VI. Anhang

1. Daten der Simulationen des Naphtyhlisochinolinium IQ-143

1) Enzymes found by iterative sequence analysis:
    1. Table S VI.1.1: List of enzymes used to build metabolic webs found to be not part of KEGG data.
2) Full list of enzymes of YANAsquare modes:
    1. Table S VI.1.2: List of enzmyes used to build metabolic web for *S. aureus* USA300.
    2. Table S VI.1.3: List of enzmyes used to build metabolic web for *S. epidermidis* RP62A.
    3. Table S VI.1.4: List of enzmyes used to build metabolic web for *H. sapiens.*
3) Synthesis and effects of the naptho-iso-quinoline IQ-143.
    1. Figure S VI.1.1: Synthesis of IQ-143.
    2. Figure S VI.1.2: Effects of IQ-143 on *S. epidermidis* RP62A.
    3. Figure S VI.1.3*:* Effects on human Cytochrome P450 enzymes.
4) Gene expression data gathered by Ohlsen et al:
    1. Table S VI.1.5: Gene expression data of *S. epidermidis* RP62A with 1,25µM IQ-143 added.
    2. Table S VI.1.5: Gene expression data of *S. epidermidis* RP62A with 0,16µM IQ-143 added.
5) Extreme modes calculated by YANAsquare models:
    1. Table S VI.1.7 to S9: Extreme modes of *S. aureus* USA300 calculated for different concentrations of IQ-143.
    2. Table S VI.1.10 to S12: Extreme modes of *S. epidermidis* RP62A calculated for different concentrations of IQ-143.
    3. Table S VI.1.13 to S15: Extreme modes of man calculated for different concentrations of IQ-143.
6) Extreme modes with changed activity after administration of IQ-143
    1. Table S VI.1.16 and S17: Higher (S16) and lower (S17) activity for *S. epidermidis* RP62A.
    2. Table S VI.1.18 and S19: Higher (S18) and lower (S19) activity for *S. aureus* USA300.

7) Measured concentrationsof nucleotides and NAD(P)H/NAD(P)$^+$.
    1. Figure S VI.1.4: Measured concentrations of NAD(P)H/NAD(P)$^+$.
    2. Figure S VI.1.5: Measured concentrations of nucleotides.
8) Calculated enzyme activities as calculated by R and YANAsquare:
    1. Table S VI.1.20: Calculated enzyme activities for *S. aureus* USA300.
    2. Table S VI.1.21: Calculated enzyme activities for *S. epidermidis* RP62A.
9) PCR Analysis
    1. Figure S VI.1.6: Results for PCR detection of *in silico* predicted additional enzymes for *S. epidermidis.*
10) Mode of action: Complex 1&3 of the oxidative phosphorylation
    1. Figure S VI.1.7: Mode of action of complex 1 of the oxidative phosphorylation
    2. Figure S VI.1.8: Mode of action of complex 1 of the oxidative phosphorylation

1. Enzymes found by iterative sequence analysis:

Table S VI.1.1: List of enzymes used to build metabolic webs found to be not part of KEGG data[1].

H. sapiens

EC- Number	Enzymname	Query Sequence: Brenda/NCBI	Hit: exPASY/NCBI	e- Value	Bit- Score
3.6.1.5	Apyrase	P49961	ENTP1_HUMAN	0,00E+000	1013
3.6.1.19	nucleoside-triphosphate diphosphatase	Q9BY32	ITPA_HUMAN	1,00E-110	400
3.6.1.14	adenosine-tetraphosphatase	Q4UK18	ATPB_HUMAN	0,00E+000	649
4.6.1.2	guanylate cyclase	P33402	GCYA2_HUMAN	0,00E+000	1308
2.4.2.8	inosinate pyrophosphorylase	P00492	HPRT_HUMAN	1,00E-123	442
2.4.2.4	thymidine phosphorylase	P19971	TYPH_HUMAN	0,00E+000	868
2.7.1.74	deoxycytidine kinase	P27707	DCK_HUMAN	e-152	539
3.5.2.5	Allantoinase	P77671	ref|NP_001376.1|	2,00E-032	136
3.6.1.41	bis(5'-nucleosyl)-tetraphosphatase	P05637	ref|NP_006230.2|	8,00E-005	44,3
2.7.4.4	nucleoside-phosphate kinase	NP_036606	NP_036606	2,00E-147	518
4.2.1.70	pseudouridylate synthase	Q96K56	Q96K56_HUMAN	0,00E+000	730

***S. epidermidis* RP62A**

EC- Number	Enzymename	Query Sequence: Brenda/NCBI	Hit: exPASY/NCBI	e- Value	Bit- Score
3.6.1.19	nucleoside-triphosphate diphosphatase	Q9BY32	Q5HQ23	8.7e-16	177
3.6.1.3	Adenosinetriphosphatase	A2QUY7	Q5HME0	7.3e-51	508
2.7.1.74	deoxycytidine kinase	P27707	Q5HRJ1	1.2e-10	136
3.1.3.5	5'-nucleotidase	Q2YUP8	Q5HKQ5	1.5e-19	244
2.4.2.22	xanthine phosphoribosyltransferase	Q04IV9	Q5HRX4	4.2e-48	486
2.4.2.4	thymidine phosphorylase	Q301G5	Q5HM85	2.4e-116	1126
2.7.1.76	epoxyadenosine kinase	Q48VP1	Q5HRJ0	2.5e-27	286

***S. aureus* USA300**

EC- Number	Enzymename	Query Sequence: Brenda/NCBI	Hit: exPASY/NCBI	e- Value	Bit- Score
2.4.2.3	uridine phosphorylase	P12758	ref|NC_007793.1	2,00E-022	100
3.2.2.3	uridine nucleosidase	Q88S31	ref|NC_007793.1	3,00E-048	186
2.7.4.4	uridine-cytidine kinase	ref|NP_036606.2	ref|NC_007793.1	9,00E-042	163

2.7.4.10	nucleoside-triphosphate-adenylate kinase	Q9UIJ7	ref|NC_007793.1	2,00E-043	169
3.6.1.19	nucleoside-triphosphate diphosphatase	Q9BY32	ref|NC_007793.1	3,00E-012	65
2.7.7.6	DNA-directed RNA polymerase	Q2FER5	ref|NC_007793.1	1,00E-159	553
3.2.2.8	riboyslpyrimidine nucleosidase	A7ZNY5	ref|NC_007793.1	3,00E-060	225
2.7.1.74	deoxycytidine kinase	P27707	ref|NC_007793.1	3,00E-008	52
3.5.4.14	deoxycytidine deaminase	O74047	ref|NC_007793.1	5,00E-021	94
3.5.2.2	Dihydropyrimidinase	A2UD01	ref|NC_007793.1	4,00E-024	106
4.2.1.70	pseudouridylate synthase	A5ISF5	ref|NC_007793.1|	1,00E-168	583
2.4.2.4	thymidine phosphorylase	A5IUT1	ref|NC_007793.1	0	716

[1] Enzymes added through iterative sequence analysis to the enzymelist derived from KEGG.

2: Full list of enzymes of YANAsquare modes

Table S VI.1.2: List of enzmyes used to build metabolic web for *S. aureus* USA300 [1].

Enzyme name	reversible?	Reaction equation
ADP-energy_to_ADP-metabolism	true	ADP-energy = ADP-metabolism
AMP-energy_to_AMP-metabolism	true	AMP-energy = AMP-metabolism
AS_Acetyl-CoA_to_L-Leucine	false	Acetyl-CoA + L-Glutamate + NAD+ = CO2 + L-Leucine + NADH + Oxo-Glutarate
AS_Acetyl-CoA_to_L-Valine	true	Acetyl-CoA + L-Glutamate = CoA-SH + Oxo-Glutarate
AS_Alanine_to_Pyruvate	true	Pyruvate + beta_Alanine = L-Alanine + Malonate_semi_aldehyde
AS_Aspartate_to_Alanine	false	L-Aspartate = CO2 + L-Alanine
AS_Aspartate_to_Arginine	false	ATP-energy + L-Aspartate = ADP-energy + Fumarate + L-Arginine
AS_Aspartate_to_Asparagine	false	ATP-energy + L-Aspartate + L-Glutamine = ADP-energy + L-Asparagine + L-Glutamate + Orthophosphate
AS_Aspartate_to_beta-Alanine	false	L-Aspartate = CO2 + beta_Alanine
AS_Aspartate_to_Homoserine	true	ATP-energy + L-Aspartate + 2 NADPH = ADP-energy + Homoserine + 2 NADP+ + Phosphate
AS_Glutamate_to_Glutamine	false	ATP-energy + L-Glutamate + NH3 = ADP-energy + L-Glutamine + Phosphate
AS_Glutamate_to_Proline	false	ATP-energy + L-Glutamate + 2 NADPH = ADP-energy + L-Proline + 2 NADP+ + 2 Phosphate
AS_Histidine_to_Glutamate	false	2 H2O + L-Histidine + THF = Formamido-THF + L-Glutamate + NH3
AS_Homoserine_to_Threonine	false	ATP-energy + H2O + Homoserine = ADP-energy + L-Threonine + Phosphate
AS_Isoleucine	false	ATP-energy + Isoleucine_ext = ADP-energy + iso-Leucine
AS_Leucine	false	ATP-energy + Leucine-ext = ADP-energy + L-Leucine
AS_Phenylalanin_to_Tyrosine	false	L-Phenylalanine + NADPH + O2 = H2O + L-Tyrosine + NADP+
AS_Saccharopine_to_Lysine	true	H2O + NAD+ + Saccharopine = L-Lysine + NADH + Oxo-Glutarate
AS_Serine_to_Cysteine	false	Acetyl-CoA + H2S + L-Serine = Acetate + CoA-SH + L-Cysteine
AS_Serine_to_Glycine	true	L-Serine + THF = 5-10-Methylene-THF + H2O + L-Glycine
AS_Serine_to_Methionine	false	5-10-Methylene-THF + L-Serine = L-Methionine + NH3 + Pyruvate + THF
AS_Serine_to_Pyruvate	false	L-Serine = NADPH + Pyruvate
AS_Threonine	false	ATP-energy + Threonine_ext = ADP-energy + L-Threonine

AS_Tryptophan_to_Tryptamine	false	L-Tryptophan = CO2 + Tryptamine
AS_Valine	false	ATP-energy + Valine-ext = ADP-energy + L-Valine
ATP-energy_to_ATP-metabolism	true	ATP-energy = ATP-metabolism
DNA-extern_to_DNA-intern	false	DNA-extern = DNA
DNA_to_DNA-blocked	false	DNA + IQ-143 = DNA_blocked + IQ-143_used
FA_Deg_C16_to_Acetyl-CoA	false	C16 + 6 FAD + 6 NAD+ = 6 Acetyl-CoA + 6 CoA-SH + 6 FADH2 + 6 NADH
FA_Syn_Acetyl-CoA_to_C16	false	6 Acetyl-CoA + 6 NADPH = 6 ACP + C16 + 6 CO2 + 6 H2O + 6 NADP+
IQ-143-extern_to_IQ-143	false	IQ-143_extern = IQ-143
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	true	2-Phospho-D-glycerate = 3-Phospho-D-glycerate
Glyc_2-phospho-D-glycerate-hydro-lyase	true	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
Glyc_6-phospho-beta-glucosidase	true	H2O + Salicin6-phosphate = Salicylalcohol + beta-D-Glucose6-phosphate
Glyc_6-phosphofructokinase	true	ATP-energy + beta-D-Fructose6-phosphate = ADP-energy + beta-D-Fructose16-bisphosphate
Glyc_acetaldehyde-dehydrogenase_NAD+	true	Acetaldehyde + H2O + NAD+ = Acetate + H+ + NADH
Glyc_Actetate-CoA-ligase	true	ATP-energy + Acetate + CoA = ADP-energy + Acetyl-CoA + Pyrophosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	true	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	true	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_ATP-alpha-D-glucokinase	true	ATP-energy + alpha-D-Glucose = ADP-energy + alpha-D-Glucose6-phosphate
Glyc_ATP-beta-D-glucokinase	true	ATP-energy + beta-D-Glucose = ADP-metabolism + beta-D-Glucose6-phosphate
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	true	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_D-Glucose-1-epimerase	true	alpha-D-Glucose = beta-D-Glucose
Glyc_D-Glucose-1-epimerase-ketol-isomerase	true	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal = Glyceronephosphate
Glyc_dihydrolipoamide-dehydrogenase	false	EnzymeN6-(dihydrolipoyl)lysine + NAD+ = EnzymeN6-(lipoyl)lysine + H+ + NADH
Glyc_fructose-bisphosphat-aldolase	true	beta-D-Fructose16-bisphosphate = (2R)-2-Hydroxy-3-(phosphonooxy)-propanal + Glyceronephosphate
Glyc_fructose-bisphosphatase	false	H2O + beta-D-Fructose16-bisphosphate = Orthophosphate + beta-D-Fructose6-phosphate
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NADP+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADPH
Glyc_lipoic_acetyltransferase	true	Acetyl-CoA + EnzymeN6-(dihydrolipoyl)lysine = CoA + Dihydrolipoyllysine-residueacetyltransferaseS-

		acetyldihydrolipoyllysine
Glyc_phosphoglycerate-kinase	true	3-Phospho-D-glycerate + ATP-energy = 3-Phospho-D-glyceroylphosphate + ADP-energy
Glyc_PTS-permease1	true	D-Glucose + ProteinN(pi)-phospho-L-histidine = Proteinhistidine + alpha-D-Glucose6-phosphate
Glyc_PTS-permease2	true	Arbutin + ProteinN(pi)-phospho-L-histidine = Arbutin6-phosphate + Proteinhistidine
Glyc_pyruvate_dehydrogenase	false	Pyruvate + Thiamindiphosphate = 2-(alpha-Hydroxyethyl)thiaminediphosphate + CO2
Glyc_Succinate-CoA-ligase	true	ATP-energy + CoA + Succinate = ADP-energy + Orthophosphate + Succinyl-CoA
N-acylneuraminate-9-phosphatase	true	H2O + alpha-D-ribose-5P = AMP-metabolism + alpha-D-Ribose1-phosphate
OP_complex1	false	2 H+ + NADH + Ubichinon = 4 H+_ext + NAD+ + Ubihydrochinon
OP_complex2	false	4 H+ + Succinate + Ubichinon = Fumarate + Ubihydrochinon
OP_complex3	false	2 H+ + Ubihydrochinon + cytochrome_BC = 4 H+_ext + Ubichinon + cytochrome_C
OP_complex4	false	2 H+ + O- + cytochrome_C = 2 H+_ext + H2O
OP_complex5	false	ADP-energy + 3 H+_ext + Phosphate = ATP-energy + 3 H+ + H2O
PurM_5-Hydroxyisourate-amidohydrolase	false	5-Hydroxyisourate + H2O = (S)(+)-Allantoin
PurM_5-nucleotidase_AMP	false	AMP-metabolism + H2O = Adenosine + Orthophosphate
PurM_5-nucleotidase_CMP	false	CMP + H2O = Cytidine + Orthophosphate
PurM_5-nucleotidase_dAMP	false	H2O + dAMP = Deoxyadenosine + Orthophosphate
PurM_5-nucleotidase_dCMP	false	H2O + dCMP = Deoxycytidine + Orthophosphate
PurM_5-nucleotidase_dGMP	false	H2O + dGMP = Deoxyguanosine + Orthophosphate
PurM_5-nucleotidase_dTMP	false	H2O + dTMP = Orthophosphate + Thymidine
PurM_5-nucleotidase_GMP	false	GMP + H2O = Guanosine + Orthophosphate
PurM_5-nucleotidase_IMP	false	H2O + IMP = Inosine + Orthophosphate
PurM_5-nucleotidase_UMP	false	H2O + UMP = Orthophosphate + Uridine
PurM_5-nucleotidase_XMP	false	H2O + Xanthosine5-phosphate = Orthophosphate + Xanthosine
PurM_adenylate-kinase_AMP	true	AMP-metabolism + ATP-energy = 2 ADP-metabolism
PurM_adenylate-kinase_dAMP	true	ATP-energy + dAMP = ADP-energy + dADP
PurM_adenylosuccinate-lyase	true	N6-(12-Dicarboxyethyl)-AMP = AMP-metabolism + Fumarate
PurM_adenylosuccinate-lyase2	true	1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole = 1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Fumarate

PurM_adenylylsulfate-kinase	true	ATP-energy + Adenylylsulfate = 3-phosphoadenylylsulfate + ADP-energy
PurM_ADP-ribose-ribophosphohydrolase	false	ADP-ribose + H2O = AMP-metabolism + D-Ribose5-phosphate
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	true	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Pyrophosphate = 5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate
PurM_AIR-carboxylase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate = Aminoimidazoleribotide + CO2
PurM_allantoinase	false	Allantoate + H2O = Allantoine
PurM_AMP-pyrophosphorylase2	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_ATP-phosphohydrolase	false	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
PurM_ATP_CDP-phosphotransferase	true	ATP-energy + CDP = ADP-energy + CTP
PurM_ATP_dADP-phosphotransferase	true	ATP-energy + dADP = ADP-energy + dATP
PurM_ATP_dCDP-phosphotransferase	true	ATP-energy + dCDP = ADP-energy + dCTP
PurM_ATP_dGDP-phosphotransferase	true	ATP-energy + dGDP = ADP-energy + dGTP
PurM_ATP_dIDP-phosphotransferase	true	ATP-energy + dIDP = ADP-energy + dITP
PurM_ATP_dTDP-phosphotransferase	true	ATP-energy + dTDP = ADP-energy + dTTP
PurM_ATP_dUDP-phosphotransferase	true	ATP-energy + dUDP = ADP-energy + dUTP
PurM_ATP_GMP-guanylate-kinase	true	ATP-energy + GMP = ADP-energy + GDP
PurM_ATP_GMP_guanylate-kinase	true	ATP-energy + dGMP = ADP-energy + dGDP
PurM_ATP_GTP-phosphotransferase	true	ATP-energy + GDP = ADP-energy + GTP
PurM_ATP_IDP-phosphotransferase	true	ATP-energy + IDP = ADP-energy + ITP
PurM_ATP_UTP-phosphotransferase	true	ATP-energy + UDP = ADP-energy + UTP
PurM_carbamate-kinase_ATP	true	ATP-energy + CO2 + NH3 = ADP-energy + Carbamoylphosphate
PurM_D-Ribose-1,5-phosphomutase	false	alpha-D-Ribose1-phosphate = D-Ribose5-phosphate
PurM_deoxyadenosine-kinase_ATP	false	ATP-energy + Deoxyadenosine = ADP-energy + dAMP
PurM_deoxycytidine-kinase_ATP	false	ATP-energy + Adenosine = ADP-energy + AMP-metabolism
PurM_deoxycytidine-kinase_ATP2	false	ATP-energy + Deoxycytidine = ADP-energy + dCMP
PurM_dGTP-diphosphohydrolase	false	H2O + dGTP = Pyrophosphate + dGMP
PurM_dITP-diphosphohydrolase	false	H2O + dITP = 2-Deoxyinosine-5-phosphate + Pyrophosphate
PurM_DNA-directed-RNA-polyermase_ATP	false	ATP-metabolism + RNA = Pyrophosphate + RNA-A

PurM_DNA-directed-RNA-polyermase_CTP	false	CTP + RNA = Pyrophosphate + RNA-C
PurM_DNA-directed-RNA-polyermase_GTP	false	GTP + RNA = Pyrophosphate + RNA-G
PurM_DNA-directed-RNA-polyermase_UTP	false	RNA + UTP = Pyrophosphate + RNA-U
PurM_GDP-reductase	false	GMP + H+-intern + NADPH = IMP + NADP+ + NH3
PurM_GMP-pyrophosphorylase2	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PurM_GTP-diphosphohydrolase	false	GTP + H2O = GMP + Pyrophosphate
PurM_GTP-pyrophosphokinase	false	ATP-energy + GTP = ADP-energy + Guanosine3-diphosphate5-triphosphate
PurM_IMP-cyclohydrolase	true	H2O + IMP = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide
PurM_IMP-dehydrogenase	false	H2O + IMP + NAD+ = H+-intern + NADH + Xanthosine5-phosphate
PurM_IMP-pyrophosphorylase	true	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
PurM_IMP_L-aspartate-ligase	true	GTP + IMP + L-Aspartate = GDP + N6-(12-Dicarboxyethyl)-AMP + Orthophosphate
PurM_ITP-diphosphohydrolase	false	H2O + ITP = IMP + Pyrophosphate
PurM_metaphosphatase	true	Guanosine3-diphosphate5-triphosphate + H2O = Guanosine_3',5'-bis(diphosphate) + Orthophosphate
PurM_nucleoside-diphosphate-phosphotransferase_ATP	true	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
PurM_nucleotide-phosphatase_Adenine	true	Adenosine + Orthophosphate = Adenine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Deoxyadenosine	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PurM_nucleotide-phosphatase_Deoxyguanosine	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PurM_nucleotide-phosphatase_Deoxyinosine	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
PurM_nucleotide-phosphatase_Deoxyuridine	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PurM_nucleotide-phosphatase_Guanosine	true	Guanosine + Orthophosphate = Guanine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Inosine	true	Inosine + Orthophosphate = Hypoxanthine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Xanthosine	true	Orthophosphate + Xanthosine = Xanthine + alpha-D-Ribose1-phosphate
PurM_PRPP-synthetase	true	ATP-energy + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy
PurM_pyruvate-phosphotransferase_ATP	false	ATP-metabolism + Pyruvate = ADP-metabolism + Phosphoenolpyruvate
PurM_pyruvate-phosphotransferase_dATP	false	Pyruvate + dATP = Phosphoenolpyruvate + dADP
PurM_pyruvate-phosphotransferase_dGTP	false	Pyruvate + dGTP = Phosphoenolpyruvate + dGDP
PurM_pyruvate-phosphotransferase_GTP	false	GTP + Pyruvate = GDP + Phosphoenolpyruvate
PurM_SAICAR-synthetase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate + ATP-metabolism + L-Aspartate = 1-(5-

		Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole + ADP-metabolism + Orthophosphate
PurM_thioredoxin-oxidoreductase_dADP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dATP	false	ATP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dCDP	false	CDP + Thioredoxin = H2O + Oxidizedthioredoxin + dCDP
PurM_thioredoxin-oxidoreductase_dCTP	false	CTP + Thioredoxin = Oxidizedthioredoxin + dCTP
PurM_thioredoxin-oxidoreductase_dGDP	false	GDP + Thioredoxin = H2O + Oxidizedthioredoxin + dGDP
PurM_thioredoxin-oxidoreductase_dGTP	false	GTP + Thioredoxin = H2O + Oxidizedthioredoxin + dGTP
PurM_thioredoxin-oxidoreductase_dUDP	false	Thioredoxin + UDP = H2O + Oxidizedthioredoxin + dUDP
PurM_thioredoxin-oxidoreductase_dUTP	false	Thioredoxin + UTP = Oxidizedthioredoxin + dUTP
PurM_urea-amidohydrolase	false	H2O + Urea = CO2 + 2 NH3
PurM_UTP-diphosphohydrolase	false	H2O + UTP = Pyrophosphate + UMP
PurM_xanthosine-phosphoribosyltransferase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP-ligase	false	ATP-energy + NH3 + Xanthosine5-phosphate = ADP-energy + GMP + Pyrophosphate
PurM_XMP-pyrophosphorylase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP_L-glutamine-amide-ligase	false	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = ADP-energy + GMP + L-Glutamate + Pyrophosphate
PurM_XTP-diphosphohydrolase	false	H2O + XTP = Pyrophosphate + Xanthosine5-phosphate
PyrM_2,3-cyclic-nucleotidase_CMP	false	23-CyclicCMP + H2O = 3-CMP
PyrM_2,3-cyclic-nucleotidase_UMP	false	23-CyclicUMP + H2O = 3-UMP
PyrM_AMP-pyrophosphorylase	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PyrM_aspartate-carbamoyltransferase	false	Carbamoylphosphate + L-Aspartate = N-Carbamoyl-L-aspartate + Orthophosphate
PyrM_ATP_dTDP_thymidylate-kinase	true	ATP-energy + dTMP = ADP-energy + dTDP
PyrM_ATP_dUDP_thymidylate-kinase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_CO2_L-glutamine-amido-ligase	false	2 ATP-energy + H2O + HCO3- + L-Glutamine = 2 ADP-energy + Carbamoylphosphate + L-Glutamate + Orthophosphate
PyrM_CTP-synthase	false	ATP-energy + NH3 + UTP = ADP-energy + CTP + Orthophosphate
PyrM_cytidilate-kinase_CTP	true	ATP-energy + CMP = ADP-energy + CDP
PyrM_cytidilate-kinase_dCMP	true	ATP-energy + dCMP = ADP-energy + dCDP
PyrM_cytidine-aminohydrolase	true	Cytidine + H2O = NH3 + Uridine

PyrM_cytidine-kinase	false	Cytidine + UTP = CMP + UDP
PyrM_cytidine-kinase_ATP	false	ATP-energy + Cytidine = ADP-energy + CMP
PyrM_cytidine-kinase_dATP	false	Cytidine + dATP = CMP + dADP
PyrM_cytidine-kinase_dCTP	false	Cytidine + dCTP-ex = CMP + dCDP-ex
PyrM_cytidine-kinase_dGTP	false	Cytidine + dGTP = CMP + dGDP
PyrM_cytidine-kinase_dTTP	false	Cytidine + dTTP-ex = CMP + dTDP-ex
PyrM_cytidine-kinase_dUTP	false	Cytidine + dUTP-ex = CMP + dUDP-ex
PyrM_cytidine-kinase_GTP	false	Cytidine + GTP = CMP + GDP
PyrM_cytidine-kinase_ITP	false	Cytidine + ITP = CMP + IDP
PyrM_cytidine-ribohydrolase	false	Cytidine + H2O = Cytosine + D-Ribose
PyrM_dCMP-aminohydrolase	true	H2O + dCMP = NH3 + dUMP
PyrM_deoxyadenosine-phosphorylase	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PyrM_Deoxycytidine-aminohydrolase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_Deoxycytidine-deaminase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_deoxyguanosine-phosphorylase	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PyrM_deoxyinosine-phosphorylase	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Inosine
PyrM_deoxyuridine-phosphorylase	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PyrM_dihydroorotase	true	(S)-Dihydroorotate + H2O = N-Carbamoyl-L-aspartate
PyrM_dihydroorotate-oxidase	true	(S)-Dihydroorotate + Oxygen = H2O2 + Orotate
PyrM_dUMP-phosphotransferase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_dUTP-diphosphatase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_dUTP-diphosphohydrolase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_GMP-pyrophosphorylase	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PyrM_nucleoside-phosphate-kinase_ATP	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-phosphate-kinase_ATP2	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-triphosphate-adenylate-kinase	true	ATP-energy + UTP = ADP-energy + UDP
PyrM_OMP-decarboxylase	false	Orotidine5-phosphate = CO2 + UMP
PyrM_orotate-phosphoribosyltransferase	true	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate

