTCACTATAGGGAGAACAGCCCTCACCAATCAC
FTL_0472	AGGTGACACTATAGAATACTTGGTGGCGCAGACTTATT	GTACGACTCACTATAGGGACCAAGCTGTTTGATACGCAA
FTL_1147	AGGTGACACTATAGAATAGAAAATGCCCAAGCAATCAT	GTACGACTCACTATAGGGATCACCACCACCAGCTACTGA
FTL_0478	AGGTGACACTATAGAATAAGTCGCATGAGTGGGTCAA	GTACGACTCACTATAGGGATGACTCGTGAAGGGTCATCA
FTL_0484	AGGTGACACTATAGAATATGCAGCTAAGGAAAGGGTTG	GTACGACTCACTATAGGGATACAACTGTGCCTGCTGGAG
FTL_1336	AGGTGACACTATAGAATATGAGTCCCATCAAGCAATGT	GTACGACTCACTATAGGGAGCGAGCATGGAGCTTACTCT
FTL_0158	AGGTGACACTATAGAATATAATGCCAAAAACCCAGAGG	GTACGACTCACTATAGGGATCCCATGACTTGACCATCAC
FTL_1527	AGGTGACACTATAGAATACGCCTCATTTGACGGTAGAT	GTACGACTCACTATAGGGAGAGCTGCTGCATCACATCTT
FTL_1504	AGGTGACACTATAGAATACCTTATCAGGAGCAGGTCCA	GTACGACTCACTATAGGGAAAGACGACTGGCAAGGTGAT
FTL_0269	AGGTGACACTATAGAATAGCCGATTTCTTTACCACCAA	GTACGACTCACTATAGGGACCATGGGTTGATAAGGATGG
FTL_0001	AGGTGACACTATAGAATAGCCTATCCATGTGGAGCAAA	GTACGACTCACTATAGGGACATAGCTTCGTCAAAACCGA