PyrM_pyrimidine-nucleoside-phosphorylase	true	Cytidine + Orthophosphate = Cytosine + alpha-D-Ribose1-phosphate
PyrM_thioredoxin-reductase	false	H+ + NADPH + Oxidizedthioredoxin = NADP+ + Thioredoxin
PyrM_thymidilate-synthase	false	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
PyrM_thymidine-kinase_dTMP	true	ATP-energy + Thymidine = ADP-energy + dTMP
PyrM_thymidine-kinase_dUMP	true	ATP-energy + Deoxyuridine = ADP-energy + dUMP
PyrM_thymidine-phosphorylase	true	Orthophosphate + Thymidine = 2-Deoxy-D-ribose1-phosphate + Thymine
PyrM_UMP-pyrophosphorylase	true	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
PyrM_uridine-kinase_ATP	false	ATP-energy + Uridine = ADP-energy + UMP
PyrM_uridine-kinase_dATP	false	Uridine + dATP = UMP + dADP
PyrM_uridine-kinase_dCTP	false	Uridine + dCTP-ex = UMP + dCDP-ex
PyrM_uridine-kinase_dGTP	false	Uridine + dGTP = UMP + dGDP
PyrM_uridine-kinase_dTTP	false	Uridine + dTTP-ex = UMP + dTDP-ex
PyrM_uridine-kinase_dUTP	false	Uridine + dUTP-ex = UMP + dUDP-ex
PyrM_uridine-kinase_GTP	false	GTP + Uridine = GDP + UMP
PyrM_uridine-kinase_ITP	false	ITP + Uridine = IDP + UMP
PyrM_uridine-kinase_UTP	false	UTP + Uridine = UDP + UMP
PyrM_uridine-phosphorylase	true	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
PyrM_uridine-ribohydrolase	false	H2O + Uridine = D-Ribose + Uracil
PyrM_UTP_L-glutamine-amido-ligase	false	ATP-energy + H2O + L-Glutamine + UTP = ADP-energy + CTP + L-Glutamate + Orthophosphate
SERP0290-zinc-transport_efflux	false	ATP-energy + H2O + Zn2+-intern = ADP-energy + Pyrophosphate + Zn2+-extern
SERP0291-zinc-transporter_import	false	ATP-energy + H2O + Zn2+-extern = ADP-energy + Pyrophosphate + Zn2+-intern
SERP0292-iron-dicitrate-transporter_import	false	ATP-energy + H2O + ferric-dicitrate_extern = ADP-energy + Pyrophosphate + ferric_dicitrate_intern
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	true	Ethanol + NAD+ = Acetaldehyde + H+ + NADH
SERP0653-PurM_FGAM-synthethase	false	5-Phosphoribosyl-N-formylglycinamide + ATP-metabolism + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ADP-metabolism + L-Glutamate + Orthophosphate
SERP0655-PurM_amidophosphoribosyltransferase	false	5-Phosphoribosylamine + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O + L-Glutamine
SERP0656-PurM_AIR_synthetase	false	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-metabolism = ADP-metabolism + Aminoimidazoleribotide + Orthophosphate

SERP0657-PurM_GAR-formyltransferase	false	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide = 5-Phosphoribosyl-N-formylglycinamide + Tetrahydrofolate
SERP0658-PurM_AICAR-formyltransferase	false	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + 10-Formyltetrahydrofolate = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide + Tetrahydrofolate
SERP0659-PurM_phosphoribosylamine-glycine-ligase	false	5-Phosphoribosylamine + ATP-metabolism + Glycine = 5-Phosphoribosylglycinamide + ADP-metabolism + Orthophosphate
SERP0686-spermidine/putrescine-transport_import	false	ATP-metabolism + H2O + putrescine_extern + spermidine_extern = ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0687-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0688-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0765-Uracil-permease-transport_import	false	H+-extern + uracil_extern = H+-intern + uracil_intern
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	false	DNA + dATP = DNA-A + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	false	DNA + dCTP = DNA-C + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	false	DNA + dGTP = DNA-G + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	false	DNA + dTTP = DNA-T + Pyrophosphate
SERP0841-PurM_PNPase_ADP	false	ADP-metabolism + RNA = Orthophosphate + RNA-A
SERP0841-PurM_PNPase_GDP	false	GDP + RNA = Orthophosphate + RNA-G
SERP1403-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143_extern + Pyrophosphate
SERP1802-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1803-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1944-MultiDrug-transport_efflux	false	IQ-143 + H+-intern = IQ-143_extern + H+-extern
SERP1951-lipoprotein-transport_efflux/import	true	ATP-energy + H2O + lipoprotein_extern = ADP-energy + Pyrophosphate + lipoprotein_intern
SERP1952-macrolide-transport_efflux	false	ATP-energy + H2O + macrolide_intern = ADP-energy + Pyrophosphate + macrolide_extern
SERP1997-formate/nitrite-transport_efflux/import	false	H+-intern + formate_internal + nitrite_external = H+-extern + formate_extern + nitrite_intern
SERP2060-glyerol-transport_import	false	ATP-energy + H2O + glycerol-3-phosphate_extern = ADP-energy + Pyrophosphate + glycerol-3-phosphate_intern
SERP2156-Glyc_L-lactate-dehydrogenase	true	(S)-Lactate + NAD+ = H+ + NADH + Pyruvate

SERP2179-choline/betaine/carnitine-transp_efflux	false	H+-extern + betaine_intern + carnitine-extern + choline-extern = H+-intern + betaine-extern + carnitine-intern + choline-intern
SERP2186-PurM_ATP_sulfate-adenylyltransferase	false	ATP-energy + Sulfate = Adenylylsulfate + Pyrophosphate
SERP2283-phopsphonate-transport_import	false	ATP-energy + H2O + phosphonate_extern = ADP-energy + Pyrophosphate + phosphonate_intern
SERP2289-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143_extern + Pyrophosphate
TCA_citrate-hydro-lyase	true	Citrate = H2O + cis-Aconitate
TCA_citrate-hydroxymutase	true	Citrate = Isocitrate
TCA_citrate_synthase	true	Citrate + CoA = Acetyl-CoA + H2O + Oxaloacetate
TCA_fumarate-hydratase	true	(S)-Malate = Fumarate + H2O
TCA_isocitrate-hydro-lyase	true	Isocitrate = H2O + cis-Aconitate
TCA_lipoic-transsuccinylase	true	EnzymeN6-(dihydrolipoyl)lysine + Succinyl-CoA = CoA + Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine
TCA_Oxidoreductase	false	Isocitrate + NAD+ = 2-Oxoglutarate + CO2 + H+ + NADH
TCA_oxoglutarate-dehydrogenase-complex1	true	2-Oxoglutarate + Thiamindiphosphate = 3-Carboxy-1-hydroxypropyl-ThPP + CO2
TCA_oxoglutarate-dehydrogenase-complex2	true	3-Carboxy-1-hydroxypropyl-ThPP + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine + Thiamindiphosphate
TCA_oxoglutarate-synthase	false	CO2 + Reducedferredoxin + Succinyl-CoA = 2-Oxoglutarate + CoA + Oxidizedferredoxin
TCA_PEP-carboxylase	true	ATP-energy + Oxaloacetate = ADP-energy + CO2 + Phosphoenolpyruvate
TCA_Pyruvate_CO2-ligase	true	ATP-energy + HCO3- + Pyruvate = ADP-energy + Orthophosphate + Oxaloacetate
TCA_pyruvate_dehydrogenase	false	2-(alpha-Hydroxyethyl)thiaminediphosphate + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine + Thiamindiphosphate

[1] List of enzymes used to build the metabolic web of *S. aureus USA 300*. This list is composed of data derived from KEGG and own annotations. Abbreviations: AS: Amino acids; FA: fatty acid synthesis and degradation; Glyc: Glycolysis and Pentose Phosphate Pathways; OP: Oxidative phosphorylation; PurM: Purine Metabolism; PyrM: Pyrimidine Metabolism; TCA: Citric acid Cycle; SERP: Enzymes measured by gene expression micro arrays.

Table S VI.1.3: List of enzmyes used to build metabolic web for *S. epidermidis* RP62A [1].

Enzyme name	reversible?	Reaction equation
ADP-energy_to_ADP-metabolism	true	ADP-energy = ADP-metabolism
AMP-energy_to_AMP-metabolism	true	AMP-energy = AMP-metabolism
AS_Acetyl-CoA_to_L-Leucine	false	Acetyl-CoA + L-Glutamate + NAD+ = CO2 + L-Leucine + NADH + Oxo-Glutarate
AS_Acetyl-CoA_to_L-Valine	true	Acetyl-CoA + L-Glutamate = CoA-SH + Oxo-Glutarate
AS_Alanine_to_Pyruvate	true	Pyruvate + beta_Alanine = L-Alanine + Malonate_semi_aldehyde
AS_Aspartate_to_Alanine	false	L-Aspartate = CO2 + L-Alanine
AS_Aspartate_to_Arginine	false	ATP-energy + L-Aspartate = ADP-energy + Fumarate + L-Arginine
AS_Aspartate_to_Asparagine	false	ATP-energy + L-Aspartate + L-Glutamine = ADP-energy + L-Asparagine + L-Glutamate + Orthophosphate
AS_Aspartate_to_beta-Alanine	false	L-Aspartate = CO2 + beta_Alanine
AS_Aspartate_to_Homoserine	true	ATP-energy + L-Aspartate + 2 NADPH = ADP-energy + Homoserine + 2 NADP+ + Phosphate
AS_Glutamate_to_Glutamine	false	ATP-energy + L-Glutamate + NH3 = ADP-energy + L-Glutamine + Phosphate
AS_Glutamate_to_Proline	false	ATP-energy + L-Glutamate + 2 NADPH = ADP-energy + L-Proline + 2 NADP+ + 2 Phosphate
AS_Histidine_to_Glutamate	false	2 H2O + L-Histidine + THF = Formamido-THF + L-Glutamate + NH3
AS_Homoserine_to_Threonine	false	ATP-energy + H2O + Homoserine = ADP-energy + L-Threonine + Phosphate
AS_Isoleucine	false	ATP-energy + Isoleucine_ext = ADP-energy + iso-Leucine
AS_Leucine	false	ATP-energy + Leucine-ext = ADP-energy + L-Leucine
AS_Phenylalanin_to_Tyrosine	false	L-Phenylalanine + NADPH + O2 = H2O + L-Tyrosine + NADP+
AS_Saccharopine_to_Lysine	true	H2O + NAD+ + Saccharopine = L-Lysine + NADH + Oxo-Glutarate
AS_Serine_to_Cysteine	false	Acetyl-CoA + H2S + L-Serine = Acetate + CoA-SH + L-Cysteine
AS_Serine_to_Glycine	true	L-Serine + THF = 5-10-Methylene-THF + H2O + L-Glycine
AS_Serine_to_Methionine	false	5-10-Methylene-THF + L-Serine = L-Methionine + NH3 + Pyruvate + THF
AS_Serine_to_Pyruvate	false	L-Serine = NADPH + Pyruvate
AS_Threonine	false	ATP-energy + Threonine_ext = ADP-energy + L-Threonine
AS_Tryptophan_to_Tryptamine	false	L-Tryptophan = CO2 + Tryptamine
AS_Valine	false	ATP-energy + Valine-ext = ADP-energy + L-Valine

ATP-energy_to_ATP-metabolism	true	ATP-energy = ATP-metabolism
DNA-extern_to_DNA-intern	false	DNA-extern = DNA
DNA_to_DNA-blocked	false	DNA + IQ-143 = DNA_blocked + IQ-143_used
FA_Deg_C16_to_Acetyl-CoA	false	C16 + 6 FAD + 6 NAD+ = 6 Acetyl-CoA + 6 CoA-SH + 6 FADH2 + 6 NADH
FA_Syn_Acetyl-CoA_to_C16	false	6 Acetyl-CoA + 6 NADPH = 6 ACP + C16 + 6 CO2 + 6 H2O + 6 NADP+
IQ-143-extern_to_IQ-143	false	IQ-143-extern = IQ-143
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	true	2-Phospho-D-glycerate = 3-Phospho-D-glycerate
Glyc_2-phospho-D-glycerate-hydro-lyase	true	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
Glyc_6-phospho-beta-glucosidase	true	H2O + Salicin6-phosphate = Salicylalcohol + beta-D-Glucose6-phosphate
Glyc_6-phosphofructokinase	true	ATP-energy + beta-D-Fructose6-phosphate = ADP-energy + beta-D-Fructose16-bisphosphate
Glyc_acetaldehyde-dehydrogenase_NAD+	true	Acetaldehyde + H2O + NAD+ = Acetate + H+ + NADH
Glyc_Actetate-CoA-ligase	true	ATP-energy + Acetate + CoA = ADP-energy + Acetyl-CoA + Pyrophosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	true	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	true	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_ATP-alpha-D-glucokinase	true	ATP-metabolism + alpha-D-Glucose = ADP-metabolism + alpha-D-Glucose6-phosphate
Glyc_ATP-beta-D-glucokinase	true	ATP-energy + beta-D-Glucose = ADP-metabolism + beta-D-Glucose6-phosphate
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	true	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_D-Glucose-1-epimerase	true	alpha-D-Glucose = beta-D-Glucose
Glyc_D-Glucose-1-epimerase-ketol-isomerase	true	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal = Glyceronephosphate
Glyc_dihydrolipoamide-dehydrogenase	false	EnzymeN6-(dihydrolipoyl)lysine + NAD+ = EnzymeN6-(lipoyl)lysine + H+ + NADH
Glyc_fructose-bisphosphat-aldolase	true	beta-D-Fructose16-bisphosphate = (2R)-2-Hydroxy-3-(phosphonooxy)-propanal + Glyceronephosphate
Glyc_fructose-bisphosphatase	false	H2O + beta-D-Fructose16-bisphosphate = Orthophosphate + beta-D-Fructose6-phosphate
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NADP+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADPH
Glyc_lipoic_acetyltransferase	true	Acetyl-CoA + EnzymeN6-(dihydrolipoyl)lysine = CoA + Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine
Glyc_phosphoglycerate-kinase	true	3-Phospho-D-glycerate + ATP-energy = 3-Phospho-D-glyceroylphosphate + ADP-energy

Glyc_PTS-permease1	true	D-Glucose + ProteinN(pi)-phospho-L-histidine = Proteinhistidine + alpha-D-Glucose6-phosphate
Glyc_PTS-permease2	true	Arbutin + ProteinN(pi)-phospho-L-histidine = Arbutin6-phosphate + Proteinhistidine
Glyc_pyruvate_dehydrogenase	false	Pyruvate + Thiamindiphosphate = 2-(alpha-Hydroxyethyl)thiaminediphosphate + CO2
Glyc_Succinate-CoA-ligase	true	ATP-energy + CoA + Succinate = ADP-energy + Orthophosphate + Succinyl-CoA
OP_complex1	false	2 H+ + NADH + Ubichinon = 4 H+_ext + NAD+ + Ubihydrochinon
OP_complex2	false	4 H+ + Succinate + Ubichinon = Fumarate + Ubihydrochinon
OP_complex3	false	2 H+ + Ubihydrochinon + cytochrome_BC = 4 H+_ext + Ubichinon + cytochrome_C
OP_complex4	false	2 H+ + O- + cytochrome_C = 2 H+_ext + H2O
OP_complex5	false	ADP-energy + 3 H+_ext + Phosphate = ATP-energy + 3 H+ + H2O
PurM_5-nucleotidase_AMP	false	AMP-metabolism + H2O = Adenosine + Orthophosphate
PurM_5-nucleotidase_CMP	false	CMP + H2O = Cytidine + Orthophosphate
PurM_5-nucleotidase_dAMP	false	H2O + dAMP = Deoxyadenosine + Orthophosphate
PurM_5-nucleotidase_dCMP	false	H2O + dCMP = Deoxycytidine + Orthophosphate
PurM_5-nucleotidase_dGMP	false	H2O + dGMP = Deoxyguanosine + Orthophosphate
PurM_5-nucleotidase_dTMP	false	H2O + dTMP = Orthophosphate + Thymidine
PurM_5-nucleotidase_GMP	false	GMP + H2O = Guanosine + Orthophosphate
PurM_5-nucleotidase_IMP	false	H2O + IMP = Inosine + Orthophosphate
PurM_5-nucleotidase_UMP	false	H2O + UMP = Orthophosphate + Uridine
PurM_5-nucleotidase_XMP	false	H2O + Xanthosine5-phosphate = Orthophosphate + Xanthosine
PurM_adenylate-kinase_AMP	true	AMP-metabolism + ATP-energy = 2 ADP-metabolism
PurM_adenylate-kinase_dAMP	true	ATP-energy + dAMP = ADP-energy + dADP
PurM_adenylosuccinate-lyase	true	N6-(12-Dicarboxyethyl)-AMP = AMP-metabolism + Fumarate
PurM_adenylosuccinate-lyase2	true	1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole = 1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Fumarate
PurM_adenylylsulfate-kinase	true	ATP-energy + Adenylylsulfate = 3-phosphoadenylylsulfate + ADP-energy
PurM_ADP-ribose-ribophosphohydrolase	false	ADP-ribose + H2O = AMP-metabolism + D-Ribose5-phosphate
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	true	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Pyrophosphate = 5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate
PurM_AIR-carboxylase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate = Aminoimidazoleribotide + CO2

PurM_AMP-pyrophosphorylase	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_AMP-pyrophosphorylase2	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_ATP-phosphohydrolase	false	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
PurM_ATP_CDP-phosphotransferase	true	ATP-energy + CDP = ADP-energy + CTP
PurM_ATP_dADP-phosphotransferase	true	ATP-energy + dADP = ADP-energy + dATP
PurM_ATP_dCDP-phosphotransferase	true	ATP-energy + dCDP = ADP-energy + dCTP
PurM_ATP_dGDP-phosphotransferase	true	ATP-energy + dGDP = ADP-energy + dGTP
PurM_ATP_dIDP-phosphotransferase	true	ATP-energy + dIDP = ADP-energy + dITP
PurM_ATP_dTDP-phosphotransferase	true	ATP-energy + dTDP = ADP-energy + dTTP
PurM_ATP_dUDP-phosphotransferase	true	ATP-energy + dUDP = ADP-energy + dUTP
PurM_ATP_GMP-guanylate-kinase	true	ATP-energy + GMP = ADP-energy + GDP
PurM_ATP_GMP_guanylate-kinase	true	ATP-energy + dGMP = ADP-energy + dGDP
PurM_ATP_GTP-phosphotransferase	true	ATP-energy + GDP = ADP-energy + GTP
PurM_ATP_IDP-phosphotransferase	true	ATP-energy + IDP = ADP-energy + ITP
PurM_ATP_UTP-phosphotransferase	true	ATP-energy + UDP = ADP-energy + UTP
PurM_carbamate-kinase_ATP	true	ATP-energy + CO2 + NH3 = ADP-energy + Carbamoylphosphate
PurM_D-Ribose-1,5-phosphomutase	false	alpha-D-Ribose1-phosphate = D-Ribose5-phosphate
PurM_deoxyadenosine-kinase_ATP	false	ATP-energy + Deoxyadenosine = ADP-energy + dAMP
PurM_deoxycytidine-kinase_ATP	false	ATP-energy + Adenosine = ADP-energy + AMP-metabolism
PurM_deoxycytidine-kinase_ATP2	false	ATP-energy + Deoxycytidine = ADP-energy + dCMP
PurM_dGTP-diphosphohydrolase	false	H2O + dGTP = Pyrophosphate + dGMP
PurM_dITP-diphosphohydrolase	false	H2O + dITP = 2-Deoxyinosine-5-phosphate + Pyrophosphate
PurM_DNA-directed-RNA-polyermase_CTP	false	CTP + RNA = Pyrophosphate + RNA-C
PurM_DNA-directed-RNA-polyermase_GTP	false	GTP + RNA = Pyrophosphate + RNA-G
PurM_DNA-directed-RNA-polyermase_UTP	false	RNA + UTP = Pyrophosphate + RNA-U
PurM_DNA-directed-RNA-polymerase_ATP	false	ATP-metabolism + RNA = Pyrophosphate + RNA-A
PurM_GDP-reductase	false	GMP + H+-intern + NADPH = IMP + NADP+ + NH3
PurM_GMP-pyrophosphorylase	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine

PurM_GMP-pyrophosphorylase2	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PurM_GTP-diphosphohydrolase	false	GTP + H2O = GMP + Pyrophosphate
PurM_GTP-pyrophosphokinase	false	ATP-energy + GTP = ADP-energy + Guanosine3-diphosphate5-triphosphate
PurM_IMP-cyclohydrolase	true	H2O + IMP = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide
PurM_IMP-dehydrogenase	false	H2O + IMP + NAD+ = H+-intern + NADH + Xanthosine5-phosphate
PurM_IMP-pyrophosphorylase	true	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
PurM_IMP_L-aspartate-ligase	true	GTP + IMP + L-Aspartate = GDP + N6-(12-Dicarboxyethyl)-AMP + Orthophosphate
PurM_ITP-diphosphohydrolase	false	H2O + ITP = IMP + Pyrophosphate
PurM_metaphosphatase	true	Guanosine3-diphosphate5-triphosphate + H2O = Guanosine_3',5'-bis(diphosphate) + Orthophosphate
PurM_nucleoside-diphosphate-phosphotransferase_ATP	true	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
PurM_nucleotide-phosphatase_Adenine	true	Adenosine + Orthophosphate = Adenine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Deoxyadenosine	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PurM_nucleotide-phosphatase_Deoxyguanosine	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PurM_nucleotide-phosphatase_Deoxyinosine	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
PurM_nucleotide-phosphatase_Deoxyuridine	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PurM_nucleotide-phosphatase_Guanosine	true	Guanosine + Orthophosphate = Guanine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Inosine	true	Inosine + Orthophosphate = Hypoxanthine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Xanthosine	true	Orthophosphate + Xanthosine = Xanthine + alpha-D-Ribose1-phosphate
PurM_PRPP-synthetase	true	ATP-energy + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy
PurM_pyruvate-phosphotransferase_ATP	false	ATP-metabolism + Pyruvate = ADP-metabolism + Phosphoenolpyruvate
PurM_pyruvate-phosphotransferase_dATP	false	Pyruvate + dATP = Phosphoenolpyruvate + dADP
PurM_pyruvate-phosphotransferase_dGTP	false	Pyruvate + dGTP = Phosphoenolpyruvate + dGDP
PurM_pyruvate-phosphotransferase_GTP	false	GTP + Pyruvate = GDP + Phosphoenolpyruvate
PurM_SAICAR-synthetase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate + ATP-metabolism + L-Aspartate = 1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole + ADP-metabolism + Orthophosphate
PurM_thioredoxin-oxidoreductase_dATP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dCDP	false	CDP + Thioredoxin = H2O + Oxidizedthioredoxin + dCDP
PurM_thioredoxin-oxidoreductase_dCTP	false	CTP + Thioredoxin = Oxidizedthioredoxin + dCTP

PurM_thioredoxin-oxidoreductase_dGDP	false	GDP + Thioredoxin = H2O + Oxidizedferredoxin + dGDP
PurM_thioredoxin-oxidoreductase_dGTP	false	GTP + Thioredoxin = H2O + Oxidizedthioredoxin + dGTP
PurM_thioredoxin-oxidoreductase_dUDP	false	Thioredoxin + UDP = H2O + Oxidizedthioredoxin + dUDP
PurM_thioredoxin-oxidoreductase_dUTP	false	Thioredoxin + UTP = Oxidizedthioredoxin + dUTP
PurM_thioredoxin-oxidoreductased_dADP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_urea-amidohydrolase	false	H2O + Urea = CO2 + 2 NH3
PurM_UTP-diphosphohydrolase	false	H2O + UTP = Pyrophosphate + UMP
PurM_xanthosine-phosphoribosyltransferase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP-pyrophosphorylase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP_L-glutamine-amide-ligase	false	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = ADP-energy + GMP + L-Glutamate + Pyrophosphate
PurM_XTP-diphosphohydrolase	false	H2O + XTP = Pyrophosphate + Xanthosine5-phosphate
PyrM_2,3-cyclic-nucleotidase_CMP	false	23-CyclicCMP + H2O = 3-CMP
PyrM_2,3-cyclic-nucleotidase_UMP	false	23-CyclicUMP + H2O = 3-UMP
PyrM_aspartate-carbamoyltransferase	false	Carbamoylphosphate + L-Aspartate = N-Carbamoyl-L-aspartate + Orthophosphate
PyrM_ATP_dTDP_thymidylate-kinase	true	ATP-energy + dTMP = ADP-energy + dTDP
PyrM_ATP_dUDP_thymidylate-kinase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_CO2_L-glutamine-amido-ligase	false	2 ATP-energy + H2O + HCO3- + L-Glutamine = 2 ADP-energy + Carbamoylphosphate + L-Glutamate + Orthophosphate
PyrM_CTP-synthase	false	ATP-energy + NH3 + UTP = ADP-energy + CTP + Orthophosphate
PyrM_cytidilate-kinase_CTP	true	ATP-energy + CMP = ADP-energy + CDP
PyrM_cytidilate-kinase_dCMP	true	ATP-energy + dCMP = ADP-energy + dCDP
PyrM_cytidine-aminohydrolase	true	Cytidine + H2O = NH3 + Uridine
PyrM_cytidine-kinase_ATP	false	ATP-energy + Cytidine = ADP-energy + CMP
PyrM_cytidine-kinase_dATP	false	Cytidine + dATP = CMP + dADP
PyrM_cytidine-kinase_dCTP	false	Cytidine + dCTP-ex = CMP + dCDP-ex
PyrM_cytidine-kinase_dGTP	false	Cytidine + dGTP = CMP + dGDP
PyrM_cytidine-kinase_dTTP	false	Cytidine + dTTP-ex = CMP + dTDP-ex
PyrM_cytidine-kinase_dUTP	false	Cytidine + dUTP-ex = CMP + dUDP-ex

PyrM_cytidine-kinase_GTP	false	Cytidine + GTP = CMP + GDP
PyrM_cytidine-kinase_ITP	false	Cytidine + ITP = CMP + IDP
PyrM_cytidine-kinase_UTP	false	Cytidine + UTP = CMP + UDP
PyrM_cytidine-ribohydrolase	false	Cytidine + H2O = Cytosine + D-Ribose
PyrM_dCMP-aminohydrolase	true	H2O + dCMP = NH3 + dUMP
PyrM_deoxyadenosine-phosphorylase	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PyrM_Deoxycytidine-aminohydrolase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_Deoxycytidine-deaminase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_deoxyguanosine-phosphorylase	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PyrM_deoxyinosine-phosphorylase	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Inosine
PyrM_deoxyuridine-phosphorylase	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PyrM_dihydroorotase	true	(S)-Dihydroorotate + H2O = N-Carbamoyl-L-aspartate
PyrM_dihydroorotate-oxidase	true	(S)-Dihydroorotate + Oxygen = H2O2 + Orotate
PyrM_dUMP-phosphotransferase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_dUTP-diphosphatase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_dUTP-diphosphohydrolase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_nucleoside-phosphate-kinase_ATP	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-phosphate-kinase_ATP2	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-triphosphate-adenylate-kinase	true	ATP-energy + UTP = ADP-energy + UDP
PyrM_OMP-decarboxylase	false	Orotidine5-phosphate = CO2 + UMP
PyrM_orotate-phosphoribosyltransferase	true	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
PyrM_pyrimidine-nucleoside-phosphorylase	true	Cytidine + Orthophosphate = Cytosine + alpha-D-Ribose1-phosphate
PyrM_thioredoxin-reductase	false	H+ + NADPH + Oxidizedthioredoxin = NADP+ + Thioredoxin
PyrM_thymidilate-synthase	false	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
PyrM_thymidine-kinase_dTMP	true	ATP-energy + Thymidine = ADP-energy + dTMP
PyrM_thymidine-kinase_dUMP	true	ATP-energy + Deoxyuridine = ADP-energy + dUMP
PyrM_thymidine-phosphorylase	true	Orthophosphate + Thymidine = 2-Deoxy-D-ribose1-phosphate + Thymine
PyrM_UMP-pyrophosphorylase	true	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil

PyrM_uridine-kinase_ATP	false	ATP-energy + Uridine = ADP-energy + UMP
PyrM_uridine-kinase_dATP	false	Uridine + dATP = UMP + dADP
PyrM_uridine-kinase_dCTP	false	Uridine + dCTP-ex = UMP + dCDP-ex
PyrM_uridine-kinase_dGTP	false	Uridine + dGTP = UMP + dGDP
PyrM_uridine-kinase_dTTP	false	Uridine + dTTP-ex = UMP + dTDP-ex
PyrM_uridine-kinase_dUTP	false	Uridine + dUTP-ex = UMP + dUDP-ex
PyrM_uridine-kinase_GTP	false	GTP + Uridine = GDP + UMP
PyrM_uridine-kinase_ITP	false	ITP + Uridine = IDP + UMP
PyrM_uridine-kinase_UTP	false	UTP + Uridine = UDP + UMP
PyrM_uridine-phosphorylase	true	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
PyrM_uridine-ribohydrolase	false	H2O + Uridine = D-Ribose + Uracil
PyrM_UTP_L-glutamine-amido-ligase	false	ATP-energy + H2O + L-Glutamine + UTP = ADP-energy + CTP + L-Glutamate + Orthophosphate
SERP0290-zinc-transport_efflux	false	ATP-energy + H2O + Zn2+-intern = ADP-energy + Pyrophosphate + Zn2+-extern
SERP0291-zinc-transporter_import	false	ATP-energy + H2O + Zn2+-extern = ADP-energy + Pyrophosphate + Zn2+-intern
SERP0292-iron-dicitrate-transporter_import	false	ATP-energy + H2O + ferric-dicitrate_extern = ADP-energy + Pyrophosphate + ferric_dicitrate_intern
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	true	Ethanol + NAD+ = Acetaldehyde + H+ + NADH
SERP0653-PurM_FGAM-synthethase	false	5-Phosphoribosyl-N-formylglycinamide + ATP-metabolism + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ADP-metabolism + L-Glutamate + Orthophosphate
SERP0655-PurM_amidophosphoribosyltransferase	false	5-Phosphoribosylamine + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O + L-Glutamine
SERP0656-PurM_AIR_synthetase	false	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-metabolism = ADP-metabolism + Aminoimidazoleribotide + Orthophosphate
SERP0657-PurM_GAR-formyltransferase	false	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide = 5-Phosphoribosyl-N-formylglycinamide + Tetrahydrofolate
SERP0658-PurM_AICAR-formyltransferase	false	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + 10-Formyltetrahydrofolate = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide + Tetrahydrofolate
SERP0659-PurM_phosphoribosylamine-glycine-ligase	false	5-Phosphoribosylamine + ATP-metabolism + Glycine = 5-Phosphoribosylglycinamide + ADP-metabolism + Orthophosphate
SERP0686-spermidine/putrescine-transport_import	false	ATP-metabolism + H2O + putrescine_extern + spermidine_extern = ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern

SERP0687-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0688-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0765-Uracil-permease-transport_import	false	H+-extern + uracil_extern = H+-intern + uracil_intern
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	false	DNA + dATP = DNA-A + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	false	DNA + dCTP = DNA-C + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	false	DNA + dGTP = DNA-G + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	false	DNA + dTTP = DNA-T + Pyrophosphate
SERP0841-PurM_PNPase_ADP	false	ADP-metabolism + RNA = Orthophosphate + RNA-A
SERP0841-PurM_PNPase_GDP	false	GDP + RNA = Orthophosphate + RNA-G
SERP1403-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143-extern + Pyrophosphate
SERP1802-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1803-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1944-MultiDrug-transport_efflux	false	IQ-143 + H+-intern = IQ-143-extern + H+-extern
SERP1951-lipoprotein-transport_efflux/import	true	ATP-energy + H2O + lipoprotein_extern = ADP-energy + Pyrophosphate + lipoprotein_intern
SERP1952-macrolide-transport_efflux	false	ATP-energy + H2O + macrolide_intern = ADP-energy + Pyrophosphate + macrolide_extern
SERP1997-formate/nitrite-transport_efflux/import	false	H+-intern + formate_internal + nitrite_external = H+-extern + formate_extern + nitrite_intern
SERP2060-glyerol-transport_import	false	ATP-energy + H2O + glycerol-3-phosphate_extern = ADP-energy + Pyrophosphate + glycerol-3-phosphate_intern
SERP2156-Glyc_L-lactate-dehydrogenase	true	(S)-Lactate + NAD+ = H+ + NADH + Pyruvate
SERP2179-choline/betaine/carnitine-transp_efflux	false	H+-extern + betaine_intern + carnitine-extern + choline-extern = H+-intern + betaine-extern + carnitine-intern + choline-intern
SERP2186-PurM_ATP_sulfate-adenylyltransferase	false	ATP-energy + Sulfate = Adenylylsulfate + Pyrophosphate
SERP2283-phopsphonate-transport_import	false	ATP-energy + H2O + phosphonate_extern = ADP-energy + Pyrophosphate + phosphonate_intern
SERP2289-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143-extern + Pyrophosphate
TCA_citrate-hydro-lyase	true	Citrate = H2O + cis-Aconitate
TCA_citrate-hydroxymutase	true	Citrate = Isocitrate

TCA_citrate_synthase	true	Citrate + CoA = Acetyl-CoA + H2O + Oxaloacetate
TCA_fumarate-hydratase	true	(S)-Malate = Fumarate + H2O
TCA_isocitrate-hydro-lyase	true	Isocitrate = H2O + cis-Aconitate
TCA_lipoic-transsuccinylase	true	EnzymeN6-(dihydrolipoyl)lysine + Succinyl-CoA = CoA + Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine
TCA_Oxidoreductase	false	Isocitrate + NAD+ = 2-Oxoglutarate + CO2 + H+ + NADH
TCA_oxoglutarate-dehydrogenase-complex1	true	2-Oxoglutarate + Thiamindiphosphate = 3-Carboxy-1-hydroxypropyl-ThPP + CO2
TCA_oxoglutarate-dehydrogenase-complex2	true	3-Carboxy-1-hydroxypropyl-ThPP + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine + Thiamindiphosphate
TCA_oxoglutarate-synthase	false	CO2 + Reducedferredoxin + Succinyl-CoA = 2-Oxoglutarate + CoA + Oxidizedferredoxin
TCA_PEP-carboxylase	true	ATP-energy + Oxaloacetate = ADP-energy + CO2 + Phosphoenolpyruvate
TCA_Pyruvate_CO2-ligase	true	ATP-energy + HCO3- + Pyruvate = ADP-energy + Orthophosphate + Oxaloacetate
TCA_pyruvate_dehydrogenase	false	2-(alpha-Hydroxyethyl)thiaminediphosphate + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine + Thiamindiphosphate
TCA_succinate-dehydrogenase	true	Acceptor + Succinate = Fumarate + Reducedacceptor

[1] List of enzymes used to build the metabolic web of *S. epidermidis* RP62A. This list is composed of data derived from KEGG and own annotations.

Abbreviations: AS: Amino acids; FA: fatty acid synthesis and degradation; Glyc: Glycolysis and Pentose Phosphate Pathways; OP: Oxidative phosphorylation; PurM: Purine Metabolism; PyrM: Pyrimidine Metabolism; TCA: Citric acid Cycle; SERP: Enzymes measured by gene expression micro array.

Table S VI.1.4: List of enzmyes used to build metabolic web for man [1].

Enzyme name	reversible?	Reaction equation
ADP-energy_to_ADP-metabolism	True	ADP-metabolism = AMP-energy
AMP-energy_to_AMP-metabolism	True	AMP-metabolism = AMP-energy
ATP-energy_to_ATP-metabolism	True	ATP-metabolism = ATP-energy
Cytochrome_1A2	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
Cytochrome_2C19	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
Cytochrome_2C8	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
Cytochrome_2C9	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
Cytochrome_2D6	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
Cytochrome_3A4	False	ATP-energy + IQ-143 = ADP-energy + IQ-143_deactivated
DNA-extern_To_DNA-intern	True	DNA-extern = DNA
EC:1.1.1.1.-rn:R00754	False	Ethanol + NAD+ = Acetaldehyde + H+ + NADH
EC:1.1.1.2-rn:R00746	False	Ethanol + NADP+ = Acetaldehyde + H+ + NADPH
EC:1.1.1.205-rn:R01130	True	H2O + IMP + NAD+ = H+ + NADH + Xanthosine5-phosphate
EC:1.1.1.27-rn:R00703	True	(S)-Lactate + NAD+ = H+ + NADH + Pyruvate
EC:1.1.1.37-rn:R00342	True	(S)-Malate + NAD+ = H+ + NADH + Oxaloacetate
EC:1.1.1.41-rn:R00709	False	Isocitrate + NAD+ = 2-Oxoglutarate + CO2 + H+ + NADH
EC:1.1.1.42-rn:R00268	True	Oxalosuccinate = 2-Oxoglutarate + CO2
EC:1.1.1.42-rn:R01899	True	Isocitrate + NADP+ = H+ + NADPH + Oxalosuccinate
EC:1.17.1.4-rn:R01768	False	H2O + Hypoxanthine + NAD+ = NADH + Xanthine
EC:1.17.1.4-rn:R02103	False	H2O + NAD+ + Xanthine = H+ + NADH + Urate
EC:1.17.3.2-rn:R01769	False	H2O + Hypoxanthine + Oxygen = H2O2 + Xanthine
EC:1.17.3.2-rn:R02107	False	H2O + Oxygen + Xanthine = H2O2 + Urate
EC:1.17.4.1-rn:R02017	False	H2O + Oxidizedthioredoxin + dADP = ADP-energy + Thioredoxin
EC:1.17.4.1-rn:R02018	False	H2O + Oxidizedthioredoxin + dUDP = Thioredoxin + UDP
EC:1.17.4.1-rn:R02019	False	H2O + Oxidizedthioredoxin + dGDP = GDP + Thioredoxin
EC:1.17.4.1-rn:R02024	False	H2O + Oxidizedthioredoxin + dCDP = CDP + Thioredoxin

EC:1.2.1.12-rn:R01061	False	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
EC:1.2.1.13-rn:R01063	False	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NADP+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADPH
EC:1.2.1.3-rn:R00710	True	Acetaldehyde + H2O + NAD+ = Acetate + H+ + NADH
EC:1.2.1.3-rn:R00711	True	Acetaldehyde + H2O + NADP+ = Acetate + H+ + NADPH
EC:1.2.4.1-rn:R00014	False	Pyruvate + Thiamindiphosphate = 2-(alpha-Hydroxyethyl)thiaminediphosphate + CO2
EC:1.2.4.1-rn:R03270	False	2-(alpha-Hydroxyethyl)thiaminediphosphate + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine + Thiamindiphosphate
EC:1.2.4.2-rn:R00621	True	2-Oxoglutarate + Thiamindiphosphate = 3-Carboxy-1-hydroxypropyl-ThPP + CO2
EC:1.2.4.2-rn:R03316	True	3-Carboxy-1-hydroxypropyl-ThPP + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine + Thiamindiphosphate
EC:1.3.1.2-rn:R00978	True	56-Dihydrouracil + NADP+ = H+ + NADPH + Uracil
EC:1.3.1.2-rn:R01415	True	56-Dihydrothymine + NADP+ = H+ + NADPH + Thymine
EC:1.3.3.1-rn:R01867	True	(S)-Dihydroorotate + Oxygen = H2O2 + Orotate
EC:1.3.5.1-rn:R02164	True	Succinate + Ubiquinone = Fumarate + Ubiquinol
EC:1.7.1.7-rn:R01134	False	IMP + NADP+ + NH3 = GMP + H+ + NADPH
EC:1.8.1.4-rn:R07618	False	EnzymeN6-(dihydrolipoyl)lysine + NAD+ = EnzymeN6-(lipoyl)lysine + H+ + NADH
EC:1.8.1.9-rn:R02016	False	NADP+ + Thioredoxin = H+ + NADPH + Oxidizedthioredoxin
EC:2.1.1.45-rn:R02101	False	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
EC:2.1.3.2-rn:R01397	False	Carbamoylphosphate + L-Aspartate = N-Carbamoyl-L-aspartate + Orthophosphate
EC:2.3.1.12-rn:R02569	True	Acetyl-CoA + EnzymeN6-(dihydrolipoyl)lysine = CoA + Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine
EC:2.3.1.61-rn:R02570	True	EnzymeN6-(dihydrolipoyl)lysine + Succinyl-CoA = CoA + Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine
EC:2.3.3.1-rn:R00351	True	Citrate + CoA = Acetyl-CoA + H2O + Oxaloacetate
EC:2.3.3.8-rn:R00352	True	ATP-energy + Citrate + CoA = ADP-energy + Acetyl-CoA + Orthophosphate + Oxaloacetate
EC:2.4.2.1-rn:R01561	True	Adenosine + Orthophosphate = Adenine + alpha-D-Ribose1-phosphate
EC:2.4.2.1-rn:R01863	True	Inosine + Orthophosphate = Hypoxanthine + alpha-D-Ribose1-phosphate
EC:2.4.2.1-rn:R01969	True	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine

EC:2.4.2.1-rn:R02147	True	Guanosine + Orthophosphate = Guanine + alpha-D-Ribose1-phosphate
EC:2.4.2.1-rn:R02297	True	Orthophosphate + Xanthosine = Xanthine + alpha-D-Ribose1-phosphate
EC:2.4.2.1-rn:R02484	True	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
EC:2.4.2.1-rn:R02557	True	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
EC:2.4.2.1-rn:R02748	True	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
EC:2.4.2.10-rn:R01870	True	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
EC:2.4.2.3-rn:R01876	True	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
EC:2.4.2.4-rn:R01570	True	Orthophosphate + Thymidine = 2-Deoxy-D-ribose1-phosphate + Thymine
EC:2.4.2.4-rn:R01969	True	2-Deoxy-D-ribose1-phosphate + Guanine = Deoxyguanosine + Orthophosphate
EC:2.4.2.4-rn:R02484	True	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
EC:2.4.2.4-rn:R02557	True	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
EC:2.4.2.4-rn:R02748	True	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
EC:2.4.2.7-rn:R00190	True	AMP-energy + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
EC:2.4.2.7-rn:R01229	True	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
EC:2.4.2.7-rn:R04378	True	AICAR + Pyrophosphate = 5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate
EC:2.4.2.8-rn:R01132	True	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
EC:2.4.2.8-rn:R02142	True	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
EC:2.4.2.9-rn:R00966	True	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
EC:2.7.1.11-rn:R04779	True	ATP-energy + beta-D-Fructose6-phosphate = ADP-energy + beta-D-Fructose16-bisphosphate
EC:2.7.1.113-rn:R01967	False	ATP-energy + Deoxyguanosine = ADP-energy + dGMP
EC:2.7.1.2-rn:R01600	True	ATP-energy + beta-D-Glucose = ADP-energy + beta-D-Glucose6-phosphate
EC:2.7.1.2-rn:R01786	True	ATP-energy + alpha-D-Glucose = ADP-energy + alpha-D-Glucose6-phosphate
EC:2.7.1.21-rn:R01567	True	ATP-energy + Thymidine = ADP-energy + dTMP
EC:2.7.1.21-rn:R02099	True	ATP-energy + Deoxyuridine = ADP-energy + dUMP
EC:2.7.1.25-rn:R00509	True	ATP-energy + Adenylylsulfate = 3-Phosphoadenylylsulfate + ADP-energy
EC:2.7.1.40-rn:R00200	False	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
EC:2.7.1.40-rn:R00430	False	GTP + Pyruvate = GDP + Phosphoenolpyruvate
EC:2.7.1.40-rn:R01138	False	Pyruvate + dATP = Phosphoenolpyruvate + dADP

EC:2.7.1.40-rn:R01858	False	Pyruvate + dGTP = Phosphoenolpyruvate + dGDP
EC:2.7.1.48-rn:R00513	False	ATP-energy + Cytidine = ADP-energy + CMP
EC:2.7.1.48-rn:R00516	False	Cytidine + UTP = CMP + UDP
EC:2.7.1.48-rn:R00517	False	Cytidine + GTP = CMP + GDP
EC:2.7.1.48-rn:R00962	False	Cytidine + ITP = CMP + IDP
EC:2.7.1.48-rn:R00964	False	ATP-energy + Uridine = ADP-energy + UMP
EC:2.7.1.48-rn:R00967	False	UTP + Uridine = UDP + UMP
EC:2.7.1.48-rn:R00968	False	GTP + Uridine = GDP + UMP
EC:2.7.1.48-rn:R00970	False	ITP + Uridine = IDP + UMP
EC:2.7.1.48-rn:R01548	False	Cytidine + dATP = CMP + dADP
EC:2.7.1.48-rn:R01549	False	Uridine + dATP = UMP + dADP
EC:2.7.1.48-rn:R01880	False	Uridine + dGTP = UMP + dGDP
EC:2.7.1.48-rn:R02091	False	Cytidine + dGTP = CMP + dGDP
EC:2.7.1.48-rn:R02096	False	Cytidine + dTTP = CMP + dTDP
EC:2.7.1.48-rn:R02097	False	Uridine + dTTP = UMP + dTDP
EC:2.7.1.48-rn:R02327	False	Uridine + dCTP = UMP + dCDP
EC:2.7.1.48-rn:R02332	False	Uridine + dUTP = UMP + dUDP
EC:2.7.1.48-rn:R02371	False	Cytidine + dCTP = CMP + dCDP
EC:2.7.1.48-rn:R02372	False	Cytidine + dUTP = CMP + dUDP
EC:2.7.1.74-rn:R00185	False	ATP-energy + Adenosine = ADP-energy + AMP-metabolism
EC:2.7.1.74-rn:R01666	False	ATP-energy + Deoxycytidine = ADP-energy + dCMP
EC:2.7.2.3-rn:R01512	True	3-Phospho-D-glycerate + ATP-energy = 3-Phospho-D-glyceroylphosphate + ADP-energy
EC:2.7.4.10-rn:R00157	True	AMP-energy + UTP = ADP-energy + UDP
EC:2.7.4.14-rn:R00158	True	ATP-energy + UMP = ADP-energy + UDP
EC:2.7.4.14-rn:R00512	True	ATP-energy + CMP = ADP-energy + CDP
EC:2.7.4.14-rn:R01665	True	ATP-energy + dCMP = ADP-energy + dCDP
EC:2.7.4.3-rn:R00127	True	AMP-metabolism + ATP-energy = 2 ADP-metabolism
EC:2.7.4.3-rn:R01547	True	ATP-energy + dAMP = ADP-energy + dADP

EC:2.7.4.4-rn:R00334	True	ATP-energy + UMP = ADP-energy + UDP
EC:2.7.4.4-rn:R02098	True	ATP-energy + dUMP = ADP-energy + dUDP
EC:2.7.4.6-rn:R00124	True	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
EC:2.7.4.6-rn:R00156	True	ATP-energy + UDP = ADP-energy + UTP
EC:2.7.4.6-rn:R00330	True	ATP-energy + GDP = ADP-energy + GTP
EC:2.7.4.6-rn:R00570	True	ATP-energy + CDP = ADP-energy + CTP
EC:2.7.4.6-rn:R00722	True	ATP-energy + IDP = ADP-energy + ITP
EC:2.7.4.6-rn:R01137	True	ATP-energy + dADP = ADP-energy + dATP
EC:2.7.4.6-rn:R01857	True	ATP-energy + dGDP = ADP-energy + dGTP
EC:2.7.4.6-rn:R02093	True	ATP-energy + dTDP = ADP-energy + dTTP
EC:2.7.4.6-rn:R02326	True	ATP-energy + dCDP = ADP-energy + dCTP
EC:2.7.4.6-rn:R02331	True	ATP-energy + dUDP = ADP-energy + dUTP
EC:2.7.4.6-rn:R03530	True	ATP-energy + dIDP = ADP-energy + dITP
EC:2.7.4.8-rn:R00332	True	ATP-energy + GMP = ADP-energy + GDP
EC:2.7.4.8-rn:R02090	True	ATP-energy + dGMP = ADP-energy + dGDP
EC:2.7.4.9-rn:R02094	True	ATP-energy + dTMP = ADP-energy + dTDP
EC:2.7.4.9-rn:R02098	True	ATP-energy + dUMP = ADP-energy + dUDP
EC:2.7.6.1-rn:R01049	True	ATP-energy + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + AMP-energy
EC:2.7.7.6-rn:R00435	True	ATP-metabolism + RNA = Pyrophosphate + RNA-A
EC:2.7.7.6-rn:R00441	True	GTP + RNA = Pyrophosphate + RNA-G
EC:2.7.7.6-rn:R00442	True	CTP + RNA = Pyrophosphate + RNA-C
EC:2.7.7.6-rn:R00443	True	RNA + UTP = Pyrophosphate + RNA-U
EC:3.1.3.11-rn:R04780	False	H2O + beta-D-Fructose16-bisphosphate = Orthophosphate + beta-D-Fructose6-phosphate
EC:3.1.3.5-rn:R00183	False	AMP-energy + H2O = Adenosine + Orthophosphate
EC:3.1.3.5-rn:R00511	False	CMP + H2O = Cytidine + Orthophosphate
EC:3.1.3.5-rn:R00963	False	H2O + UMP = Orthophosphate + Uridine
EC:3.1.3.5-rn:R01126	False	H2O + IMP = Inosine + Orthophosphate
EC:3.1.3.5-rn:R01227	False	GMP + H2O = Guanosine + Orthophosphate

EC:3.1.3.5-rn:R01569	False	H2O + dTMP = Orthophosphate + Thymidine
EC:3.1.3.5-rn:R01664	False	H2O + dCMP = Deoxycytidine + Orthophosphate
EC:3.1.3.5-rn:R01968	False	H2O + dGMP = Deoxyguanosine + Orthophosphate
EC:3.1.3.5-rn:R02088	False	H2O + dAMP = Deoxyadenosine + Orthophosphate
EC:3.1.3.5-rn:R02719	False	H2O + Xanthosine5-phosphate = Orthophosphate + Xanthosine
EC:3.1.3.9-rn:R01788	False	H2O + alpha-D-Glucose6-phosphate = Orthophosphate + alpha-D-Glucose
EC:3.1.4.17-rn:R00191	False	35-CyclicAMP + H2O = AMP-energy
EC:3.1.4.17-rn:R01234	False	35-CyclicGMP + H2O = GMP
EC:3.5.1.6-rn:R00905	False	3-Ureidopropionate + H2O = CO2 + NH3 + beta-Alanine
EC:3.5.1.6-rn:R04666	False	3-Ureidoisobutyrate + H2O = 3-Aminoisobutanoate + CO2 + NH3
EC:3.5.2.2-rn:R02269	True	56-Dihydrouracil + H2O = 3-Ureidopropionate
EC:3.5.2.2-rn:R03055	True	56-Dihydrothymine + H2O = 3-Ureidoisobutyrate
EC:3.5.2.3-rn:R01993	True	(S)-Dihydroorotate + H2O = N-Carbamoyl-L-aspartate
EC:3.5.2.5-rn:R02425	False	Allantoate + H2O = Allantoine
EC:3.5.3.4-rn:R02422	False	Allantoate + H2O = (-)-Ureidoglycolate + Urea
EC:3.5.4.10-rn:R01127	True	H2O + IMP = FAICAR
EC:3.5.4.12-rn:R01663	True	H2O + dCMP = NH3 + dUMP
EC:3.5.4.3-rn:R01676	False	Guanine + H2O = NH3 + Xanthine
EC:3.5.4.4-rn:R01560	False	Adenosine + H2O = Inosine + NH3
EC:3.5.4.4-rn:R02556	False	Deoxyadenosine + H2O = Deoxyinosine + NH3
EC:3.5.4.5-rn:R01878	True	Cytidine + H2O = NH3 + Uridine
EC:3.5.4.5-rn:R02485	True	Deoxycytidine + H2O = Deoxyuridine + NH3
EC:3.5.4.6-rn:R00181	False	AMP-energy + H2O = IMP + NH3
EC:3.6.1.11-rn:R03409	True	Guanosine3-diphosphate5-triphosphate + H2O = Guanosine35-bis(diphosphate) + Orthophosphate
EC:3.6.1.13-rn:R01054	False	ADP-ribose + H2O = AMP-energy + D-Ribose5-phosphate
EC:3.6.1.17-rn:R00184	True	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = AMP-energy + ATP-energy
EC:3.6.1.17-rn:R00969	True	H2O + P1P4-Bis(5-uridyl)tetraphosphate = UMP + UTP
EC:3.6.1.17-rn:R01232	True	H2O + P1P4-Bis(5-guanosyl)tetraphosphate = GMP + GTP

EC:3.6.1.17-rn:R02805	True	H2O + P1P4-Bis(5-xanthosyl)tetraphosphate = XTP + Xanthosine5-phosphate
EC:3.6.1.19-rn:R00426	False	GTP + H2O = GMP + Pyrophosphate
EC:3.6.1.19-rn:R00662	False	H2O + UTP = Pyrophosphate + UMP
EC:3.6.1.19-rn:R00720	False	H2O + ITP = IMP + Pyrophosphate
EC:3.6.1.19-rn:R01855	False	H2O + dGTP = Pyrophosphate + dGMP
EC:3.6.1.19-rn:R02100	False	H2O + dUTP = Pyrophosphate + dUMP
EC:3.6.1.19-rn:R02720	False	H2O + XTP = Pyrophosphate + Xanthosine5-phosphate
EC:3.6.1.19-rn:R03531	False	H2O + dITP = 2-Deoxyinosine5-phosphate + Pyrophosphate
EC:3.6.1.23-RN:R02100	False	H2O + dUTP = Pyrophosphate + dUMP
EC:3.6.1.29-rn:R00187	True	H2O + P1P3-Bis(5-adenosyl)triphosphate = ADP-energy + AMP-energy
EC:3.6.1.3-rn:R00086	False	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
EC:3.6.1.41-rn:R00125	False	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = 2 ADP-energy
EC:3.6.1.5-rn:R00086	False	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
EC:3.6.1.5-rn:R00122	False	ADP-energy + Ca2+IN + H2O = AMP-energy + Orthophosphate
EC:3.6.1.5-rn:R00155	False	Ca2+IN + H2O + UDP = Orthophosphate + UMP
EC:3.6.1.5-rn:R00159	False	Ca2+IN + H2O + UTP = Orthophosphate + UDP
EC:3.6.1.5-rn:R00328	False	Ca2+IN + GDP + H2O = GMP + Orthophosphate
EC:3.6.1.5-rn:R00335	False	Ca2+IN + GTP + H2O = GDP + Orthophosphate
EC:3.6.1.5-rn:R00514	False	CDP + Ca2+IN + H2O = CMP + Orthophosphate
EC:3.6.1.5-rn:R00569	False	CTP + Ca2+IN + H2O = CDP + Orthophosphate
EC:3.6.1.5-rn:R00719	False	Ca2+IN + H2O + ITP = IDP + Orthophosphate
EC:3.6.1.5-rn:R00961	False	Ca2+IN + H2O + IDP = IMP + Orthophosphate
EC:3.6.1.5-rn:R02092	False	Ca2+IN + H2O + dTDP = Orthophosphate + dTMP
EC:3.6.1.5-rn:R02095	False	Ca2+IN + H2O + dTTP = Orthophosphate + dTDP
EC:3.6.1.6-rn:R00155	False	Ca2+IN + H2O + UDP = Orthophosphate + UMP
EC:3.6.1.6-rn:R00328	False	Ca2+IN + GDP + H2O = GMP + Orthophosphate
EC:3.6.1.6-rn:R00961	False	Ca2+IN + H2O + IDP = IMP + Orthophosphate
EC:3.6.1.7-rn:R01515	False	3-Phospho-D-glyceroylphosphate + H2O = 3-Phospho-D-glycerate + Orthophosphate

EC:3.6.1.8-rn:R00086	False	ATP-metabolism + Ca2+IN + H2O = ADP-energy + Orthophosphate
EC:3.6.1.8-rn:R00087	False	ATP-metabolism + Ca2+IN + H2O = AMP-energy + Orthophosphate
EC:3.6.1.8-rn:R00426	False	Ca2+IN + GTP-extern + H2O = GMP + Pyrophosphate
EC:3.6.1.8-rn:R00720	False	Ca2+IN + H2O + ITP-extern = IMP + Pyrophosphate
EC:3.6.1.9-rn:R00507	False	3-Phosphoadenylylsulfate + H2O = Adenosine35-bisphosphate + Sulfate
EC:4.1.1.21-rn:R04209	True	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate = Aminoimidazoleribotide + CO2
EC:4.1.1.23-rn:R00965	True	Orotidine5-phosphate = CO2 + UMP
EC:4.1.1.32-rn:R00431	True	GTP + Oxaloacetate = CO2 + GDP + Phosphoenolpyruvate
EC:4.1.1.32-rn:R00726	True	ITP + Oxaloacetate = CO2 + IDP + Phosphoenolpyruvate
EC:4.1.2.13-rn:R01070	True	beta-D-Fructose16-bisphosphate = (2R)-2-Hydroxy-3-(phosphonooxy)-propanal + Glyceronephosphate
EC:4.1.3.6-rn:R00362	False	Citrate = Acetate + Oxaloacetate
EC:4.2.1.11-rn:R00658	True	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
EC:4.2.1.2-rn:R01082	True	(S)-Malate = Fumarate + H2O
EC:4.2.1.3-rn:R01324	True	Citrate = Isocitrate
EC:4.2.1.3-rn:R01325	True	Citrate = H2O + cis-Aconitate
EC:4.2.1.3-rn:R01900	True	Isocitrate = H2O + cis-Aconitate
EC:4.2.1.70-rn:R01055	True	D-Ribose5-phosphate + Uracil = H2O + Pseudouridine5-phosphate
EC:4.3.2.2-rn:R01083	True	N6-(12-Dicarboxyethyl)-AMP = AMP-energy + Fumarate
EC:4.3.2.2-rn:R04559	True	1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole = AICAR + Fumarate
EC:4.6.1.1-rn:R00089	False	ATP-energy = 35-CyclicAMP + Pyrophosphate
EC:4.6.1.1-rn:R00434	False	GTP = 35-CyclicGMP + Pyrophosphate
EC:4.6.1.2-rn:R00434	False	GTP = 35-CyclicGMP + Pyrophosphate
EC:5.1.3.3-rn:R01602	True	alpha-D-Glucose = beta-D-Glucose
EC:5.3.1.1-rn:R01015	True	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal = Glyceronephosphate
EC:5.3.1.9-rn:R02739	True	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
EC:5.3.1.9-rn:R02740	True	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
EC:5.3.1.9-rn:R03321	True	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
EC:5.4.2.1-rn:R01518	True	2-Phospho-D-glycerate = 3-Phospho-D-glycerate

EC:5.4.2.1-rn:R01662	False	3-Phospho-D-glyceroylphosphate = 23-Bisphospho-D-glycerate
EC:5.4.2.2-rn:R00959	True	D-Glucose1-phosphate = alpha-D-Glucose6-phosphate
EC:5.4.2.4-rn:R01516	False	23-Bisphospho-D-glycerate + H2O = 3-Phospho-D-glycerate + Orthophosphate
EC:6.2.1.1-rn:R00235	True	ATP-energy + Acetate + CoA = AMP-energy + Acetyl-CoA + Pyrophosphate
EC:6.2.1.4-rn:R00432	True	CoA + GTP + Succinate = GDP + Orthophosphate + Succinyl-CoA
EC:6.2.1.4-rn:R00727	True	CoA + ITP + Succinate = IDP + Orthophosphate + Succinyl-CoA
EC:6.2.1.5-rn:R00405	True	ATP-energy + CoA + Succinate = ADP-energy + Orthophosphate + Succinyl-CoA
EC:6.3.2.6-rn:R04591	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate + ATP-metabolism + L-Aspartate = 1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole + ADP-metabolism + Orthophosphate
EC:6.3.4.1-rn:R01230	False	ATP-energy + NH3 + Xanthosine5-phosphate = AMP-energy + GMP + Pyrophosphate
EC:6.3.4.2-rn:R00571	False	ATP-energy + NH3 + UTP = ADP-energy + CTP + Orthophosphate
EC:6.3.4.2-rn:R00573	False	ATP-energy + H2O + L-Glutamine + UTP = ADP-energy + CTP + L-Glutamate + Orthophosphate
EC:6.3.4.4-rn:R01135	True	GTP + IMP + L-Aspartate = GDP + N6-(12-Dicarboxyethyl)-AMP + Orthophosphate
EC:6.3.5.2-rn:R01231	False	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = AMP-energy + GMP + L-Glutamate + Pyrophosphate
EC:6.3.5.5-rn:R00575	False	2 ATP-energy + H2O + HCO3- + L-Glutamine = 2 ADP-energy + Carbamoylphosphate + L-Glutamate + Orthophosphate
EC:6.4.1.1-rn:R00344	True	ATP-energy + HCO3- + Pyruvate = ADP-energy + Orthophosphate + Oxaloacetate
SERP0653-EC:6.3.5.3-rn:R04463	False	5-Phosphoribosyl-N-formylglycinamide + ATP-energy + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ADP-energy + L-Glutamate + Orthophosphate
SERP0653-EC:6.3.5.3-rn:R04463_blocked	False	5-Phosphoribosyl-N-formylglycinamide + ATP-energy + IQ-143 + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine_blo + ADP-energy + IQ-143_used + L-Glutamate + Orthophosphate
SERP0655-EC:2.4.2.14-rn:R01072	False	5-Phosphoribosylamine + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O + L-Glutamine
SERP0655-EC:2.4.2.14-rn:R01072_blocked	False	5-Phosphoribosylamine + IQ-143 + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate_blocked + IQ-143_used + H2O + L-Glutamine
SERP0656-EC:6.3.3.1-rn:R04208	False	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-energy = ADP-energy + Aminoimidazoleribotide + Orthophosphate
SERP0656-EC:6.3.3.1-rn:R04208_blocked	False	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-energy + IQ-143 = 5-Phosphoribosyl-N-formylglycinamide_blocked + IQ-143_used + Tetrahydrofolate
SERP0657-EC:2.1.2.2-rn:R04325	False	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide = 5-Phosphoribosyl-N-formylglycinamide + Tetrahydrofolate
SERP0657-EC:2.1.2.2-rn:R04325_blocked	False	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide + IQ-143 = 5-Phosphoribosyl-N-formylglycinamide_blocked + IQ-143_used + Tetrahydrofolate

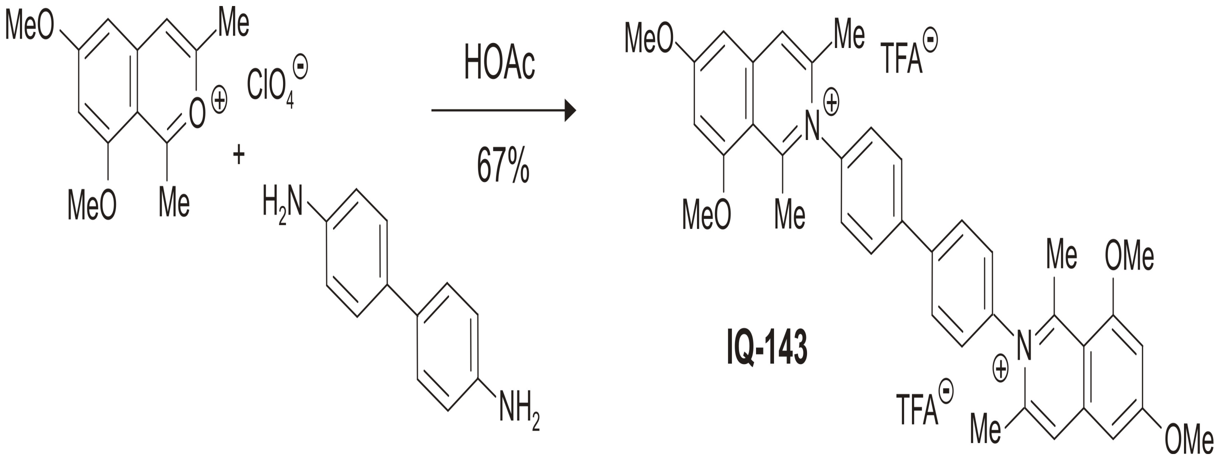
SERP0658-EC:2.1.2.3-rn:R04560	False	10-Formyltetrahydrofolate + AICAR = FAICAR + Tetrahydrofolate
SERP0658-EC:2.1.2.3-rn:R04560_blocked	false	10-Formyltetrahydrofolate + AICAR + IQ-143 = FAICAR-blocked + IQ-143_used + Tetrahydrofolate
SERP0659-EC:6.3.4.13-rn:R04144	False	5-Phosphoribosylamine + ATP-energy + Glycine = 5-Phosphoribosylglycinamide + ADP-energy + Orthophosphate
SERP0659-EC:6.3.4.13-rn:R04144_blocked	False	5-Phosphoribosylamine + ATP-energy + IQ-143 + Glycine = 5-Phosphoribosylglycinamide + ADP-energy + IQ-143_used + Orthophosphate
SERP0831-EC:2.7.7.7-rn:R00375	True	DNA + dATP = DNA-A + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00375_blocked	False	DNA + IQ-143+ dATP = DNA-A_blocked + IQ-_used + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00376	True	DNA + dGTP = DNA-G + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00376_blocked	False	DNA + IQ-143+ dGTP = DNA-G_blocked + IQ-_used + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00377	True	DNA + dCTP = DNA-C + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00377_blocked	False	DNA + IQ-143+ dCTP = DNA-C_blocked + IQ-_used + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00378	True	DNA + dTTP = DNA-T + Pyrophosphate
SERP0831-EC:2.7.7.7-rn:R00378_blocked	False	DNA + IQ-143+ dTTP = DNA-T_blocked + IQ-_used + Pyrophosphate
SERP0841-EC:2.7.7.8-rn:R00437	False	ADP-metabolism + RNA = Orthophosphate + RNA-A
SERP0841-EC:2.7.7.8-rn:R00437_blocked	False	ADP-metabolism + IQ-143+ RNA = IQ-_used + Orthophosphate + RNA-A_blocked
SERP0841-EC:2.7.7.8-rn:R00438	False	RNA + UDP = Orthophosphate + RNA-U
SERP0841-EC:2.7.7.8-rn:R00438_blocked	False	IQ-143+ RNA + UDP = IQ-_used + Orthophosphate + RNA-U_blocked
SERP0841-EC:2.7.7.8-rn:R00439	False	GDP + RNA = Orthophosphate + RNA-G
SERP0841-EC:2.7.7.8-rn:R00439_blocked	False	IQ-143+ GDP + RNA = IQ-_used + Orthophosphate + RNA-G_blocked
SERP0841-EC:2.7.7.8-rn:R00440	False	CDP + RNA = Orthophosphate + RNA-C
SERP0841-EC:2.7.7.8-rn:R00440_blocked	False	CDP + IQ-143+ RNA = IQ-_used + Orthophosphate + RNA-C_blocked
SERP2186-EC:2.7.7.4-rn:R00529	False	ATP-energy + Sulfate = Adenylylsulfate + Pyrophosphate
SERP2186-EC:2.7.7.4-rn:R00529_blocked	False	ATP-energy + IQ-143+ Sulfate = Adenylylsulfate_blocked + IQ-_used + Pyrophosphate

[1] List of enzymes used to build the metabolic web of *H. sapiens*. This list is composed of data derived from KEGG and own annotations.

Abbreviations: SERP: Enzymes measured by gene expression micro array (see point IV, supplementary materials).

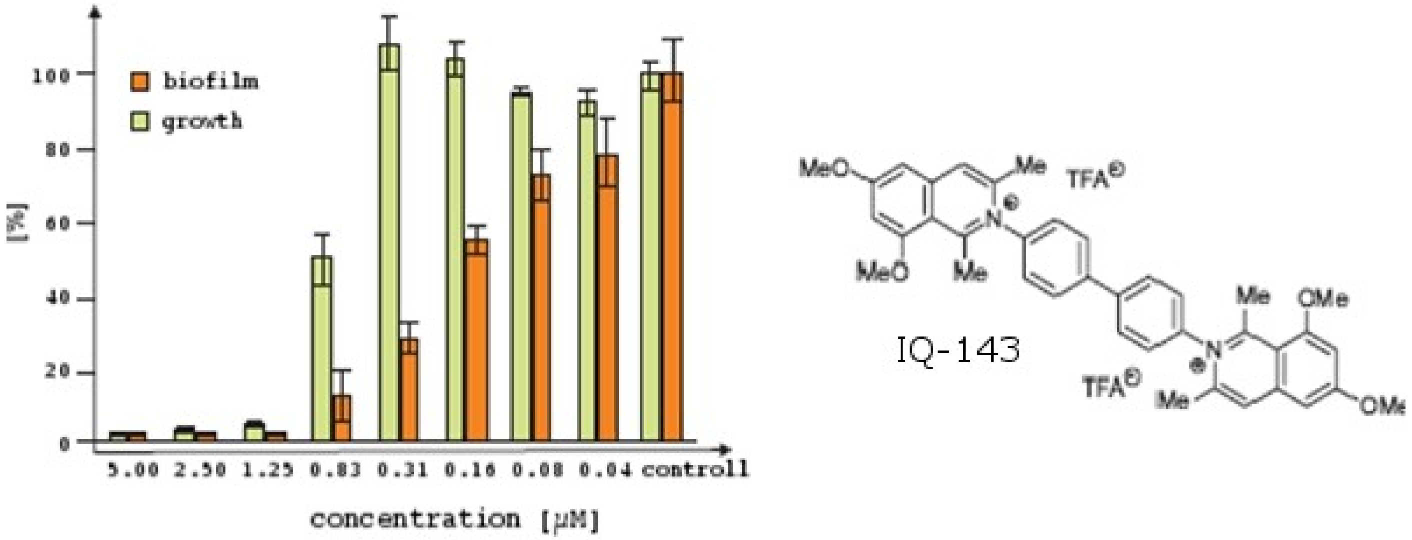
3: Synthesis and effects of the isoquinoline IQ-143.

Figure S VI.1.1: Synthesis of IQ-143 according to Bringmann et al 2007 [49]:



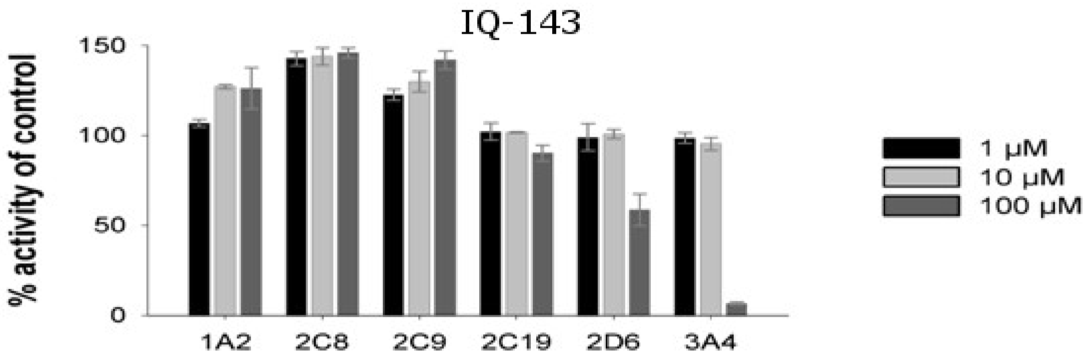
The compound IQ-143 was synthesized according to the method above by T. Gulder [49].

Figure S VI.1.2: Effects of IQ-143 on *S. epidermidis* RP62A (Bringmann et al. 2007 [49])



[1] Growth inhibition of different concentrations of IQ-143[49].

Figure S VI.1.3: Effects of IQ143 on human Cytochrome- P- enzymes[1].



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[1] Percentage of cytochrome activation is shown on the y-axis, the six key cytochromes in man were incubated in vitro with different concentrations of IQ-143 (see materials and methods). Only one human cytochrome (3A4) is inhibited at high concentrations, two other (2C19 and 2D6) are reduced.

4: Gene expression data gathered by the Ohlsen group.

Table S VI.1.5: This data shows the effects of 1.25µM IQ-143 on *S. epidermidis* RP62A as measured by the Ohlsen group.

Concentration: 1.25µM

id	Name	Mean (Stats)	Median (Stats)	SD (Stats)	CV (Stats)	Count (Stats)	Min (Stats)	Max (Stats)	Max-Min (Stats)	One Sample t-Test (Adv)
SERP0630	2-succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylic acid synthase-2-oxoglutarate decarboxylase (menD) [4.1.1.71] {Staphylococcus epidermidis RP62A}	**2.224**	2.210	**0.026**	1.155	**6**	2.092	2.475	0.383	**0.000000**
SERP0372	6-pyruvoyl tetrahydrobiopterin synthase, putative {Staphylococcus epidermidis RP62A}	**4.007**	3.599	**0.126**	3.157	**6**	3.104	6.170	3.067	**0.000081**
SERP1803	ABC transporter, ATP-binding protein {Staphylococcus epidermidis RP62A}	**2.276**	2.301	**0.023**	1.004	**6**	2.132	2.407	0.275	**0.000000**
SERP1802	ABC transporter, ATP-binding protein {Staphylococcus epidermidis RP62A}	**2.449**	2.401	**0.143**	5.827	**6**	1.655	4.008	2.352	**0.001138**
SERP1403	ABC transporter, permease-ATP-binding protein {Staphylococcus epidermidis RP62A}	**2.050**	2.063	**0.044**	2.145	**6**	1.758	2.307	0.549	**0.000012**
SERP2311	acetyltransferase, GNAT family {Staphylococcus epidermidis RP62A}	**2.739**	2.676	**0.072**	2.638	**6**	2.089	3.366	1.276	**0.000025**
SERP1996	acetyltransferase, GNAT family {Staphylococcus epidermidis RP62A}	**3.323**	3.258	**0.075**	2.261	**6**	2.669	4.270	1.601	**0.000013**
SERP0389	alcohol dehydrogenase, iron-containing [1.1.1.1] {Staphylococcus epidermidis RP62A}	**3.358**	3.070	**0.081**	2.418	**5**	2.803	4.153	1.349	**0.000132**
SERP2112	alcohol dehydrogenase, zinc-containing [1.1.1.1] {Staphylococcus epidermidis RP62A}	**4.080**	4.015	**0.038**	0.934	**3**	3.771	4.485	0.714	**0.001296**
SERP0963	aspartokinase, alpha and beta subunits (lysC) [2.7.2.4] {Staphylococcus epidermidis RP62A}	**3.391**	4.010	**0.187**	5.527	**5**	1.726	5.326	3.599	**0.003192**

SERP2244	capA-related protein {Staphylococcus epidermidis RP62A}	**2.716**	2.786	**0.056**	2.052	**6**	2.175	3.060	0.885	**0.000007**
SERP2179	choline-carnitine-betaine transporter {Staphylococcus epidermidis RP62A}	**2.225**	2.389	**0.133**	5.995	**6**	1.364	3.077	1.714	**0.001402**
SERP1144	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.019**	1.955	**0.046**	2.256	**6**	1.796	2.372	0.576	**0.000015**
SERP1215	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.131**	2.031	**0.067**	3.147	**6**	1.851	2.872	1.021	**0.000071**
SERP1405	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.168**	1.966	**0.126**	5.791	**6**	1.676	3.721	2.045	**0.001237**
SERP1998	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.001**	1.980	**0.048**	2.385	**5**	1.765	2.341	0.576	**0.000146**
SERP2079	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.146**	2.163	**0.016**	0.765	**4**	2.040	2.222	0.182	**0.000033**
SERP0916	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.047**	2.046	**0.032**	1.540	**6**	1.874	2.211	0.337	**0.000002**
SERP0241	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.198**	2.161	**0.057**	2.580	**6**	1.927	2.658	0.731	**0.000026**
SERP2527	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.248**	2.206	**0.075**	3.358	**5**	1.919	2.951	1.032	**0.000479**
SERP2068	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.305**	2.365	**0.109**	4.735	**5**	1.662	3.329	1.667	**0.001751**
SERP2178	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.837**	3.109	**0.134**	4.721	**6**	1.848	3.853	2.005	**0.000419**
SERP0591	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.731**	2.772	**0.165**	6.029	**5**	1.513	4.288	2.774	**0.004065**
SERP1053	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.491**	2.209	**0.123**	4.947	**6**	1.857	3.731	1.874	**0.000530**
SERP2110	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.800**	2.845	**0.047**	1.670	**6**	2.468	3.195	0.727	**0.000003**
SERP0182	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**2.920**	3.009	**0.051**	1.744	**6**	2.468	3.282	0.814	**0.000003**
SERP0467	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**3.526**	3.286	**0.061**	1.723	**5**	3.059	4.180	1.122	**0.000036**
SERP1015	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**4.525**	4.557	**0.022**	0.489	**6**	4.208	4.821	0.613	**0.000000**

SERP1145	conserved hypothetical protein TIGR00046 {Staphylococcus epidermidis RP62A}	**2.131**	2.097	**0.041**	1.903	**6**	1.897	2.485	0.588	**0.000006**
SERP0672	cytochrome bd ubiquinol oxidase, subunit I (cydA) [1.10.3.-] {Staphylococcus epidermidis RP62A}	**12.078**	12.680	**0.126**	1.043	**6**	8.463	16.268	7.804	**0.000004**
SERP0673	cytochrome bd ubiquinol oxidase, subunit II (cydB) [1.10.3.-] {Staphylococcus epidermidis RP62A}	**8.390**	8.002	**0.104**	1.241	**6**	6.402	12.612	6.210	**0.000004**
SERP0831	DNA polymerase III, alpha subunit, Gram-positive type [2.7.7.7] {Staphylococcus epidermidis RP62A}	**2.156**	2.202	**0.051**	2.343	**6**	1.787	2.392	0.605	**0.000016**
SERP1433	DNA-damage-inducible protein P (dinP) {Staphylococcus epidermidis RP62A}	**2.806**	2.470	**0.134**	4.760	**6**	2.073	4.190	2.117	**0.000434**
SERP1944	drug resistance transporter, EmrB-QacA family {Staphylococcus epidermidis RP62A}	**2.212**	2.075	**0.086**	3.888	**6**	1.857	3.106	1.250	**0.000187**
SERP0263	endonuclease III, putative {Staphylococcus epidermidis RP62A}	**3.752**	3.678	**0.090**	2.406	**4**	3.089	4.743	1.655	**0.001048**
SERP0729	excinuclease ABC, C subunit (uvrC) {Staphylococcus epidermidis RP62A}	**2.994**	2.973	**0.053**	1.781	**6**	2.639	3.644	1.005	**0.000004**
SERP0373	exsB protein {Staphylococcus epidermidis RP62A}	**4.199**	3.926	**0.098**	2.327	**6**	3.286	5.554	2.268	**0.000020**
SERP0371	exsD protein {Staphylococcus epidermidis RP62A}	**3.878**	3.623	**0.092**	2.360	**6**	3.118	5.312	2.194	**0.000019**
SERP2366	formate acetyltransferase (pflB) [2.3.1.54] {Staphylococcus epidermidis RP62A}	**4.184**	4.481	**0.167**	3.994	**4**	2.586	5.904	3.318	**0.005026**
SERP1997	formate-nitrite transporter family protein {Staphylococcus epidermidis RP62A}	**2.553**	2.619	**0.109**	4.263	**6**	1.648	3.556	1.909	**0.000260**
SERP0413	GGDEF domain protein {Staphylococcus epidermidis RP62A}	**2.015**	2.008	**0.075**	3.743	**6**	1.531	2.563	1.032	**0.000181**
SERP1760	glucosamine--fructose-6-phosphate aminotransferase, isomerizing (glmS) [2.6.1.16] {Staphylococcus epidermidis RP62A}	**2.710**	2.666	**0.030**	1.091	**6**	2.555	3.084	0.529	**0.000000**

SERP2060	glycerol-3-phosphate transporter (glpT) {Staphylococcus epidermidis RP62A}	**2.700**	2.823	**0.055**	2.049	**5**	2.340	3.148	0.809	**0.000064**
SERP0363	glycosyl transferase, group 2 family protein {Staphylococcus epidermidis RP62A}	**2.484**	2.734	**0.110**	4.444	**6**	1.732	3.224	1.491	**0.000320**
SERP1208	GTP-binding protein, GTP1-OBG family {Staphylococcus epidermidis RP62A}	**2.165**	2.053	**0.069**	3.177	**6**	1.857	2.694	0.837	**0.000072**
SERP1696	HD domain protein {Staphylococcus epidermidis RP62A}	**3.237**	3.657	**0.196**	6.044	**5**	1.505	4.604	3.099	**0.004312**
SERP1206	Holliday junction DNA helicase RuvA (ruvA) {Staphylococcus epidermidis RP62A}	**2.071**	1.999	**0.067**	3.219	**6**	1.716	2.726	1.009	**0.000083**
SERP0350	hypothetical protein {Staphylococcus epidermidis RP62A}	**2.444**	2.615	**0.103**	4.226	**4**	1.754	2.976	1.222	**0.004882**
SERP2321	immunodominant antigen B, putative {Staphylococcus epidermidis RP62A}	**2.030**	1.957	**0.064**	3.159	**6**	1.750	2.525	0.775	**0.000079**
SERP0629	isochorismate synthase family protein {Staphylococcus epidermidis RP62A}	**2.266**	2.222	**0.043**	1.882	**6**	2.017	2.662	0.646	**0.000005**
SERP1796	lactose phosphotransferase system repressor (lacR) {Staphylococcus epidermidis RP62A}	**6.112**	5.855	**0.186**	3.045	**6**	4.076	13.083	9.007	**0.000145**
SERP0043	lysozyme domain protein {Staphylococcus epidermidis RP62A}	**2.715**	2.909	**0.095**	3.502	**5**	2.030	3.437	1.408	**0.000520**
SERP1230	membrane protein, putative {Staphylococcus epidermidis RP62A}	**2.628**	2.768	**0.122**	4.653	**6**	1.735	3.656	1.921	**0.000391**
SERP2520	methicillin-resistance regulatory protein MecR1 (mecR1) {Staphylococcus epidermidis RP62A}	**2.547**	2.449	**0.144**	5.669	**6**	1.792	3.745	1.953	**0.000988**
SERP0084	NADH dehydrogenase I, F subunit (nuoF) [1.6.5.3] {Staphylococcus epidermidis RP62A}	**2.264**	2.307	**0.082**	3.643	**6**	1.659	2.939	1.280	**0.000133**
SERP1980	nitrite extrusion protein {Staphylococcus epidermidis RP62A}	**2.001**	1.867	**0.101**	5.069	**6**	1.583	2.802	1.218	**0.000768**
SERP0119	Orn-Lys-Arg decarboxylase {Staphylococcus epidermidis RP62A}	**2.127**	2.002	**0.129**	6.051	**6**	1.596	3.221	1.625	**0.001550**

SERP1151	oxygen-independent coproporphyrinogen III oxidase, putative {Staphylococcus epidermidis RP62A}	**2.177**	2.215	**0.055**	2.526	**6**	1.774	2.521	0.747	**0.000023**
SERP2064	PAP2 family protein {Staphylococcus epidermidis RP62A}	**3.337**	3.422	**0.106**	3.174	**4**	2.448	4.328	1.880	**0.002203**
SERP0828	phosphatidate cytidylyltransferase (cdsA) [2.7.7.41] {Staphylococcus epidermidis RP62A}	**2.400**	2.377	**0.096**	4.020	**6**	1.697	3.170	1.472	**0.000202**
SERP2283	phosphonate ABC transporter, permease protein {Staphylococcus epidermidis RP62A}	**2.654**	2.680	**0.048**	1.802	**3**	2.367	2.948	0.581	**0.004214**
SERP1721	phosphotyrosine protein phosphatase [3.1.3.48] {Staphylococcus epidermidis RP62A}	**2.917**	2.959	**0.021**	0.720	**6**	2.704	3.090	0.387	**0.000000**
SERP0841	polyribonucleotide nucleotidyltransferase (pnp) [2.7.7.8] {Staphylococcus epidermidis RP62A}	**2.698**	2.867	**0.052**	1.936	**6**	2.214	3.007	0.792	**0.000005**
SERP0448	preprotein translocase, SecG subunit (secG) {Staphylococcus epidermidis RP62A}	**2.288**	2.146	**0.122**	5.353	**6**	1.851	3.921	2.070	**0.000811**
SERP1324	proline dehydrogenase (putA) [1.5.99.8] {Staphylococcus epidermidis RP62A}	**3.816**	3.585	**0.063**	1.642	**3**	3.445	4.501	1.056	**0.003845**
SERP1909	PTS system, IIBC components {Staphylococcus epidermidis RP62A}	**4.222**	3.952	**0.073**	1.726	**3**	3.727	5.109	1.382	**0.004493**
SERP0002	ribonuclease P protein component (rnpA) [3.1.26.5] {Staphylococcus epidermidis RP62A}	**3.710**	3.617	**0.088**	2.385	**6**	2.929	5.049	2.120	**0.000019**
SERP0179	ribosomal protein L1 (rplA) {Staphylococcus epidermidis RP62A}	**2.036**	2.177	**0.066**	3.263	**6**	1.590	2.374	0.784	**0.000091**
SERP0840	ribosomal protein S15 (rpsO) {Staphylococcus epidermidis RP62A}	**2.022**	2.054	**0.038**	1.901	**6**	1.713	2.231	0.518	**0.000007**
SERP0826	ribosome recycling factor (frr) {Staphylococcus epidermidis RP62A}	**2.333**	2.373	**0.026**	1.128	**6**	2.084	2.479	0.395	**0.000000**
SERP1435	RNA methyltransferase, TrmA family {Staphylococcus epidermidis RP62A}	**2.011**	1.964	**0.034**	1.670	**6**	1.840	2.243	0.403	**0.000003**

SERP2401	serine protease {Staphylococcus epidermidis RP62A}	**4.396**	4.388	**0.055**	1.256	**6**	3.783	5.175	1.392	**0.000001**
SERP2201	sodium:solute symporter family protein {Staphylococcus epidermidis RP62A}	**2.415**	2.369	**0.069**	2.859	**6**	1.970	3.109	1.139	**0.000039**
SERP0118	spermidine N1-acetyltransferase, putative {Staphylococcus epidermidis RP62A}	**2.133**	2.376	**0.165**	7.712	**6**	1.342	3.297	1.955	**0.004476**
SERP0686	spermidine-putrescine ABC transporter, ATP-binding protein (potA) {Staphylococcus epidermidis RP62A}	**2.401**	2.361	**0.098**	4.070	**6**	1.883	3.363	1.481	**0.000215**
SERP0687	spermidine-putrescine ABC transporter, permease protein PotB (potB) {Staphylococcus epidermidis RP62A}	**2.181**	2.208	**0.040**	1.844	**6**	1.905	2.401	0.497	**0.000005**
SERP0688	spermidine-putrescine ABC transporter, permease protein PotC (potC) {Staphylococcus epidermidis RP62A}	**2.103**	2.075	**0.053**	2.497	**6**	1.853	2.441	0.589	**0.000023**
SERP1722	Sua5-YciO-YrdC-YwlC family protein {Staphylococcus epidermidis RP62A}	**2.841**	2.762	**0.071**	2.494	**6**	2.382	3.539	1.157	**0.000019**
SERP1673	threonine dehydratase (ilvA) [4.2.1.16] {Staphylococcus epidermidis RP62A}	**4.317**	4.223	**0.121**	2.799	**6**	3.211	6.798	3.587	**0.000050**
SERP0110	transcriptional regulator, LysR family {Staphylococcus epidermidis RP62A}	**2.646**	2.526	**0.158**	5.980	**6**	1.744	4.892	3.148	**0.001250**
SERP0264	transcriptional regulator, MerR family {Staphylococcus epidermidis RP62A}	**3.488**	3.412	**0.092**	2.624	**6**	2.836	5.172	2.336	**0.000028**
SERPA0009	transcriptional regulator, putative {Staphylococcus epidermidis RP62A}	**2.177**	2.237	**0.084**	3.839	**5**	1.664	2.616	0.952	**0.000830**
SERP1797	transcriptional regulator, Sir2 family {Staphylococcus epidermidis RP62A}	**15.612**	16.124	**0.047**	0.300	**6**	13.009	17.749	4.740	**0.000000**
SERP2289	transporter, putative {Staphylococcus epidermidis RP62A}	**2.131**	1.971	**0.102**	4.782	**6**	1.682	2.985	1.303	**0.000523**
SERP2240	transposase, IS200 family {Staphylococcus epidermidis RP62A}	**3.218**	3.381	**0.114**	3.541	**6**	2.241	4.693	2.452	**0.000112**
SERP2245	tributyrin esterase EstA, putative {Staphylococcus epidermidis RP62A}	**2.307**	2.531	**0.096**	4.156	**6**	1.550	2.774	1.224	**0.000245**
SERP0806	tRNA (guanine-N1)-methyltransferase (trmD) [2.1.1.31] {Staphylococcus epidermidis RP62A}	**2.973**	2.973	**0.019**	0.627	**6**	2.809	3.174	0.365	**0.000000**

SERP0765	uracil permease (uraA) {Staphylococcus epidermidis RP62A}	**3.120**	2.763	**0.224**	7.164	**6**	1.901	6.819	4.918	**0.002906**
SERP0825	uridylate kinase (pyrH) [2.7.4.-] {Staphylococcus epidermidis RP62A}	**2.225**	2.255	**0.039**	1.753	**6**	1.926	2.429	0.504	**0.000004**
SERP2547	YjeF-related protein {Staphylococcus epidermidis RP62A}	**2.074**	2.081	**0.057**	2.732	**6**	1.744	2.522	0.778	**0.000037**
SERP0292	ABC transporter, ATP-binding protein (sitA) {Staphylococcus epidermidis RP62A}	**0.452**	0.430	**0.057**	12.654	**6**	0.404	0.531	0.127	**0.000026**
SERP1951	ABC transporter, ATP-binding protein {Staphylococcus epidermidis RP62A}	**0.469**	0.457	**0.032**	6.918	**6**	0.437	0.536	0.099	**0.000002**
SERP0291	ABC transporter, permease protein (sitB) {Staphylococcus epidermidis RP62A}	**0.436**	0.450	**0.052**	12.029	**6**	0.355	0.504	0.150	**0.000013**
SERP1952	ABC transporter, permease protein {Staphylococcus epidermidis RP62A}	**0.395**	0.386	**0.068**	17.286	**6**	0.319	0.502	0.183	**0.000029**
SERP0290	ABC transporter, substrate-binding protein (sitC) {Staphylococcus epidermidis RP62A}	**0.454**	0.449	**0.034**	7.582	**6**	0.407	0.519	0.112	**0.000002**
SERP2192	phosophoadenylyl-sulfate reductase (cysH) [1.8.4.8] {Staphylococcus epidermidis RP62A}	**0.415**	0.428	**0.046**	11.132	**6**	0.351	0.460	0.109	**0.000005**
SERP0659	phosphoribosylamine--glycine ligase (purD) [6.3.4.13] {Staphylococcus epidermidis RP62A}	**0.389**	0.392	**0.086**	22.178	**6**	0.296	0.532	0.236	**0.000082**
SERP0658	phosphoribosylaminoimidazolecarboxamide formyltransferase-IMP cyclohydrolase (purH) {Staphylococcus epidermidis RP62A}	**0.429**	0.439	**0.086**	20.004	**6**	0.317	0.545	0.229	**0.000136**
SERP0656	phosphoribosylformylglycinamidine cyclo-ligase (purM) [6.3.3.1] {Staphylococcus epidermidis RP62A}	**0.427**	0.424	**0.077**	18.090	**6**	0.342	0.519	0.176	**0.000079**
SERP0653	phosphoribosylformylglycinamidine synthase I (purQ) [6.3.5.3] {Staphylococcus epidermidis RP62A}	**0.483**	0.491	**0.101**	20.965	**6**	0.370	0.646	0.275	**0.000612**

SERP0654	phosphoribosylformylglycinamidine synthase II (purL) [6.3.5.3] {Staphylococcus epidermidis RP62A}	**0.456**	0.441	**0.080**	17.525	**6**	0.381	0.593	0.213	**0.000138**
SERP0652	phosphoribosylformylglycinamidine synthase, PurS protein (purS) {Staphylococcus epidermidis RP62A}	**0.481**	0.486	**0.116**	24.197	**6**	0.331	0.727	0.396	**0.001134**
SERP0657	phosphoribosylglycinamide formyltransferase (purN) [2.1.2.2] {Staphylococcus epidermidis RP62A}	**0.427**	0.426	**0.090**	21.199	**6**	0.338	0.534	0.196	**0.000170**
SERP0655	amidophosphoribosyltransferase (purF) [2.4.2.14] {Staphylococcus epidermidis RP62A}	**0.432**	0.436	**0.089**	20.572	**6**	0.340	0.544	0.204	**0.000168**
SERP1285	glycerophosphoryl diester phosphodiesterase, putative {Staphylococcus epidermidis RP62A}	**0.493**	0.501	**0.044**	8.898	**6**	0.435	0.555	0.120	**0.000012**
SERP0256	conserved domain protein {Staphylococcus epidermidis RP62A}	**0.473**	0.452	**0.111**	23.487	**6**	0.370	0.730	0.361	**0.000818**
SERP2187	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**0.366**	0.378	**0.060**	16.537	**6**	0.286	0.416	0.130	**0.000011**
SERP0173	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**0.422**	0.415	**0.069**	16.328	**6**	0.341	0.509	0.168	**0.000043**
SERP0171	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**0.435**	0.422	**0.089**	20.486	**6**	0.338	0.546	0.208	**0.000176**
SERP0330	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	**0.470**	0.499	**0.098**	20.781	**6**	0.341	0.609	0.268	**0.000429**
SERP2186	sulfate adenylyltransferase (sat) [2.7.7.4] {Staphylococcus epidermidis RP62A}	**0.343**	0.349	**0.043**	12.442	**6**	0.284	0.377	0.093	**0.000001**
SERP2191	sulfite reductase (NADPH) flavoprotein alpha-component (cysJ) [1.8.1.2] {Staphylococcus epidermidis RP62A}	**0.440**	0.443	**0.026**	5.950	**6**	0.398	0.467	0.069	**0.000000**
SERP2190	sulfite reductase (NADPH) hemoprotein beta-component (cysI) [1.8.1.2] {Staphylococcus epidermidis RP62A}	**0.375**	0.378	**0.024**	6.363	**6**	0.339	0.394	0.055	**0.000000**
SERP0172	RNA methyltransferase, TrmH family, group 3 {Staphylococcus epidermidis RP62A}	**0.451**	0.430	**0.091**	20.152	**6**	0.374	0.661	0.287	**0.000242**

SERP0174	RNA polymerase sigma factor sigW, putative {Staphylococcus epidermidis RP62A}	**0.423**	0.403	**0.083**	19.562	**6**	0.353	0.600	0.247	**0.000105**
SERP0357	transcriptional regulator, DeoR family {Staphylococcus epidermidis RP62A}	**0.360**	0.374	**0.081**	22.581	**6**	0.284	0.455	0.172	**0.000042**
SERP0170	cysteinyl-tRNA synthetase (cysS) [6.1.1.16] {Staphylococcus epidermidis RP62A}	**0.454**	0.436	**0.084**	18.468	**6**	0.362	0.616	0.254	**0.000169**
SERP1195	D-tyrosyl-tRNA(Tyr) deacylase (dtd) [3.1.-.-] {Staphylococcus epidermidis RP62A}	**0.342**	0.335	**0.043**	12.551	**6**	0.301	0.391	0.089	**0.000001**
SERP0169	serine acetyltransferase (cysE) [2.3.1.30] {Staphylococcus epidermidis RP62A}	**0.443**	0.420	**0.067**	15.201	**6**	0.390	0.588	0.199	**0.000051**
SERP2188	siroheme synthase, putative {Staphylococcus epidermidis RP62A}	**0.347**	0.359	**0.046**	13.172	**6**	0.287	0.388	0.101	**0.000002**
SERP2189	uroporphyrin-III C-methyltransferase, putative {Staphylococcus epidermidis RP62A}	**0.378**	0.374	**0.053**	14.127	**6**	0.311	0.447	0.136	**0.000007**
SERP1258	citrate synthase (gltA) [2.3.3.1] {Staphylococcus epidermidis RP62A}	**0.472**	0.475	**0.048**	10.257	**6**	0.397	0.537	0.140	**0.000015**
SERP2156	L-lactate dehydrogenase (ldh) [1.1.1.27] {Staphylococcus epidermidis RP62A}	**0.486**	0.478	**0.049**	10.144	**6**	0.429	0.570	0.141	**0.000020**
SERP0358	1-phosphofructokinase (fruK) [2.7.1.56] {Staphylococcus epidermidis RP62A}	**0.351**	0.360	**0.085**	24.130	**6**	0.253	0.443	0.190	**0.000046**

Table S VI.1.6: This data shows the effects of 0.16µM IQ-143 on *S. epidermidis* RP62A as measured by the Ohlsen group.

Concentration: 0.16µM

	Name	Mean (Stats)	Median (Stats)	SD (Stats)	CV (Stats)	Count (Stats)	Min (Stats)	Max (Stats)	Max-Min (Stats)	One Sample t-Test (Adv)
SERP2178	conserved hypothetical protein {Staphylococcus epidermidis RP62A}	4.464	4.406	0.071	1.599	12	3.383	5.570	2.187	0.000000
SERP2179	choline-carnitine-betaine transporter {Staphylococcus epidermidis RP62A}	8.477	7.071	0.149	1.762	12	5.884	17.771	11.888	0.000000
SERP2176	choline dehydrogenase (betA) [1.1.99.1] {Staphylococcus epidermidis RP62A}	22.286	29.051	0.322	1.444	12	3.685	53.000	49.315	0.000000
SERP2177	betaine aldehyde dehydrogenase (betB) [1.2.1.8] {Staphylococcus epidermidis RP62A}	38.110	36.852	0.088	0.231	12	27.884	55.324	27.441	0.000000
SERP2294	intercellular adhesion protein D (icaD) {Staphylococcus epidermidis RP62A}	0.340	0.316	0.177	52.277	7	0.221	0.667	0.445	0.000426
SERP2293	intercellular adhesion protein A (icaA) {Staphylococcus epidermidis RP62A}	0.239	0.237	0.288	120.615	6	0.086	0.555	0.469	0.003229
SERP1792	tagatose 1	0.462	0.511	0.116	25.142	11	0.293	0.632	0.339	0.000002
SERP1794	galactose-6-phosphate isomerase	0.426	0.399	0.158	37.077	10	0.260	0.711	0.451	0.000040
SERP1793	tagatose-6-phosphate kinase (lacC) [2.7.1.144] {Staphylococcus epidermidis RP62A}	0.494	0.479	0.114	23.172	6	0.367	0.686	0.319	0.001230
SERP1795	galactose-6-phosphate isomerase	0.464	0.478	0.170	36.552	5	0.277	0.758	0.481	0.011668
SERP1791	PTS system	0.485	0.500	0.111	22.828	9	0.320	0.644	0.324	0.000027
SERP0572	oligopeptide ABC transporter	0.493	0.609	0.219	44.522	11	0.148	0.788	0.640	0.000920
SERP0571	oligopeptide ABC transporter	0.490	0.579	0.209	42.644	10	0.270	1.064	0.794	0.001134

SERP0570	oligopeptide ABC transporter	0.449	0.418	0.282	62.788	9	0.197		1.126	0.929		0.005989
SERP0290	ABC transporter	0.407	0.399	0.292	71.665	8	0.181		1.147	0.967		0.006904
SERP0292	ABC transporter	0.488	0.543	0.288	58.952	10	0.221		1.389		1.168	0.007665
SERP0291	ABC transporter	0.437	0.544	0.253	57.919	9	0.202		1.080	0.878		0.002769
SERP1790	PTS system	0.669	0.655	0.054	8.091	9	0.510	0.789		0.278		0.000011

5: Extreme modes calculated by our YANAsquare models:

Table S VI.1.7: Extreme Modes of *S. aureus* USA300 without IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	-0,65	1	true	1	(1 PyrM_GMP-pyrophosphorylase)
4	1,00	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
5	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
6	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
7	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
8	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
9	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
10	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
11	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
12	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
13	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
14	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
15	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
16	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
17	0,96	1	true	1	(1 TCA_fumarate-hydratase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
21	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
22	1,00	1	true	1	(1 AS_Serine_to_Glycine)
23	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
24	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)

25	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
26	1,00	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
27	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)
28	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
29	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
30	-1,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
31	1,00	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
32	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
33	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
34	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
35	0,96	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
36	1,00	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
38	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
39	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
40	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
41	1,00	1	true	1	(1 Glyc_Succinate-CoA-ligase)
42	1,00	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
43	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
44	1,00	1	true	1	(1 PurM_metaphosphatase)
45	1,00	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
46	1,00	1	true	1	(1 Glyc_PTS-permease2)
47	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
48	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)
49	-0,87	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
50	-0,33	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
51	-0,33	1	true	1	(1 PurM_XMP-pyrophosphorylase)

52	-0,33	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
53	-0,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
54	-0,33	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
55	0,73	1	true	1	(1 PurM_adenylate-kinase_dAMP)
56	0,72	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
57	1,28	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PyrM_AMP-pyrophosphorylase)
58	-0,50	10	true	6	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP)
59	0,37	6	true	4	(-1 AMP-energy_to_AMP-metabolism) (2 ATP-energy_to_ATP-metabolism) (-1 PurM_adenylate-kinase_AMP) (-2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
60	0,38	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
61	0,72	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP)
62	0,51	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_6-phospho-beta-glucosidase) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_D-Glucose-1-epimerase) (2 Glyc_PTS-permease1) (-1 PurM_adenylate-kinase_AMP)
63	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
64	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
65	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
67	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
68	1,00	2	false	2	(1 PurM_ATP-phosphohydrolase) (1 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
69	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
70	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
71	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
72	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
73	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
74	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
75	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)
76	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)

77	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
78	0,53	1	false	1	(1 PyrM_dUTP-diphosphatase)
79	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
80	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
81	1,28	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
82	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
83	1,00	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
84	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
85	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
86	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
87	1,00	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
90	0,13	1	false	1	(1 DNA-extern_to_DNA-intern)
91	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
92	0,67	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
93	0,38	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
94	0,16	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
95	1,00	1	false	1	(1 PurM_ITP-diphosphohydrolase)
96	0,31	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
97	0,58	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
98	1,00	2	false	2	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0686-spermidine/putrescine-transport_import)
99	1,00	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)

100	0,38	1	false	1	(1 PurM_dITP-diphosphohydrolase)
101	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
102	0,58	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
103	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
104	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
105	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
106	1,00	1	false	1	(1 AS_Valine)
107	0,49	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
108	1,00	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
109	0,72	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
110	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
111	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
112	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
113	1,00	1	false	1	(1 AS_Serine_to_Methionine)
114	1,00	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,12	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
117	0,12	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
118	1,00	1	false	1	(1 PyrM_cytidine-kinase)
119	0,38	1	false	1	(1 AS_Leucine)
120	0,38	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,22	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)

123	1,00	1	false	1	(1 PyrM_CTP-synthase)
124	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,50	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	0,60	1	false	1	(1 PurM_allantoinase)
131	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
132	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
133	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
134	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
135	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
136	1,00	1	false	1	(1 AS_Isoleucine)
137	0,55	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
138	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
139	0,38	1	false	1	(1 PurM_5-nucleotidase_dTMP)
140	0,12	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,38	1	false	1	(1 PyrM_uridine-kinase_ATP)
142	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
143	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
144	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
145	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
146	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
147	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
148	0,60	1	false	1	(1 AS_Aspartate_to_Asparagine)
149	0,41	1	false	1	(1 PyrM_cytidine-kinase_ATP)

150	0,81	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
151	0,64	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
152	1,00	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)
153	1,00	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
154	0,57	1	false	1	(1 PurM_XTP-diphosphohydrolase)
155	0,45	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
156	1,00	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
157	1,00	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
158	0,22	1	false	1	(1 PurM_GTP-pyrophosphokinase)
159	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
160	1,00	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
161	0,27	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
162	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
163	1,00	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
164	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (2 PurM_thioredoxin-oxidoreductase_dATP)
165	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
166	0,25	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
167	1,25	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
168	1,00	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
169	0,25	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
170	1,00	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
171	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
172	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_DNA-directed-RNA-polyermase_ATP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)

173	0,50	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
174	0,49	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
175	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
176	1,00	1	false	1	(1 PurM_5-nucleotidase_GMP)
177	1,00	1	false	1	(1 PyrM_cytidine-kinase_ITP)
178	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
179	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
180	0,75	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
181	1,00	3	false	3	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 PurM_pyruvate-phosphotransferase_ATP) (-1 TCA_PEP-carboxylase)
182	1,00	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
183	0,16	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0687-spermidine/putrescine-transport_import)
184	0,27	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
185	1,00	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
186	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
187	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
188	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
189	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
190	1,04	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
191	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
192	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	1,00	1	false	1	(1 PurM_XMP-ligase)
196	1,08	1	false	1	(1 PyrM_cytidine-kinase_dATP)
197	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
198	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. aureus* USA300 without IQ-143.

Table S VI.1.8: Extreme Modes of *S. aureus* USA300 with 0.16µM IQ-143[1.]

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	-0,66	1	true	1	(1 PyrM_GMP-pyrophosphorylase)
4	1,00	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
5	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
6	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
7	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
8	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
9	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
10	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
11	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
12	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
13	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
14	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
15	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
16	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
17	0,98	1	true	1	(1 TCA_fumarate-hydratase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
21	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
22	1,00	1	true	1	(1 AS_Serine_to_Glycine)
23	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
24	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
25	-0,57	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)

26	1,00	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
27	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)
28	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
29	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
30	-1,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
31	1,00	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
32	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
33	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
34	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
35	0,98	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
36	1,00	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
38	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
39	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
40	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
41	1,00	1	true	1	(1 Glyc_Succinate-CoA-ligase)
42	1,00	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
43	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
44	1,00	1	true	1	(1 PurM_metaphosphatase)
45	0,50	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
46	1,00	1	true	1	(1 Glyc_PTS-permease2)
47	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
48	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)
49	-0,39	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
50	0,39	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
51	0,39	1	true	1	(1 PurM_XMP-pyrophosphorylase)
52	0,39	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)

53	0,39	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
54	0,39	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
55	0,79	1	true	1	(1 PurM_adenylate-kinase_dAMP)
56	0,88	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
57	1,12	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PyrM_AMP-pyrophosphorylase)
58	0,51	10	true	6	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP)
59	0,37	6	true	4	(-1 AMP-energy_to_AMP-metabolism) (2 ATP-energy_to_ATP-metabolism) (-1 PurM_adenylate-kinase_AMP) (-2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
60	0,38	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
61	0,88	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP)
62	0,60	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_6-phospho-beta-glucosidase) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_D-Glucose-1-epimerase) (2 Glyc_PTS-permease1) (-1 PurM_adenylate-kinase_AMP)
63	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
64	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
65	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
67	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
68	1,00	2	false	2	(1 PurM_ATP-phosphohydrolase) (1 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
69	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
70	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
71	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
72	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
73	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
74	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
75	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)
76	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)
77	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)

78	0,51	1	false	1	(1 PyrM_dUTP-diphosphatase)
79	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
80	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
81	1,12	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
82	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
83	0,54	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
84	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
85	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
86	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
87	1,00	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
90	1,00	1	false	1	(1 DNA-extern_to_DNA-intern)
91	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
92	0,67	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
93	0,00	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
94	0,23	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
95	1,00	1	false	1	(1 PurM_ITP-diphosphohydrolase)
96	0,33	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
97	0,61	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
98	1,00	2	false	2	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0686-spermidine/putrescine-transport_import)
99	1,00	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
100	2,02	1	false	1	(1 PurM_dITP-diphosphohydrolase)

101	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
102	0,62	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
103	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
104	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
105	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
106	1,00	1	false	1	(1 AS_Valine)
107	0,40	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
108	1,00	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
109	0,88	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
110	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
111	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
112	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
113	1,00	1	false	1	(1 AS_Serine_to_Methionine)
114	1,00	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
117	2,02	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
118	1,00	1	false	1	(1 PyrM_cytidine-kinase)
119	0,00	1	false	1	(1 AS_Leucine)
120	2,02	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	1,00	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,50	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 PurM_allantoinase)
131	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
132	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
133	0,47	1	false	1	(1 PyrM_uridine-kinase_dATP)
134	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
135	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
136	1,00	1	false	1	(1 AS_Isoleucine)
137	0,57	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
138	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
139	0,00	1	false	1	(1 PurM_5-nucleotidase_dTMP)
140	0,00	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,00	1	false	1	(1 PyrM_uridine-kinase_ATP)
142	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
143	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
144	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
145	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
146	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
147	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
148	0,57	1	false	1	(1 AS_Aspartate_to_Asparagine)
149	0,27	1	false	1	(1 PyrM_cytidine-kinase_ATP)
150	0,70	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)

151	0,72	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
152	1,00	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)
153	1,00	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
154	0,54	1	false	1	(1 PurM_XTP-diphosphohydrolase)
155	0,43	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
156	1,00	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
157	1,00	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
158	1,00	1	false	1	(1 PurM_GTP-pyrophosphokinase)
159	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
160	1,00	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
161	0,21	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
162	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
163	1,00	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
164	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (2 PurM_thioredoxin-oxidoreductase_dATP)
165	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
166	0,25	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
167	1,10	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
168	1,00	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
169	0,25	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
170	1,00	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
171	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
172	0,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_DNA-directed-RNA-polyermase_ATP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
173	0,50	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)

174	0,40	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
175	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
176	1,00	1	false	1	(1 PurM_5-nucleotidase_GMP)
177	1,00	1	false	1	(1 PyrM_cytidine-kinase_ITP)
178	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
179	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
180	0,90	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
181	1,00	3	false	3	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 PurM_pyruvate-phosphotransferase_ATP) (-1 TCA_PEP-carboxylase)
182	1,00	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
183	0,23	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0687-spermidine/putrescine-transport_import)
184	0,21	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
185	1,00	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
186	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
187	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
188	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
189	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
190	1,02	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
191	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
192	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	1,00	1	false	1	(1 PurM_XMP-ligase)
196	0,55	1	false	1	(1 PyrM_cytidine-kinase_dATP)
197	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
198	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. aureus* USA300 with 0.16µM IQ-143.

Table S VI.1.9: Extreme Modes of *S. aureus* USA300 with 1.25µM IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	-0,66	1	true	1	(1 PyrM_GMP-pyrophosphorylase)
4	1,00	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
5	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
6	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
7	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
8	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
9	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
10	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
11	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
12	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
13	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
14	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
15	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
16	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
17	0,97	1	true	1	(1 TCA_fumarate-hydratase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
19	0,46	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
21	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
22	1,00	1	true	1	(1 AS_Serine_to_Glycine)
23	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
24	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
25	-0,59	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)

26	1,00	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
27	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)
28	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
29	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
30	-1,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
31	1,00	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
32	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
33	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
34	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
35	0,97	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
36	1,00	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
38	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
39	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
40	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
41	1,00	1	true	1	(1 Glyc_Succinate-CoA-ligase)
42	1,00	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
43	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
44	1,00	1	true	1	(1 PurM_metaphosphatase)
45	1,00	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
46	1,00	1	true	1	(1 Glyc_PTS-permease2)
47	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
48	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)
49	-0,36	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
50	0,40	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
51	0,40	1	true	1	(1 PurM_XMP-pyrophosphorylase)
52	0,40	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)

53	0,40	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
54	0,40	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
55	0,95	1	true	1	(1 PurM_adenylate-kinase_dAMP)
56	0,92	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
57	1,08	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PyrM_AMP-pyrophosphorylase)
58	-0,50	10	true	6	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP)
59	-0,64	6	true	4	(-1 AMP-energy_to_AMP-metabolism) (2 ATP-energy_to_ATP-metabolism) (-1 PurM_adenylate-kinase_AMP) (-2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
60	0,36	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
61	0,92	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP)
62	-0,48	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_6-phospho-beta-glucosidase) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_D-Glucose-1-epimerase) (2 Glyc_PTS-permease1) (-1 PurM_adenylate-kinase_AMP)
63	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
64	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
65	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
67	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
68	1,00	2	false	2	(1 PurM_ATP-phosphohydrolase) (1 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
69	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
70	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
71	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
72	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
73	0,39	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
74	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
75	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)
76	2,30	1	false	1	(1 SERP1952-macrolide-transport_efflux)
77	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)

78	0,27	1	false	1	(1 PyrM_dUTP-diphosphatase)
79	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
80	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
81	1,08	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
82	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
83	0,43	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
84	0,22	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
85	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
86	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
87	1,00	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
90	1,04	1	false	1	(1 DNA-extern_to_DNA-intern)
91	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
92	0,67	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
93	0,02	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
94	0,39	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
95	1,00	1	false	1	(1 PurM_ITP-diphosphohydrolase)
96	0,49	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
97	1,52	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
98	1,00	2	false	2	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0686-spermidine/putrescine-transport_import)
99	2,68	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
100	0,47	1	false	1	(1 PurM_dITP-diphosphohydrolase)

101	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
102	0,16	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
103	2,40	1	false	1	(1 PurM_5-nucleotidase_UMP)
104	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
105	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
106	1,00	1	false	1	(1 AS_Valine)
107	1,41	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
108	1,00	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
109	0,92	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
110	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
111	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
112	2,87	1	false	1	(1 PurM_UTP-diphosphohydrolase)
113	1,00	1	false	1	(1 AS_Serine_to_Methionine)
114	1,00	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,36	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
117	0,83	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
118	1,00	1	false	1	(1 PyrM_cytidine-kinase)
119	0,54	1	false	1	(1 AS_Leucine)
120	1,01	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
121	0,28	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	1,97	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,72	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,50	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 PurM_allantoinase)
131	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
132	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
133	0,45	1	false	1	(1 PyrM_uridine-kinase_dATP)
134	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
135	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
136	1,00	1	false	1	(1 AS_Isoleucine)
137	0,85	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
138	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
139	0,59	1	false	1	(1 PurM_5-nucleotidase_dTMP)
140	0,96	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	1,14	1	false	1	(1 PyrM_uridine-kinase_ATP)
142	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
143	2,20	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
144	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
145	2,20	1	false	1	(1 AS_Glutamate_to_Glutamine)
146	2,20	1	false	1	(1 PurM_urea-amidohydrolase)
147	2,20	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
148	2,66	1	false	1	(1 AS_Aspartate_to_Asparagine)
149	1,27	1	false	1	(1 PyrM_cytidine-kinase_ATP)
150	0,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)

151	1,55	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
152	1,00	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)
153	1,00	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
154	0,00	1	false	1	(1 PurM_XTP-diphosphohydrolase)
155	0,15	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
156	1,00	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
157	1,00	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
158	2,06	1	false	1	(1 PurM_GTP-pyrophosphokinase)
159	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
160	1,00	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
161	0,05	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
162	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
163	1,00	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
164	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (2 PurM_thioredoxin-oxidoreductase_dATP)
165	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
166	0,22	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
167	1,20	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
168	1,00	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
169	0,22	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
170	1,00	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
171	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
172	0,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_DNA-directed-RNA-polyermase_ATP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
173	0,50	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)

174	0,48	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
175	0,28	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
176	1,00	1	false	1	(1 PurM_5-nucleotidase_GMP)
177	1,00	1	false	1	(1 PyrM_cytidine-kinase_ITP)
178	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
179	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
180	0,80	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
181	1,00	3	false	3	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 PurM_pyruvate-phosphotransferase_ATP) (-1 TCA_PEP-carboxylase)
182	1,00	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
183	0,53	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0687-spermidine/putrescine-transport_import)
184	0,05	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
185	1,00	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
186	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
187	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
188	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
189	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
190	1,03	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
191	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
192	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
193	0,35	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	1,00	1	false	1	(1 PurM_XMP-ligase)
196	0,52	1	false	1	(1 PyrM_cytidine-kinase_dATP)
197	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
198	2,82	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. aureus* USA300 with 1.25µM IQ-143.

Table S VI.1.10: Extreme Modes of *S. epidermidis* RP62A without IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	0,70	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
4	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
5	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
6	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
7	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
8	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
9	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
10	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
11	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
12	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
13	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
14	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
15	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
16	1,00	1	true	1	(1 TCA_fumarate-hydratase)
17	0,91	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
21	1,00	1	true	1	(1 AS_Serine_to_Glycine)
22	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
23	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
24	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
25	-0,52	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
26	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)

27	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
28	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
29	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
30	-1,33	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
31	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
32	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
33	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
34	1,00	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
35	0,91	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
36	-1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
38	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
39	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
40	0,50	1	true	1	(1 Glyc_Succinate-CoA-ligase)
41	0,50	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
42	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
43	1,00	1	true	1	(1 PurM_metaphosphatase)
44	1,05	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
45	0,73	1	true	1	(1 PurM_GMP-pyrophosphorylase)
46	1,00	3	true	3	(1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase)
47	1,00	6	true	6	(1 ATP-energy_to_ATP-metabolism) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_ATP-alpha-D-glucokinase) (-1 Glyc_ATP-beta-D-glucokinase) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase)
48	0,75	1	true	1	(1 Glyc_PTS-permease2)
49	1,00	4	true	4	(-1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_PTS-permease1)
50	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
51	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)

52	-1,34	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
53	0,79	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
54	0,53	1	true	1	(1 PurM_XMP-pyrophosphorylase)
55	0,53	1	true	1	(1 TCA_succinate-dehydrogenase)
56	0,53	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
57	0,53	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
58	0,53	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
59	0,92	1	true	1	(1 PurM_adenylate-kinase_dAMP)
60	1,08	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
61	-0,65	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
62	0,92	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase)
63	-0,48	14	true	8	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
64	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
65	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
67	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
68	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
69	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_ATP-phosphohydrolase)
70	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
71	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
72	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
73	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
74	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
75	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
76	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)

77	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)
78	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
79	0,55	1	false	1	(1 PyrM_dUTP-diphosphatase)
80	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
81	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
82	1,00	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
83	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
84	1,00	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
85	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
86	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
87	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
90	0,96	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
91	1,00	1	false	1	(1 DNA-extern_to_DNA-intern)
92	0,67	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
93	0,36	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
94	0,41	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
95	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
96	0,30	1	false	1	(1 PurM_ITP-diphosphohydrolase)
97	0,35	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0688-spermidine/putrescine-transport_import)
98	1,00	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
99	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1

					PurM_adenylate-kinase_AMP) (2 SERP0686-spermidine/putrescine-transport_import)
100	0,36	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
101	1,00	1	false	1	(1 PurM_dITP-diphosphohydrolase)
102	0,35	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
103	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
104	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
105	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
106	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
107	0,48	1	false	1	(1 AS_Valine)
108	1,00	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
109	0,92	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
110	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
111	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
112	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
113	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
114	1,00	1	false	1	(1 AS_Serine_to_Methionine)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,19	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
117	0,19	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
118	1,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
119	0,36	1	false	1	(1 AS_Leucine)
120	0,36	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,48	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,75	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
131	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
132	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
133	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
134	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
135	1,00	1	false	1	(1 AS_Isoleucine)
136	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
137	0,52	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
138	1,00	1	false	1	(1 PurM_5-nucleotidase_dTMP)
139	0,36	1	false	1	(1 PyrM_uridine-kinase_ATP)
140	0,19	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,36	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
142	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
143	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
144	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
145	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
146	1,00	1	false	1	(1 AS_Aspartate_to_Asparagine)
147	1,00	1	false	1	(1 PyrM_cytidine-kinase_ATP)
148	0,64	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
149	0,48	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
150	0,91	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)

151	0,56	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
152	1,00	1	false	1	(1 PurM_XTP-diphosphohydrolase)
153	1,00	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
154	0,60	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
155	0,48	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
156	1,00	1	false	1	(1 PurM_GTP-pyrophosphokinase)
157	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
158	0,48	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
159	1,00	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
160	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
161	0,66	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
162	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dATP)
163	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
164	1,00	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
165	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
166	0,25	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
167	0,51	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
168	0,25	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
169	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
170	1,00	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
171	0,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
172	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
173	0,48	1	false	1	(1 PurM_5-nucleotidase_GMP)
174	0,25	1	false	1	(1 PyrM_cytidine-kinase_ITP)

175	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
176	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
177	1,00	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
178	1,00	16	false	9	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_pyruvate-phosphotransferase_ATP) (-2 TCA_PEP-carboxylase)
179	0,48	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
180	1,00	6	false	6	(-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_ATP-alpha-D-glucokinase) (1 Glyc_ATP-beta-D-glucokinase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_D-Glucose-1-epimerase) (1 PurM_DNA-directed-RNA-polymerase_ATP)
181	1,00	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0687-spermidine/putrescine-transport_import)
182	0,41	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
183	0,48	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
184	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
185	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
186	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductased_dADP)
187	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
188	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
189	1,00	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
190	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
191	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
192	1,00	1	false	1	(1 PyrM_cytidine-kinase_UTP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	0,56	1	false	1	(1 PyrM_cytidine-kinase_dATP)
196	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
197	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. epidermidis* RP62A without IQ-143.

Table S VI.1.11: Extreme Modes of *S. epidermidis* RP62A with 0.16µM IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	0,70	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
4	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
5	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
6	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
7	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
8	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
9	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
10	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
11	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
12	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
13	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
14	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
15	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
16	1,00	1	true	1	(1 TCA_fumarate-hydratase)
17	0,91	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
21	1,00	1	true	1	(1 AS_Serine_to_Glycine)
22	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
23	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
24	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
25	-0,52	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
26	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)

27	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
28	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
29	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
30	-1,33	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
31	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
32	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
33	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
34	1,00	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
35	0,91	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
36	-1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
38	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
39	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
40	0,50	1	true	1	(1 Glyc_Succinate-CoA-ligase)
41	0,50	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
42	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
43	1,00	1	true	1	(1 PurM_metaphosphatase)
44	1,05	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
45	0,73	1	true	1	(1 PurM_GMP-pyrophosphorylase)
46	1,00	3	true	3	(1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase)
47	1,00	6	true	6	(1 ATP-energy_to_ATP-metabolism) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_ATP-alpha-D-glucokinase) (-1 Glyc_ATP-beta-D-glucokinase) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase)
48	0,75	1	true	1	(1 Glyc_PTS-permease2)
49	1,00	4	true	4	(-1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_PTS-permease1)
50	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
51	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)

52	-1,34	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
53	0,79	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
54	0,53	1	true	1	(1 PurM_XMP-pyrophosphorylase)
55	0,53	1	true	1	(1 TCA_succinate-dehydrogenase)
56	0,53	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
57	0,53	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
58	0,53	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
59	0,92	1	true	1	(1 PurM_adenylate-kinase_dAMP)
60	1,08	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
61	-0,65	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
62	0,92	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase)
63	-0,48	14	true	8	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
64	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
65	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
67	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
68	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
69	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_ATP-phosphohydrolase)
70	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
71	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
72	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
73	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
74	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
75	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
76	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)

77	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)
78	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
79	0,55	1	false	1	(1 PyrM_dUTP-diphosphatase)
80	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
81	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
82	1,00	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
83	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
84	1,00	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
85	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
86	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
87	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
90	0,96	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
91	1,00	1	false	1	(1 DNA-extern_to_DNA-intern)
92	0,67	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
93	0,36	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
94	0,41	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
95	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
96	0,30	1	false	1	(1 PurM_ITP-diphosphohydrolase)
97	0,35	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0688-spermidine/putrescine-transport_import)
98	1,00	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
99	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1

					PurM_adenylate-kinase_AMP) (2 SERP0686-spermidine/putrescine-transport_import)
100	0,36	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
101	1,00	1	false	1	(1 PurM_dITP-diphosphohydrolase)
102	0,35	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
103	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
104	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
105	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
106	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
107	0,48	1	false	1	(1 AS_Valine)
108	1,00	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
109	0,92	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
110	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
111	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
112	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
113	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
114	1,00	1	false	1	(1 AS_Serine_to_Methionine)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,19	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
117	0,19	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
118	1,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
119	0,36	1	false	1	(1 AS_Leucine)
120	0,36	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,48	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,75	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
131	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
132	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
133	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
134	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
135	1,00	1	false	1	(1 AS_Isoleucine)
136	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
137	0,52	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
138	1,00	1	false	1	(1 PurM_5-nucleotidase_dTMP)
139	0,36	1	false	1	(1 PyrM_uridine-kinase_ATP)
140	0,19	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,36	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
142	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
143	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
144	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
145	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
146	1,00	1	false	1	(1 AS_Aspartate_to_Asparagine)
147	1,00	1	false	1	(1 PyrM_cytidine-kinase_ATP)
148	0,64	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
149	0,48	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
150	0,91	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)

151	0,56	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
152	1,00	1	false	1	(1 PurM_XTP-diphosphohydrolase)
153	1,00	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
154	0,60	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
155	0,48	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
156	1,00	1	false	1	(1 PurM_GTP-pyrophosphokinase)
157	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
158	0,48	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
159	1,00	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
160	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
161	0,66	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
162	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dATP)
163	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
164	1,00	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
165	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
166	0,25	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
167	0,51	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
168	0,25	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
169	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
170	1,00	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
171	0,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
172	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
173	0,48	1	false	1	(1 PurM_5-nucleotidase_GMP)
174	0,25	1	false	1	(1 PyrM_cytidine-kinase_ITP)

175	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
176	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
177	1,00	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
178	1,00	16	false	9	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_pyruvate-phosphotransferase_ATP) (-2 TCA_PEP-carboxylase)
179	0,48	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
180	1,00	6	false	6	(-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_ATP-alpha-D-glucokinase) (1 Glyc_ATP-beta-D-glucokinase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_D-Glucose-1-epimerase) (1 PurM_DNA-directed-RNA-polymerase_ATP)
181	1,00	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0687-spermidine/putrescine-transport_import)
182	0,41	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
183	0,48	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
184	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
185	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
186	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductased_dADP)
187	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
188	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
189	1,00	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
190	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
191	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
192	1,00	1	false	1	(1 PyrM_cytidine-kinase_UTP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	0,56	1	false	1	(1 PyrM_cytidine-kinase_dATP)
196	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
197	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. epidermidis* RP62A with 0.16µMIQ-143.

Table S VI.1.12: Extreme Modes of *S. epidermidis* RP62A with 1.25µM IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	-0,67	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
4	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
5	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
6	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
7	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
8	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
9	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
10	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
11	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
12	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
13	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
14	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
15	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
16	1,00	1	true	1	(1 TCA_fumarate-hydratase)
17	1,01	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
19	0,39	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
21	1,00	1	true	1	(1 AS_Serine_to_Glycine)
22	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
23	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
24	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
25	-0,52	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
26	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)

27	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
28	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
29	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
30	-1,33	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
31	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
32	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
33	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
34	1,00	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
35	1,00	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
36	1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
38	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
39	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
40	0,75	1	true	1	(1 Glyc_Succinate-CoA-ligase)
41	0,75	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
42	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
43	1,00	1	true	1	(1 PurM_metaphosphatase)
44	1,11	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
45	0,67	1	true	1	(1 PurM_GMP-pyrophosphorylase)
46	1,00	3	true	3	(1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase)
47	1,00	6	true	6	(1 ATP-energy_to_ATP-metabolism) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_ATP-alpha-D-glucokinase) (-1 Glyc_ATP-beta-D-glucokinase) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase)
48	1,12	1	true	1	(1 Glyc_PTS-permease2)
49	1,00	4	true	4	(-1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_PTS-permease1)
50	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
51	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)

52	-1,74	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
53	0,79	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
54	0,53	1	true	1	(1 PurM_XMP-pyrophosphorylase)
55	0,53	1	true	1	(1 TCA_succinate-dehydrogenase)
56	0,53	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
57	0,53	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
58	0,53	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
59	0,92	1	true	1	(1 PurM_adenylate-kinase_dAMP)
60	1,08	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
61	-0,92	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
62	0,92	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase)
63	0,45	14	true	8	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
64	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
65	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
67	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
68	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
69	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_ATP-phosphohydrolase)
70	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
71	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
72	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
73	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
74	2,62	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
75	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
76	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)

77	2,07	1	false	1	(1 SERP1952-macrolide-transport_efflux)
78	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
79	0,28	1	false	1	(1 PyrM_dUTP-diphosphatase)
80	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
81	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
82	1,00	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
83	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
84	3,07	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
85	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
86	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
87	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
90	0,96	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
91	1,00	1	false	1	(1 DNA-extern_to_DNA-intern)
92	0,67	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
93	0,17	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
94	1,09	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
95	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
96	0,48	1	false	1	(1 PurM_ITP-diphosphohydrolase)
97	0,69	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0688-spermidine/putrescine-transport_import)
98	1,00	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
99	1,97	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1

					PurM_adenylate-kinase_AMP) (2 SERP0686-spermidine/putrescine-transport_import)
100	0,01	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
101	1,00	1	false	1	(1 PurM_dITP-diphosphohydrolase)
102	0,08	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
103	2,30	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
104	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
105	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
106	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
107	1,48	1	false	1	(1 AS_Valine)
108	1,00	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
109	0,96	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
110	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
111	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
112	2,06	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
113	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
114	1,00	1	false	1	(1 AS_Serine_to_Methionine)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,00	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
117	0,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
118	1,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
119	0,89	1	false	1	(1 AS_Leucine)
120	0,39	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
121	0,28	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,20	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,72	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,12	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
131	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
132	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
133	0,44	1	false	1	(1 AS_Serine_to_Pyruvate)
134	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
135	1,00	1	false	1	(1 AS_Isoleucine)
136	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
137	0,83	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
138	1,00	1	false	1	(1 PurM_5-nucleotidase_dTMP)
139	0,77	1	false	1	(1 PyrM_uridine-kinase_ATP)
140	0,00	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	1,49	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
142	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
143	2,87	1	false	1	(1 PyrM_OMP-decarboxylase)
144	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
145	2,20	1	false	1	(1 PurM_urea-amidohydrolase)
146	2,20	1	false	1	(1 AS_Aspartate_to_Asparagine)
147	2,20	1	false	1	(1 PyrM_cytidine-kinase_ATP)
148	0,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
149	2,69	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
150	0,00	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)

151	1,23	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
152	1,00	1	false	1	(1 PurM_XTP-diphosphohydrolase)
153	1,00	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
154	0,43	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
155	0,17	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
156	1,00	1	false	1	(1 PurM_GTP-pyrophosphokinase)
157	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
158	1,60	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
159	1,00	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
160	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
161	0,26	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
162	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dATP)
163	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
164	1,00	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
165	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
166	0,25	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
167	1,58	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
168	0,25	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
169	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
170	1,00	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
171	0,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
172	0,88	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
173	0,55	1	false	1	(1 PurM_5-nucleotidase_GMP)
174	0,28	1	false	1	(1 PyrM_cytidine-kinase_ITP)

175	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
176	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
177	1,00	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
178	1,00	16	false	9	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_pyruvate-phosphotransferase_ATP) (-2 TCA_PEP-carboxylase)
179	1,00	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
180	1,00	6	false	6	(-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_ATP-alpha-D-glucokinase) (1 Glyc_ATP-beta-D-glucokinase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_D-Glucose-1-epimerase) (1 PurM_DNA-directed-RNA-polymerase_ATP)
181	1,00	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0687-spermidine/putrescine-transport_import)
182	0,41	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
183	0,48	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
184	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
185	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
186	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductased_dADP)
187	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
188	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
189	1,00	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
190	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
191	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
192	2,68	1	false	1	(1 PyrM_cytidine-kinase_UTP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	0,56	1	false	1	(1 PyrM_cytidine-kinase_dATP)
196	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
197	0,49	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. epidermidis* RP62A with 1.25µM IQ-143.

Table S VI.1.13: Extreme Modes of *H. sapiens* without IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Net reaction
1	0.01655153401230347	1	true	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = AMP-energy + ATP-energy
2	0.9718829672703104	2	true	2	ADP-energy + GTP = ATP-energy + GDP
3	0.03494402270226615	1	true	1	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
4	0.015529980226903106	1	true	1	ATP-energy + UMP = ADP-energy + UDP
5	0.01125584770243826	1	true	1	ATP-energy + GMP = ADP-energy + GDP
6	6.774006132614918E-4	3	true	3	ATP-energy + CDP + RNA-U = ADP-energy + RNA-C + UTP
7	0.025167558640849963	3	true	3	ATP-energy + CDP + RNA-G = ADP-energy + GTP + RNA-C
8	0.028076999689041093	1	true	1	ATP-energy + UMP = ADP-energy + UDP
9	5.899637709720906E-4	1	true	1	ATP-metabolism = ATP-energy
10	0.018001729088897522	1	true	1	Orotidine5-phosphate = CO2 + UMP
11	0.01554561791018938	2	true	2	ATP-energy + H2O = ADP-energy + Orthophosphate
12	0.029944097937886216	1	true	1	AMP-metabolism = AMP-energy
13	0.9527511006480274	4	true	4	ADP-energy + GTP = ATP-energy + GDP
14	0.9876120638225723	4	true	4	2 ATP-energy + HCO3- + Pyruvate = 2 ADP-energy + CO2 + Orthophosphate + Phosphoenolpyruvate
15	0.014188190744323315	2	true	2	no net reaction
16	0.02118596232367509	1	true	1	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
17	0.010106457228134413	1	true	1	ATP-energy + CMP = ADP-energy + CDP
18	0.009358474654924787	1	true	1	ATP-energy + UDP = ADP-energy + UTP
19	0.07943073523980781	1	true	1	H2O + P1P3-Bis(5-adenosyl)triphosphate = ADP-energy + AMP-energy
20	0.010044051015754452	2	true	2	no net reaction
21	0.01824437762284048	2	true	2	no net reaction
22	0.0012509594977667682	3	true	3	no net reaction
23	0.9602115557760446	3	true	3	no net reaction
24	0.01645565948549066	1	true	1	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
25	0.0021665356272504432	3	true	3	ATP-energy + CDP + RNA-A = ADP-energy + ATP-metabolism + RNA-C
26	0.0943099346725943	1	true	1	(S)-Malate = Fumarate + H2O
27	0.012948684236533947	1	true	1	H2O + P1P4-Bis(5-guanosyl)tetraphosphate = GMP + GTP
28	0.045555583674236844	1	true	1	ATP-energy + GDP = ADP-energy + GTP
29	0.013937927079011314	1	true	1	AMP-metabolism + ATP-energy = 2 ADP-metabolism
30	0.04317061235472264	1	true	1	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
31	0.00793872622557823	2	true	2	GTP + IMP + L-Aspartate = AMP-energy + Fumarate + GDP + Orthophosphate
32	0.02717156409365451	2	true	2	no net reaction
33	0.005678293834417758	2	true	2	no net reaction

34	0.009930339633110297	1	true	1	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
35	0.03209480095504813	5	true	5	(S)-Malate + ATP-energy + Pyruvate = (S)-Lactate + ADP-energy + CO2 + Phosphoenolpyruvate
36	0.04450111475800855	1	true	1	ADP-metabolism = AMP-energy
37	0.01989702660635051	1	true	1	AMP-energy + UTP = ADP-energy + UDP
38	0.01692849626786197	1	true	1	H2O + P1P4-Bis(5-uridyl)tetraphosphate = UMP + UTP
39	0.06952355118557085	5	true	5	(S)-Malate + ATP-energy + Xanthosine5-phosphate = ADP-energy + CO2 + H2O + IMP + Phosphoenolpyruvate
40	0.008330465255968367	4	true	4	no net reaction
41	0.005058992507136817	5	true	5	no net reaction
42	5.505708648326779E-4	4	true	4	5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate + ADP-metabolism + Fumarate + Orthophosphate = ATP-metabolism + Aminoimidazoleribotide + CO2 + L-Aspartate + Pyrophosphate
43	0.08181961410412486	1	true	1	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
44	0.005050457086610116	3	false	3	ADP-energy + Pyrophosphate = ATP-energy + Orthophosphate
45	0.018167680737062875	1	false	1	ADP-energy + Ca2+IN + H2O = AMP-energy + Orthophosphate
46	0.015324950057069353	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
47	4.7720160015451984E-4	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
48	0.003578665589720975	3	false	3	ADP-energy + IQ-143+ GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-G_blocked
49	0.001221154736165464	4	false	4	ATP-energy + H2O = ADP-energy + Orthophosphate
50	0.009096800791878135	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
51	0.03951104134964545	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
52	0.00523060743484105	1	false	1	Ca2+IN + GTP-extern + H2O = GMP + Pyrophosphate
53	0.9968666667562996	3	false	3	ATP-energy + Uridine = ADP-energy + UMP
54	0.0032694373666711796	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
55	0.0039695467237707005	1	false	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = 2 ADP-energy
56	0.0121455865991974	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
57	0.01140728480657438	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
58	0.06216909045003616	4	false	4	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
59	0.007239691436841333	4	false	4	ADP-energy + DNA-C + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + CDP + DNA-extern + Thioredoxin
60	0.016436038228987426	2	false	2	GTP + H2O = GMP + Pyrophosphate
61	0.0017676334216116807	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
62	0.010915335683589156	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
63	0.00806401832991821	1	false	1	ATP-metabolism + Ca2+IN + H2O = AMP-energy + Orthophosphate
64	0.008111073626983156	1	false	1	CDP + Ca2+IN + H2O = CMP + Orthophosphate
65	0.00551366953277066	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
66	0.004837438314087672	2	false	2	ADP-ribose + ATP-energy + H2O = 5-Phospho-alpha-D-ribose1-diphosphate + 2 AMP-energy

67	0.002719567373834275	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + Guanine + H2O = NH3 + Pyrophosphate + Xanthosine5-phosphate
68	0.004433263231509499	3	false	3	ADP-energy + Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + Orthophosphate + RNA-U
69	0.0017683832496308005	11	false	11	ATP-energy + DNA-G + NH3 + Uracil = ADP-energy + DNA-C + Guanine + Orthophosphate
70	0.006389732960451755	6	false	6	ADP-energy + CO2 + H2O + Phosphoenolpyruvate + Pyrophosphate + Xanthosine5-phosphate = (S)-Malate + 5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + Urate
71	0.03245474140844962	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
72	0.02876252165783144	1	false	1	ATP-metabolism + Ca2+IN + H2O = ADP-energy + Orthophosphate
73	0.02655006243116209	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
74	0.005829600642677901	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
75	0.015879066073576364	6	false	6	5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + CO2 + H+ + H2O + Hypoxanthine + Phosphoenolpyruvate = (S)-Malate + ATP-energy + Pyrophosphate + Xanthosine5-phosphate
76	0.01305179100730347	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
77	0.0012688045742796916	4	false	4	ADP-energy + DNA-G + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + GDP + Thioredoxin
78	9.123969621090966E-4	2	false	2	2 ATP-energy + Sulfate = 3-Phosphoadenylylsulfate + ADP-energy + Pyrophosphate
79	0.009300834767392185	1	false	1	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
80	0.0022206474374074636	1	false	1	Ca2+IN + H2O + ITP-extern = IMP + Pyrophosphate
81	0.008825953610068216	1	false	1	H2O + UTP = Pyrophosphate + UMP
82	0.008979317355852112	7	false	7	ADP-energy + CO2 + IMP + NH3 + Phosphoenolpyruvate = (S)-Malate + ATP-energy + GMP
83	0.001492299580795775	5	false	5	no net reaction
84	0.00848849181548772	2	false	2	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
85	0.021681261743009217	2	false	2	GMP + H2O = Guanine + alpha-D-Ribose1-phosphate
86	0.057702289633061454	2	false	2	DNA-G + IQ-143= DNA-G_blocked + IQ-_used
87	0.0012961275747516154	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
88	0.010894109338160374	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
89	0.030690514747585662	2	false	2	DNA-A + IQ-143= DNA-A_blocked + IQ-_used
90	0.0074227893781351195	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-U_blocked
91	0.010613528041014009	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
92	0.8837780364757674	1	false	1	ATP-energy + IQ-143+ Sulfate = Adenylylsulfate_blocked + IQ-_used + Pyrophosphate
93	0.024348581021184867	1	false	1	GTP + Pyruvate = GDP + Phosphoenolpyruvate
94	0.007376710993599267	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP
95	0.004201194469749314	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
96	0.0341601707739696	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
97	0.0019757778213018717	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
98	4.581880484155754E-5	1	false	1	H2O + UMP = Orthophosphate + Uridine
99	0.004142418877938869	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate

100	6.64663831680401E-4	8	false	8	510-Methylenetetrahydrofolate + DNA-C + H2O = DNA-T + Dihydrofolate + NH3
101	3.174750994855424E-4	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
102	0.001804175549338094	3	false	3	ATP-energy + H2O = AMP-energy + Pyrophosphate
103	0.02591033431757106	1	false	1	ATP-energy + NH3 + Xanthosine5-phosphate = AMP-energy + GMP + Pyrophosphate
104	2.335524305914216E-4	2	false	2	GTP + NH3 + Uridine = CMP + GDP + H2O
105	0.006859798908416703	4	false	4	2 ATP-energy + HCO3- + L-Aspartate + L-Glutamine + Oxygen = 2 ADP-energy + H2O2 + L-Glutamate + Orotate + 2 Orthophosphate
106	0.09430912891069909	1	false	1	Ca2+IN + GTP + H2O = GDP + Orthophosphate
107	0.01513046193649914	2	false	2	NH3 + UTP + Uridine = CMP + H2O + UDP
108	0.0031978007666132457	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
109	0.9866322844197013	3	false	3	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
110	0.004823885645214965	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
111	0.02008514117824356	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
112	0.0037166464650704167	4	false	4	no net reaction
113	0.027461291380987185	2	false	2	NH3 + UTP = CDP + Orthophosphate
114	1.238309503881485E-4	1	false	1	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = AMP-energy + GMP + L-Glutamate + Pyrophosphate
115	0.0069347528912339085	3	false	3	ADP-energy + ADP-metabolism + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-A_blocked
116	0.0014966550786249533	12	false	12	5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + DNA-A + NH3 + Uracil = ADP-energy + AMP-energy + DNA-C + Orthophosphate + Pyrophosphate
117	0.00961678170064062	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + H2O + Hypoxanthine + Oxygen = H2O2 + Pyrophosphate + Xanthosine5-phosphate
118	0.003486425047949271	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
119	0.004048704451746876	1	false	1	GTP + Uridine = GDP + UMP
120	7.601547877701398E-4	2	false	2	H2O + IMP = Hypoxanthine + alpha-D-Ribose1-phosphate
121	0.0023616325357191936	2	false	2	CMP + 2 H2O = NH3 + Orthophosphate + Uridine
122	0.010139460239020348	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
123	0.013870108901137601	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
124	0.008015444330371158	1	false	1	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
125	0.0030630428480734606	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
126	0.007861645349033441	2	false	2	ATP-energy + H2O = AMP-energy + Pyrophosphate
127	0.026861811545211167	3	false	3	ATP-energy + H2O = ADP-energy + Orthophosphate
128	0.015648974186699194	3	false	3	ADP-energy + ADP-metabolism + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-A
129	0.02750206970242519	1	false	1	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
130	0.006421668756456889	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
131	0.017854367612828104	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + IQ-_used + Orthophosphate + RNA-C_blocked

132	0.007359227270793189	2	false	2	2 H2O + P1P4-Bis(5-xanthosyl)tetraphosphate = Pyrophosphate + 2 Xanthosine5-phosphate
133	0.0025019821493916794	2	false	2	GTP + H2O = GMP + Pyrophosphate
134	0.02467670775406272	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
135	0.005500357152584456	1	false	1	ATP-energy + Uridine = ADP-energy + UMP
136	0.006538273927002236	4	false	4	DNA-A + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + Thioredoxin
137	4.8528168517425474E-4	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
138	0.0058922524232456475	2	false	2	H2O + Oxygen + Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O2 + Urate
139	0.00868422262778401	2	false	2	H2O + L-Glutamine + UTP = CDP + L-Glutamate + Orthophosphate
140	0.015653147128281475	2	false	2	DNA-T + IQ-143= DNA-T_blocked + IQ-_used
141	0.0289175789015248	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
142	0.017844171075269033	1	false	1	Ca2+IN + H2O + UTP = Orthophosphate + UDP
143	9.747119662268933E-4	7	false	7	ADP-energy + DNA-C + 2 H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + NH3 + Thioredoxin + UDP
144	0.023538204503250504	7	false	7	ADP-energy + CO2 + Phosphoenolpyruvate + Thioredoxin = (S)-Malate + ATP-energy + Oxidizedthioredoxin
145	0.03866035115109223	1	false	1	GTP + H2O = GMP + Pyrophosphate
146	0.010487485921525264	1	false	1	AMP-energy + H2O = IMP + NH3
147	0.0022429419981450094	3	false	3	AMP-energy + ATP-energy + Pyrophosphate + alpha-D-Ribose1-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + AMP-metabolism + Orthophosphate
148	0.015311481162256335	3	false	3	ADP-energy + GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-G
149	0.012361030082629898	1	false	1	UTP + Uridine = UDP + UMP
150	0.0038361570176190796	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
151	0.024077724104495934	2	false	2	DNA-C + IQ-143= DNA-C_blocked + IQ-_used
152	0.004517643364860158	11	false	11	DNA-C + Guanine + H2O = DNA-G + NH3 + Uracil
153	0.004049895406326054	1	false	1	Allantoate + H2O = Allantoine
154	0.0011179498930405929	32	false	19	5 ADP-energy + CO2 + H2O + Orthophosphate + 4 Phosphoenolpyruvate + Pyruvate + Ubiquinone = 3 (S)-Malate + 5 ATP-energy + Fumarate + Ubiquinol
155	0.004243888613050029	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP

[1] This data shows the elementary mode Analysis for *H. sapiens* without IQ-143:

Table S VI.1.14: Extreme Modes of *H. sapiens* with 0.16µM IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Net reaction
1	0.005130030045226164	1	true	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = AMP-energy + ATP-energy
2	0.4397620271448569	2	true	2	ADP-energy + GTP = ATP-energy + GDP
3	0.09480536073977541	1	true	1	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
4	0.03823934247721361	1	true	1	ATP-energy + UMP = ADP-energy + UDP
5	0.009104482032904815	1	true	1	ATP-energy + GMP = ADP-energy + GDP
6	0.007704237115931267	3	true	3	ATP-energy + CDP + RNA-U = ADP-energy + RNA-C + UTP
7	0.0017270300754455015	3	true	3	ATP-energy + CDP + RNA-G = ADP-energy + GTP + RNA-C
8	0.05725996742131523	1	true	1	ATP-energy + UMP = ADP-energy + UDP
9	0.024214500034897335	1	true	1	ATP-metabolism = ATP-energy
10	0.009442734667085562	1	true	1	Orotidine5-phosphate = CO2 + UMP
11	0.01202298234818866	2	true	2	ATP-energy + H2O = ADP-energy + Orthophosphate
12	0.011202803201679434	1	true	1	AMP-metabolism = AMP-energy
13	0.9979458833338856	4	true	4	ADP-energy + GTP = ATP-energy + GDP
14	0.9941042589766935	4	true	4	2 ATP-energy + HCO3- + Pyruvate = 2 ADP-energy + CO2 + Orthophosphate + Phosphoenolpyruvate
15	0.011028459588632078	2	true	2	no net reaction
16	0.020505076858065685	1	true	1	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
17	0.020231747454989013	1	true	1	ATP-energy + CMP = ADP-energy + CDP
18	0.02088527667504403	1	true	1	ATP-energy + UDP = ADP-energy + UTP
19	0.004049843361527694	1	true	1	H2O + P1P3-Bis(5-adenosyl)triphosphate = ADP-energy + AMP-energy
20	0.006013692692126038	2	true	2	no net reaction
21	0.007596162022488362	2	true	2	no net reaction
22	0.004653191538830148	3	true	3	no net reaction
23	0.973957437873535	3	true	3	no net reaction
24	0.015164298309223834	1	true	1	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
25	7.342594063648455E-4	3	true	3	ATP-energy + CDP + RNA-A = ADP-energy + ATP-metabolism + RNA-C
26	0.007375314266941269	1	true	1	(S)-Malate = Fumarate + H2O
27	0.008856758026085099	1	true	1	H2O + P1P4-Bis(5-guanosyl)tetraphosphate = GMP + GTP
28	0.044765835448331015	1	true	1	ATP-energy + GDP = ADP-energy + GTP
29	0.007429803106260624	1	true	1	AMP-metabolism + ATP-energy = 2 ADP-metabolism
30	0.04581608968990736	1	true	1	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
31	0.009072609077389049	2	true	2	GTP + IMP + L-Aspartate = AMP-energy + Fumarate + GDP + Orthophosphate
32	0.0018817352810703847	2	true	2	no net reaction
33	0.001122515017348391	2	true	2	no net reaction

34	0.06639499216836431	1	true	1	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
35	0.03186315028386555	5	true	5	(S)-Malate + ATP-energy + Pyruvate = (S)-Lactate + ADP-energy + CO2 + Phosphoenolpyruvate
36	0.002501413320115886	1	true	1	ADP-metabolism = AMP-energy
37	0.004531527096812593	1	true	1	AMP-energy + UTP = ADP-energy + UDP
38	0.024179372922236708	1	true	1	H2O + P1P4-Bis(5-uridyl)tetraphosphate = UMP + UTP
39	0.0026795687764290532	5	true	5	(S)-Malate + ATP-energy + Xanthosine5-phosphate = ADP-energy + CO2 + H2O + IMP + Phosphoenolpyruvate
40	0.005717595903887207	4	true	4	no net reaction
41	0.028842907966356357	5	true	5	no net reaction
42	0.0011252802077290625	4	true	4	5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate + ADP-metabolism + Fumarate + Orthophosphate = ATP-metabolism + Aminoimidazoleribotide + CO2 + L-Aspartate + Pyrophosphate
43	0.005496024523628518	1	true	1	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
44	3.5454087822606173E-4	3	false	3	ADP-energy + Pyrophosphate = ATP-energy + Orthophosphate
45	0.038917876242217875	1	false	1	ADP-energy + Ca2+IN + H2O = AMP-energy + Orthophosphate
46	0.0013525861946372952	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
47	0.002492485469045347	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
48	0.002626741631829521	3	false	3	ADP-energy + IQ-143+ GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-G_blocked
49	0.004093079518189935	4	false	4	ATP-energy + H2O = ADP-energy + Orthophosphate
50	0.0013834190967744187	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
51	0.06249878824378918	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
52	0.02767266096177401	1	false	1	Ca2+IN + GTP-extern + H2O = GMP + Pyrophosphate
53	0.9217398821749008	3	false	3	ATP-energy + Uridine = ADP-energy + UMP
54	0.030031470687912343	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
55	0.06378578683142644	1	false	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = 2 ADP-energy
56	0.03379212500206907	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
57	0.003730768499201065	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
58	0.0017552338135035095	4	false	4	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
59	0.014714368899165442	4	false	4	ADP-energy + DNA-C + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + CDP + DNA-extern + Thioredoxin
60	0.005362707333533834	2	false	2	GTP + H2O = GMP + Pyrophosphate
61	0.02427660710520141	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
62	0.009934934521844463	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
63	0.008655018738876752	1	false	1	ATP-metabolism + Ca2+IN + H2O = AMP-energy + Orthophosphate
64	0.05689430909157689	1	false	1	CDP + Ca2+IN + H2O = CMP + Orthophosphate
65	0.017796655470858735	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
66	0.0014726423314010972	2	false	2	ADP-ribose + ATP-energy + H2O = 5-Phospho-alpha-D-ribose1-diphosphate + 2 AMP-energy

67	0.0042776150948071745	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + Guanine + H2O = NH3 + Pyrophosphate + Xanthosine5-phosphate
68	0.028939063589240477	3	false	3	ADP-energy + Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + Orthophosphate + RNA-U
69	0.0019344000178397325	11	false	11	ATP-energy + DNA-G + NH3 + Uracil = ADP-energy + DNA-C + Guanine + Orthophosphate
70	0.004886284569103672	6	false	6	ADP-energy + CO2 + H2O + Phosphoenolpyruvate + Pyrophosphate + Xanthosine5-phosphate = (S)-Malate + 5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + Urate
71	0.013029597677572946	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
72	0.011362712812997389	1	false	1	ATP-metabolism + Ca2+IN + H2O = ADP-energy + Orthophosphate
73	9.490223452437441E-4	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
74	0.008945411265786518	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
75	0.037504588669099004	6	false	6	5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + CO2 + H+ + H2O + Hypoxanthine + Phosphoenolpyruvate = (S)-Malate + ATP-energy + Pyrophosphate + Xanthosine5-phosphate
76	0.021714933706790007	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
77	0.00473388172511402	4	false	4	ADP-energy + DNA-G + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + GDP + Thioredoxin
78	0.0049789841623851805	2	false	2	2 ATP-energy + Sulfate = 3-Phosphoadenylylsulfate + ADP-energy + Pyrophosphate
79	0.02462816689965397	1	false	1	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
80	0.05674045026156782	1	false	1	Ca2+IN + H2O + ITP-extern = IMP + Pyrophosphate
81	0.012680697978049826	1	false	1	H2O + UTP = Pyrophosphate + UMP
82	0.007168636006845586	7	false	7	ADP-energy + CO2 + IMP + NH3 + Phosphoenolpyruvate = (S)-Malate + ATP-energy + GMP
83	0.010391719615760908	5	false	5	no net reaction
84	0.005244773454489482	2	false	2	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
85	0.03392668547022826	2	false	2	GMP + H2O = Guanine + alpha-D-Ribose1-phosphate
86	0.001402994837579885	2	false	2	DNA-G + IQ-143= DNA-G_blocked + IQ-_used
87	0.0027033208390069285	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
88	0.011498488414621533	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
89	0.0061472460822511454	2	false	2	DNA-A + IQ-143= DNA-A_blocked + IQ-_used
90	0.0018108729538574009	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-U_blocked
91	0.011049185312248078	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
92	0.028842651739239833	1	false	1	ATP-energy + IQ-143+ Sulfate = Adenylylsulfate_blocked + IQ-_used + Pyrophosphate
93	0.05461213055700753	1	false	1	GTP + Pyruvate = GDP + Phosphoenolpyruvate
94	0.014964491850709916	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP
95	0.007781740827399131	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
96	0.06305805710461365	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
97	0.0173973276128907	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
98	0.04225034421881002	1	false	1	H2O + UMP = Orthophosphate + Uridine
99	0.021249692031397704	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate

100	0.004424086757605639	8	false	8	510-Methylenetetrahydrofolate + DNA-C + H2O = DNA-T + Dihydrofolate + NH3
101	0.005398561772016364	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
102	3.3045236095607944E-4	3	false	3	ATP-energy + H2O = AMP-energy + Pyrophosphate
103	0.013104590439268482	1	false	1	ATP-energy + NH3 + Xanthosine5-phosphate = AMP-energy + GMP + Pyrophosphate
104	0.0015242489203124432	2	false	2	GTP + NH3 + Uridine = CMP + GDP + H2O
105	6.166920175361135E-4	4	false	4	2 ATP-energy + HCO3- + L-Aspartate + L-Glutamine + Oxygen = 2 ADP-energy + H2O2 + L-Glutamate + Orotate + 2 Orthophosphate
106	0.008111785491578982	1	false	1	Ca2+IN + GTP + H2O = GDP + Orthophosphate
107	0.004761078016804143	2	false	2	NH3 + UTP + Uridine = CMP + H2O + UDP
108	0.00726859053151796	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
109	0.978557363640139	3	false	3	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
110	0.009356081770501179	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
111	0.007757346401982335	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
112	0.007899099267346443	4	false	4	no net reaction
113	0.003637222532724582	2	false	2	NH3 + UTP = CDP + Orthophosphate
114	0.024721054946452714	1	false	1	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = AMP-energy + GMP + L-Glutamate + Pyrophosphate
115	0.002172243679348207	3	false	3	ADP-energy + ADP-metabolism + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-A_blocked
116	3.426474497347787E-5	12	false	12	5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + DNA-A + NH3 + Uracil = ADP-energy + AMP-energy + DNA-C + Orthophosphate + Pyrophosphate
117	0.018897696087057603	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + H2O + Hypoxanthine + Oxygen = H2O2 + Pyrophosphate + Xanthosine5-phosphate
118	0.008940149045068346	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
119	0.00829517643691624	1	false	1	GTP + Uridine = GDP + UMP
120	1.198011158797252E-4	2	false	2	H2O + IMP = Hypoxanthine + alpha-D-Ribose1-phosphate
121	0.022565897110051525	2	false	2	CMP + 2 H2O = NH3 + Orthophosphate + Uridine
122	0.04362319987102781	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
123	7.527538197071859E-5	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
124	0.0054598110854725546	1	false	1	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
125	0.0031234091917802242	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
126	0.008061512557000716	2	false	2	ATP-energy + H2O = AMP-energy + Pyrophosphate
127	0.0010510169904632827	3	false	3	ATP-energy + H2O = ADP-energy + Orthophosphate
128	7.294308598648769E-4	3	false	3	ADP-energy + ADP-metabolism + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-A
129	0.025992562132787334	1	false	1	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
130	0.015591813645899566	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
131	0.019361033089730917	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + IQ-_used + Orthophosphate + RNA-C_blocked

132	0.004785085285212376	2	false	2	2 H2O + P1P4-Bis(5-xanthosyl)tetraphosphate = Pyrophosphate + 2 Xanthosine5-phosphate
133	0.009332045603517969	2	false	2	GTP + H2O = GMP + Pyrophosphate
134	0.014022959237212751	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
135	0.015626722755678557	1	false	1	ATP-energy + Uridine = ADP-energy + UMP
136	0.006122072625027286	4	false	4	DNA-A + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + Thioredoxin
137	1.5673110828329229E-4	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
138	0.0034552749225255086	2	false	2	H2O + Oxygen + Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O2 + Urate
139	0.002503619054793238	2	false	2	H2O + L-Glutamine + UTP = CDP + L-Glutamate + Orthophosphate
140	0.005954231138678656	2	false	2	DNA-T + IQ-143= DNA-T_blocked + IQ-_used
141	0.01594636277704542	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
142	0.042874775592222525	1	false	1	Ca2+IN + H2O + UTP = Orthophosphate + UDP
143	0.0025932956925613926	7	false	7	ADP-energy + DNA-C + 2 H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + NH3 + Thioredoxin + UDP
144	0.002449448426728229	7	false	7	ADP-energy + CO2 + Phosphoenolpyruvate + Thioredoxin = (S)-Malate + ATP-energy + Oxidizedthioredoxin
145	0.008968343979364857	1	false	1	GTP + H2O = GMP + Pyrophosphate
146	0.03491931732673392	1	false	1	AMP-energy + H2O = IMP + NH3
147	0.004039751031648775	3	false	3	AMP-energy + ATP-energy + Pyrophosphate + alpha-D-Ribose1-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + AMP-metabolism + Orthophosphate
148	0.010084535436451492	3	false	3	ADP-energy + GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-G
149	0.005047005030052842	1	false	1	UTP + Uridine = UDP + UMP
150	0.010647652395587737	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
151	0.005301580724417554	2	false	2	DNA-C + IQ-143= DNA-C_blocked + IQ-_used
152	0.00838356805192797	11	false	11	DNA-C + Guanine + H2O = DNA-G + NH3 + Uracil
153	0.00599529324361292	1	false	1	Allantoate + H2O = Allantoine
154	0.004394616104792082	32	false	19	5 ADP-energy + CO2 + H2O + Orthophosphate + 4 Phosphoenolpyruvate + Pyruvate + Ubiquinone = 3 (S)-Malate + 5 ATP-energy + Fumarate + Ubiquinol
155	0.06899209623572422	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP

[1] This data shows the elementary mode Analysis for *H. sapiens* with 0.16µM IQ-143:

Table S VI.1.15: Extreme Modes of *H. sapiens* with 1.25µM IQ-143[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Net reaction
1	0.04786344329223191	1	true	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = AMP-energy + ATP-energy
2	9.969914267465851E-4	2	true	2	ADP-energy + GTP = ATP-energy + GDP
3	0.043535723909962964	1	true	1	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
4	0.0024175638614146733	1	true	1	ATP-energy + UMP = ADP-energy + UDP
5	0.015989171210082476	1	true	1	ATP-energy + GMP = ADP-energy + GDP
6	0.02610634288231406	3	true	3	ATP-energy + CDP + RNA-U = ADP-energy + RNA-C + UTP
7	0.0024562865309492032	3	true	3	ATP-energy + CDP + RNA-G = ADP-energy + GTP + RNA-C
8	5.19077773227683E-4	1	true	1	ATP-energy + UMP = ADP-energy + UDP
9	0.017423153536418656	1	true	1	ATP-metabolism = ATP-energy
10	0.04700909087115568	1	true	1	Orotidine5-phosphate = CO2 + UMP
11	0.022066422914005845	2	true	2	ATP-energy + H2O = ADP-energy + Orthophosphate
12	0.01030019410617422	1	true	1	AMP-metabolism = AMP-energy
13	0.004261111240344895	4	true	4	ADP-energy + GTP = ATP-energy + GDP
14	0.013080093351799937	4	true	4	2 ATP-energy + HCO3- + Pyruvate = 2 ADP-energy + CO2 + Orthophosphate + Phosphoenolpyruvate
15	0.0012275664668326414	2	true	2	no net reaction
16	0.00433006585860185	1	true	1	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
17	0.019781052892711704	1	true	1	ATP-energy + CMP = ADP-energy + CDP
18	0.0010147643752992375	1	true	1	ATP-energy + UDP = ADP-energy + UTP
19	0.006170733778273374	1	true	1	H2O + P1P3-Bis(5-adenosyl)triphosphate = ADP-energy + AMP-energy
20	0.016076798397335335	2	true	2	no net reaction
21	0.011940090048190632	2	true	2	no net reaction
22	0.025841353292343383	3	true	3	no net reaction
23	0.028192008364815835	3	true	3	no net reaction
24	0.005615818134375838	1	true	1	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
25	0.007894959793193546	3	true	3	ATP-energy + CDP + RNA-A = ADP-energy + ATP-metabolism + RNA-C
26	0.041824191955041945	1	true	1	(S)-Malate = Fumarate + H2O
27	0.04015022028649451	1	true	1	H2O + P1P4-Bis(5-guanosyl)tetraphosphate = GMP + GTP
28	0.12142369551244281	1	true	1	ATP-energy + GDP = ADP-energy + GTP
29	0.021965147209823566	1	true	1	AMP-metabolism + ATP-energy = 2 ADP-metabolism
30	0.030048932370557502	1	true	1	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
31	0.002086001036413987	2	true	2	GTP + IMP + L-Aspartate = AMP-energy + Fumarate + GDP + Orthophosphate
32	0.006743979293639235	2	true	2	no net reaction
33	0.012944044905924934	2	true	2	no net reaction

34	0.00441884231341827	1	true	1	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
35	0.003571153435644736	5	true	5	(S)-Malate + ATP-energy + Pyruvate = (S)-Lactate + ADP-energy + CO2 + Phosphoenolpyruvate
36	0.004534729677700966	1	true	1	ADP-metabolism = AMP-energy
37	0.032044253587553806	1	true	1	AMP-energy + UTP = ADP-energy + UDP
38	7.099999894971676E-4	1	true	1	H2O + P1P4-Bis(5-uridyl)tetraphosphate = UMP + UTP
39	0.010679959181318699	5	true	5	(S)-Malate + ATP-energy + Xanthosine5-phosphate = ADP-energy + CO2 + H2O + IMP + Phosphoenolpyruvate
40	0.007486618692184921	4	true	4	no net reaction
41	0.013612737316568868	5	true	5	no net reaction
42	0.0016902796065854098	4	true	4	5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate + ADP-metabolism + Fumarate + Orthophosphate = ATP-metabolism + Aminoimidazoleribotide + CO2 + L-Aspartate + Pyrophosphate
43	0.03245607435050746	1	true	1	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
44	0.03648286865370309	3	false	3	ADP-energy + Pyrophosphate = ATP-energy + Orthophosphate
45	0.06904247945993924	1	false	1	ADP-energy + Ca2+IN + H2O = AMP-energy + Orthophosphate
46	0.003848199268884356	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
47	0.005319774297396718	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
48	0.02341366278916257	3	false	3	ADP-energy + IQ-143+ GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-G_blocked
49	4.675662664771485E-4	4	false	4	ATP-energy + H2O = ADP-energy + Orthophosphate
50	0.0053543977035213075	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
51	0.010394427608318435	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
52	0.03227190121903123	1	false	1	Ca2+IN + GTP-extern + H2O = GMP + Pyrophosphate
53	0.0015538189262196411	3	false	3	ATP-energy + Uridine = ADP-energy + UMP
54	0.0012552736251809637	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
55	0.02581182905210888	1	false	1	H2O + P1P4-Bis(5-adenosyl)tetraphosphate = 2 ADP-energy
56	0.005194653803581528	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
57	0.005633159716414093	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
58	0.014057220558407302	4	false	4	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
59	0.006242782616069031	4	false	4	ADP-energy + DNA-C + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + CDP + DNA-extern + Thioredoxin
60	0.004282826338055878	2	false	2	GTP + H2O = GMP + Pyrophosphate
61	0.001134341575070752	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
62	0.0010239360615290627	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
63	0.027356029648537894	1	false	1	ATP-metabolism + Ca2+IN + H2O = AMP-energy + Orthophosphate
64	0.0030045698055946035	1	false	1	CDP + Ca2+IN + H2O = CMP + Orthophosphate
65	0.016130726483697178	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
66	0.03019053483656997	2	false	2	ADP-ribose + ATP-energy + H2O = 5-Phospho-alpha-D-ribose1-diphosphate + 2 AMP-energy

67	0.0053798800333575425	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + Guanine + H2O = NH3 + Pyrophosphate + Xanthosine5-phosphate
68	0.14524612475598087	3	false	3	ADP-energy + Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + Orthophosphate + RNA-U
69	0.00922704665219487	11	false	11	ATP-energy + DNA-G + NH3 + Uracil = ADP-energy + DNA-C + Guanine + Orthophosphate
70	0.001072276755925583	6	false	6	ADP-energy + CO2 + H2O + Phosphoenolpyruvate + Pyrophosphate + Xanthosine5-phosphate = (S)-Malate + 5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + Urate
71	0.0031409560779063206	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
72	0.008811456227530878	1	false	1	ATP-metabolism + Ca2+IN + H2O = ADP-energy + Orthophosphate
73	0.007136260273736927	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
74	0.0013534572263430578	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
75	0.008475650468189877	6	false	6	5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + CO2 + H+ + H2O + Hypoxanthine + Phosphoenolpyruvate = (S)-Malate + ATP-energy + Pyrophosphate + Xanthosine5-phosphate
76	0.02931985124428904	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
77	0.012858209684887156	4	false	4	ADP-energy + DNA-G + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + GDP + Thioredoxin
78	0.012414781170910327	2	false	2	2 ATP-energy + Sulfate = 3-Phosphoadenylylsulfate + ADP-energy + Pyrophosphate
79	0.02071046953045297	1	false	1	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
80	0.01105236496032247	1	false	1	Ca2+IN + H2O + ITP-extern = IMP + Pyrophosphate
81	0.016748309469321043	1	false	1	H2O + UTP = Pyrophosphate + UMP
82	6.818332352701573E-4	7	false	7	ADP-energy + CO2 + IMP + NH3 + Phosphoenolpyruvate = (S)-Malate + ATP-energy + GMP
83	0.002331856128874543	5	false	5	no net reaction
84	0.018780980362019584	2	false	2	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
85	0.006564626807817553	2	false	2	GMP + H2O = Guanine + alpha-D-Ribose1-phosphate
86	0.9999576902783548	2	false	2	DNA-G + IQ-143= DNA-G_blocked + IQ-_used
87	0.007141838537199963	4	false	4	AMP-energy + H2O + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine + NH3
88	5.023155754058095E-4	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
89	0.9404019561579331	2	false	2	DNA-A + IQ-143= DNA-A_blocked + IQ-_used
90	0.003684070716048704	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C + UDP = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-U_blocked
91	0.00900774932214976	3	false	3	5-Phospho-alpha-D-ribose1-diphosphate + H2O = Pyrophosphate + alpha-D-Ribose1-phosphate
92	0.9052578090052474	1	false	1	ATP-energy + IQ-143+ Sulfate = Adenylylsulfate_blocked + IQ-_used + Pyrophosphate
93	0.0023795055965034617	1	false	1	GTP + Pyruvate = GDP + Phosphoenolpyruvate
94	0.02743226904519125	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP
95	0.0021222770499396137	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
96	0.044015805264594254	1	false	1	Ca2+IN + GDP + H2O = GMP + Orthophosphate
97	0.0030431229120700953	2	false	2	ATP-energy + H2O = ADP-energy + Orthophosphate
98	0.016630177019761216	1	false	1	H2O + UMP = Orthophosphate + Uridine
99	0.003106060318267767	2	false	2	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate

100	0.023123882315774336	8	false	8	510-Methylenetetrahydrofolate + DNA-C + H2O = DNA-T + Dihydrofolate + NH3
101	0.002200615066273004	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
102	0.007652047024873321	3	false	3	ATP-energy + H2O = AMP-energy + Pyrophosphate
103	0.011688263659672793	1	false	1	ATP-energy + NH3 + Xanthosine5-phosphate = AMP-energy + GMP + Pyrophosphate
104	0.0033953448234627093	2	false	2	GTP + NH3 + Uridine = CMP + GDP + H2O
105	0.0031390977125216324	4	false	4	2 ATP-energy + HCO3- + L-Aspartate + L-Glutamine + Oxygen = 2 ADP-energy + H2O2 + L-Glutamate + Orotate + 2 Orthophosphate
106	0.014404549605998684	1	false	1	Ca2+IN + GTP + H2O = GDP + Orthophosphate
107	0.023822985645377437	2	false	2	NH3 + UTP + Uridine = CMP + H2O + UDP
108	0.005334194545468796	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
109	0.006813723317181775	3	false	3	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
110	0.0123874464089746	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
111	0.004462246738856868	2	false	2	ATP-energy + Ca2+IN + H2O = ADP-energy + Orthophosphate
112	0.00387935641331405	4	false	4	no net reaction
113	4.530603317655091E-4	2	false	2	NH3 + UTP = CDP + Orthophosphate
114	0.02115380878234141	1	false	1	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = AMP-energy + GMP + L-Glutamate + Pyrophosphate
115	0.0013293192726026026	3	false	3	ADP-energy + ADP-metabolism + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + CDP + IQ-_used + Orthophosphate + RNA-A_blocked
116	0.001546238801111044	12	false	12	5-Phospho-alpha-D-ribose1-diphosphate + ATP-energy + DNA-A + NH3 + Uracil = ADP-energy + AMP-energy + DNA-C + Orthophosphate + Pyrophosphate
117	0.006849424772078727	2	false	2	5-Phospho-alpha-D-ribose1-diphosphate + H2O + Hypoxanthine + Oxygen = H2O2 + Pyrophosphate + Xanthosine5-phosphate
118	0.04704490543092743	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
119	0.009287293737837987	1	false	1	GTP + Uridine = GDP + UMP
120	0.006619911129784106	2	false	2	H2O + IMP = Hypoxanthine + alpha-D-Ribose1-phosphate
121	0.02191206586226513	2	false	2	CMP + 2 H2O = NH3 + Orthophosphate + Uridine
122	0.0158196922577456	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
123	0.01415519903558382	2	false	2	ATP-energy + Uridine = ADP-energy + UMP
124	0.01644168087774822	1	false	1	ATP-energy + Pyruvate = ADP-energy + Phosphoenolpyruvate
125	7.815613069988014E-4	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
126	0.053833488904838744	2	false	2	ATP-energy + H2O = AMP-energy + Pyrophosphate
127	0.001402091186954224	3	false	3	ATP-energy + H2O = ADP-energy + Orthophosphate
128	0.2188669341228312	3	false	3	ADP-energy + ADP-metabolism + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-A
129	0.02926510063971466	1	false	1	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
130	0.010179196296325466	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
131	0.0111746841194863	3	false	3	ADP-energy + IQ-143+ Pyrophosphate + RNA-C = ATP-energy + IQ-_used + Orthophosphate + RNA-C_blocked

132	0.021019182823906024	2	false	2	2 H2O + P1P4-Bis(5-xanthosyl)tetraphosphate = Pyrophosphate + 2 Xanthosine5-phosphate
133	0.021994073293478134	2	false	2	GTP + H2O = GMP + Pyrophosphate
134	0.06968296119203132	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
135	0.04474208869152774	1	false	1	ATP-energy + Uridine = ADP-energy + UMP
136	0.03445053484672955	4	false	4	DNA-A + H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + Thioredoxin
137	0.006484915953373527	3	false	3	ATP-energy + NH3 + Uridine = ADP-energy + CMP + H2O
138	0.008035694031373719	2	false	2	H2O + Oxygen + Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O2 + Urate
139	0.004374721814733973	2	false	2	H2O + L-Glutamine + UTP = CDP + L-Glutamate + Orthophosphate
140	0.9648928850467682	2	false	2	DNA-T + IQ-143= DNA-T_blocked + IQ-_used
141	0.004871280551854706	1	false	1	ATP-energy + IQ-143= ADP-energy + IQ-_deactivated
142	0.012602828385737341	1	false	1	Ca2+IN + H2O + UTP = Orthophosphate + UDP
143	0.010884819015411384	7	false	7	ADP-energy + DNA-C + 2 H2O + Oxidizedthioredoxin + Pyrophosphate = ATP-energy + DNA-extern + NH3 + Thioredoxin + UDP
144	0.00878438293861894	7	false	7	ADP-energy + CO2 + Phosphoenolpyruvate + Thioredoxin = (S)-Malate + ATP-energy + Oxidizedthioredoxin
145	0.014298632472019679	1	false	1	GTP + H2O = GMP + Pyrophosphate
146	0.042079271834483456	1	false	1	AMP-energy + H2O = IMP + NH3
147	0.012812062622998388	3	false	3	AMP-energy + ATP-energy + Pyrophosphate + alpha-D-Ribose1-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy + AMP-metabolism + Orthophosphate
148	0.536120821107934	3	false	3	ADP-energy + GDP + Pyrophosphate + RNA-C = ATP-energy + CDP + Orthophosphate + RNA-G
149	0.014607669409517632	1	false	1	UTP + Uridine = UDP + UMP
150	0.007971935340850722	3	false	3	2 ATP-energy + H2O = 2 ADP-energy + Pyrophosphate
151	0.9837572375860835	2	false	2	DNA-C + IQ-143= DNA-C_blocked + IQ-_used
152	0.005321509682737813	11	false	11	DNA-C + Guanine + H2O = DNA-G + NH3 + Uracil
153	0.0033649574875739274	1	false	1	Allantoate + H2O = Allantoine
154	0.003864486961261848	32	false	19	5 ADP-energy + CO2 + H2O + Orthophosphate + 4 Phosphoenolpyruvate + Pyruvate + Ubiquinone = 3 (S)-Malate + 5 ATP-energy + Fumarate + Ubiquinol
155	0.014927222858377998	1	false	1	Ca2+IN + H2O + UDP = Orthophosphate + UMP

[1] This data shows the elementary mode Analysis for *H. sapiens* with 1.25µM IQ-143:

6: Extreme modes with changed activity after administration of IQ-143

Table S VI.1.16: Extreme modes (EMs) with a significantly higher activity in *S. epidermidis* after IQ-143 administration[1].

EM Number	Pathlength	Reactions
17	1	(1 TCA_fumarate-hydratase)
35	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
36	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
40	1	(1 PurM_IMP_L-aspartate-ligase)
41	1	(1 Glyc_Succinate-CoA-ligase)
48	1	(1 PurM_ATP_dCDP-phosphotransferase)
63	1	(1 PurM_adenylylsulfate-kinase)
74	1	(1 PyrM_uridine-kinase_dTTP)
77	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
84	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
94	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
96	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
97	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
99	1	(1 PyrM_dUTP-diphosphohydrolase)
103	1	(1 PurM_5-nucleotidase_UMP)
107	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
112	1	(1 PurM_UTP-diphosphohydrolase)
119	1	(1 AS_Leucine)
139	1	(1 PurM_5-nucleotidase_dTMP)
141	1	(1 PyrM_uridine-kinase_ATP)
143	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-

		oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
147	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
149	1	(1 PyrM_cytidine-kinase_ATP)
151	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
158	1	(1 PurM_GTP-pyrophosphokinase)
172	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_DNA-directed-RNA-polyermase_ATP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
179	1	(1 PyrM_cytidine-kinase_GTP)
192	1	(1 PurM_5-nucleotidase_CMP)

[1] The listed EMs of *S. epidermidis* showed a higher activity when 0,16µM and 1,25µM IQ-143were administered.

Left column: Number of specific mode in the full EM model (Tables S10-S12).

Middle colum: Number of enzymes involved in formation of affected EM.

Table S VI.1.17: EMs with a significantly lower activity in *S. epidermidis* after IQ-143 administration[1].

EM Number	Pathlength	Reactions
3	1	(1 PurM_ATP_IDP-phosphotransferase)
19	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
45	1	(1 PurM_GMP-pyrophosphorylase)
52	1	(1 PyrM_UMP-pyrophosphorylase)
61	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
79	1	(1 PyrM_dUTP-diphosphatase)
93	1	(1 SERP0841-PurM_PNPase_GDP)
100	1	(1 PyrM_dUTP-diphosphohydrolase)
102	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
116	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
117	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
122	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
127	1	(1 PyrM_uridine-kinase_UTP)
133	1	(1 AS_Serine_to_Pyruvate)
140	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
148	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
150	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)
154	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
155	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3

		TCA_citrate_synthase)
161	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
197	1	(1 PyrM_uridine-kinase_GTP)

[1] The listed EMs of *S. epidermidis* showed a lower activity when 0,16µM and 1,25µM IQ-143were administered.

Left column: Number of specific mode in the full EM model (Tables S10-S12).

Middle colum: Number of enzymes involved in formation of affected EM.

Table S VI.1.18: EMs with a significantly higher activity in *S. aureus* after IQ-143 administration[1].

EM Number	Pathlength	Reactions
49	1	(1 PyrM_UMP-pyrophosphorylase)
50	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
51	1	(1 PurM_XMP-pyrophosphorylase)
52	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
53	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
54	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
61	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP)
79	1	(1 AS_Aspartate_to_beta-Alanine)
90	1	(1 DNA-extern_to_DNA-intern)
96	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
98	2	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0686-spermidine/putrescine-transport_import)
103	1	(1 PurM_5-nucleotidase_UMP)
109	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
116	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
122	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
130	1	(1 PurM_allantoinase)
137	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
139	1	(1 PurM_5-nucleotidase_dTMP)
140	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)

141	1	(1 PyrM_uridine-kinase_ATP)
143	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
146	1	(1 PurM_urea-amidohydrolase)
147	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
148	1	(1 AS_Aspartate_to_Asparagine)
149	1	(1 PyrM_cytidine-kinase_ATP)
151	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
158	1	(1 PurM_GTP-pyrophosphokinase)
180	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
198	1	(1 PyrM_uridine-kinase_GTP)

[1] The listed EMs of *S. aureus* showed a higher activity after administration of 0,16µM and 1,25µM IQ-143.

Left column: Number of specific mode in the full EM model (Tables S7-S9).

Middle colum: Number of enzymes involved in formation of affected EM.

Table S VI.1.19: EMs with a significantly lower activity in *S. aureus* after IQ-143 administration[1].

EM Number	Pathlength	Reactions
19	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
25	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
58	6	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP)
73	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
82	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
93	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)

102	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
133	1	(1 PyrM_uridine-kinase_dATP)
150	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
154	1	(1 PurM_XTP-diphosphohydrolase)
161	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
184	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
196	1	(1 PyrM_cytidine-kinase_dATP)

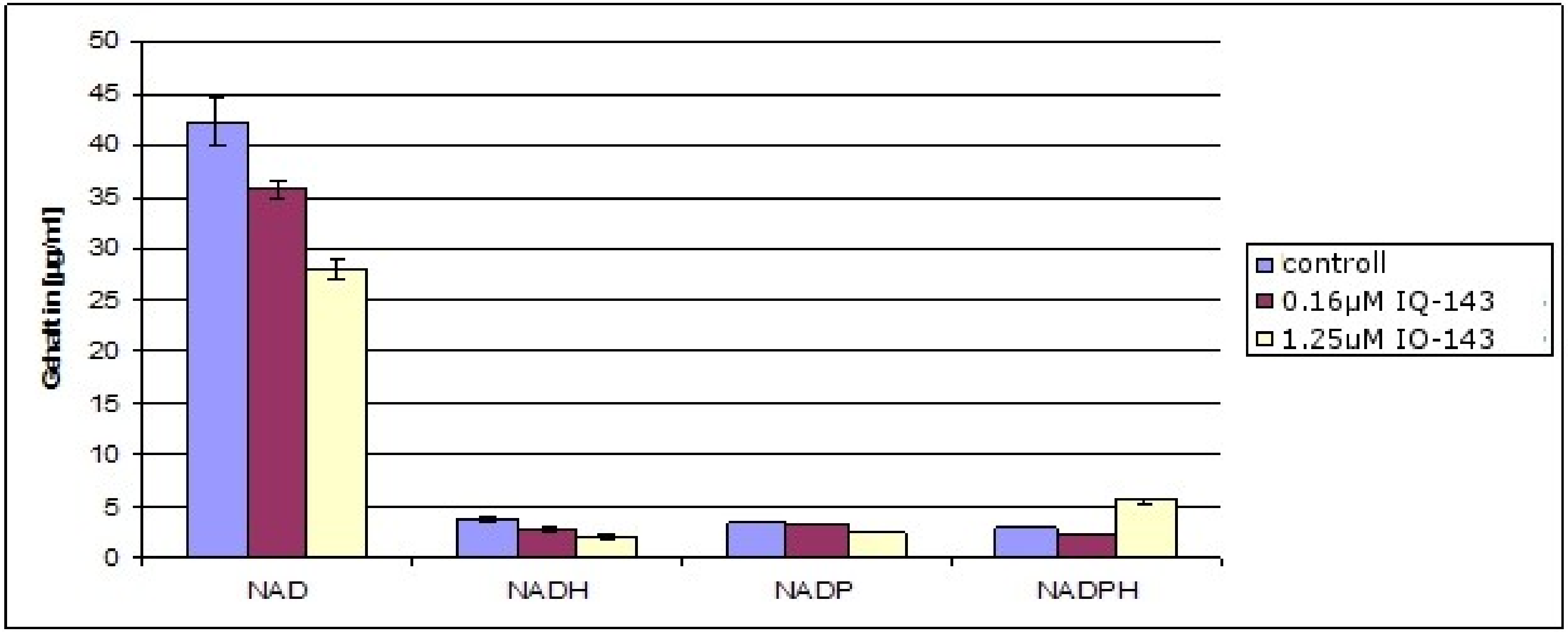
[1] The listed EMs of *S. aureus* showed a lower activity after administration of 0,16µM and 1,25µM IQ-143.

Left column: Number of specific mode in the full EM model (Tables S7-S9).

Middle colum: Number of enzymes involved in formation of affected EM.

7: Measured concentrations of nucleotides and NAD(P)H/NAD(P)$^+$

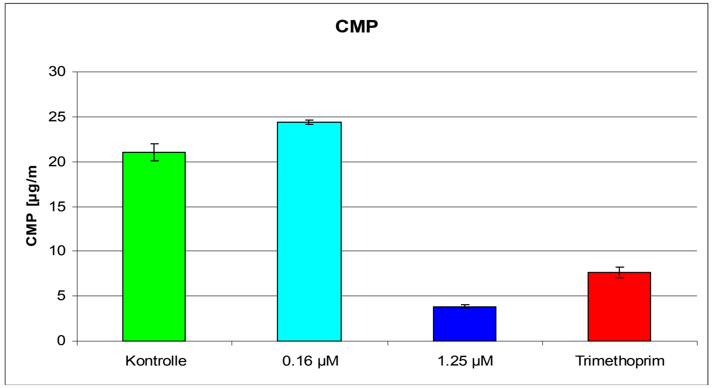
Figure S VI.1.4: Measured concentrations of NAD(P)H/NAD(P)$^+$

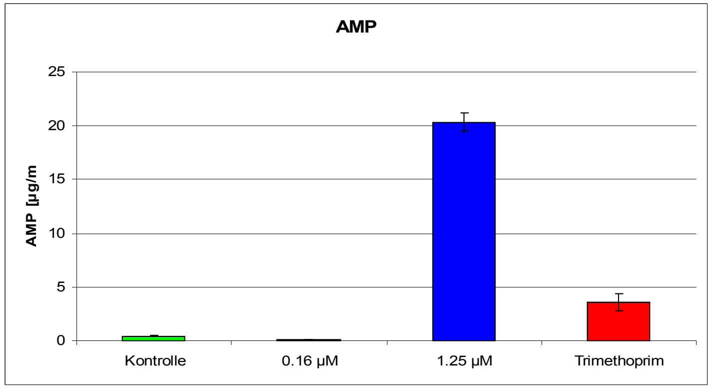


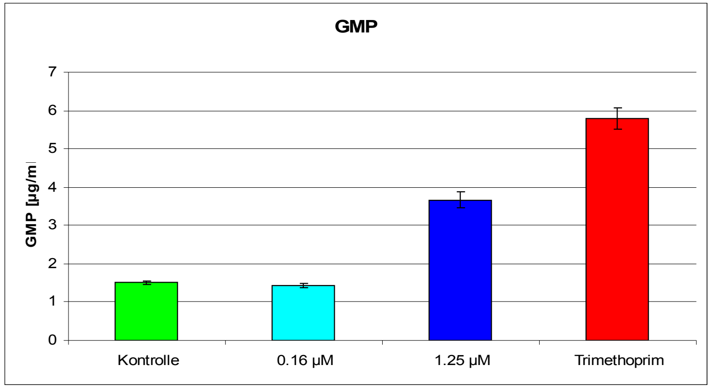
Calibration:

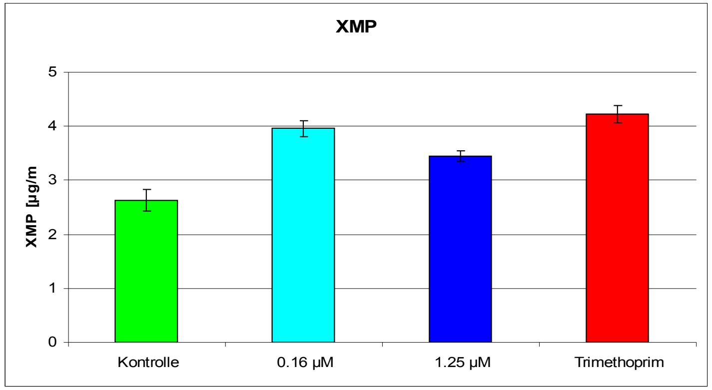
	Staph. control		Staph. 0.16 µm IQ-143		Staph. 1.25 µM IQ-143	
[µg/ml]	MW	sdv	MW	sdv	MW	sdv
NAD	42.19	2.45	44.08	0.93	34.38	0.06
NADH	3.71	0.25	2.63	0.04	1.95	0.09
NADP	3.47	0.06	3.24	0.11	2.42	0.12
NADPH	2.87	0.98	2.25	0.90	5.56	0.87

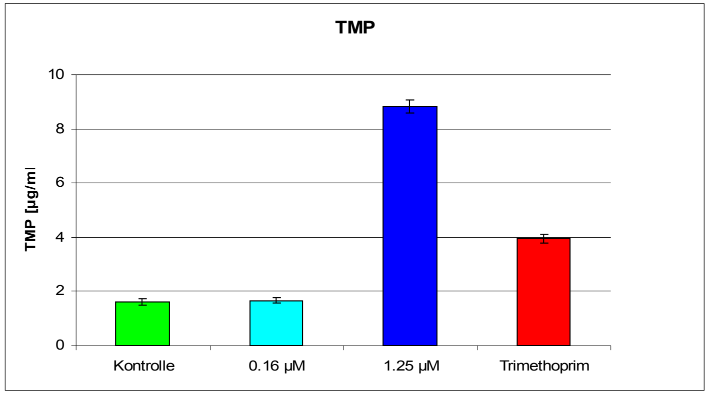
Figure S VI.1.5: Measured concentrations of nucleotides.











Calibration:

	Staph. Kontrolle		Staph. 0.16 µm		Staph. 1.25 µM		Trimethoprim	
	MW	sdv	MW	sdv	MW	sdv	MW	sdv
CMP	21.03	0.96	24.41	0.24	3.86	0.19	7.66	0.56
AMP	0.42	0.06	0.12	0.02	20.37	0.80	3.58	0.84
GMP	1.51	0.05	1.44	0.05	3.55	0.21	5.79	0.29
XMP	2.62	0.2	3.96	0.16	3.44	0.11	4.22	0.16
TMP	1.61	0.12	1.67	0.11	8.81	0.24	3.96	0.15

8: Calculated enzyme actvities

Table S VI.1.20: Calculated enzyme activities for *S. aureus* USA300.

S. AUREUS	0.00 µM	0.00 µM	0.16 µM	0.16 µM	1.25 µM	1.25 µM
Name	Raw flux	Normalized flux	Raw flux	Normalized flux	Raw flux	Normalized flux
ADP-energy_to_ADP-metabolism	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
AMP-energy_to_AMP-metabolism	0.2884	0.1444	0.3869	0.1314	0.4212	0.1960
AS_Acetyl-CoA_to_L-Leucine	0.0822	0.0411	0.0781	0.0265	0.0685	0.0319
AS_Acetyl-CoA_to_L-Valine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Alanine_to_Pyruvate	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Aspartate_to_Alanine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Aspartate_to_Arginine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Aspartate_to_Asparagine	0.0474	0.0237	0.0437	0.0148	0.1770	0.0823
AS_Aspartate_to_beta-Alanine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Aspartate_to_Homoserine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Glutamate_to_Glutamine	0.0790	0.0396	0.0766	0.0260	0.1464	0.0681
AS_Glutamate_to_Proline	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Histidine_to_Glutamate	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Homoserine_to_Threonine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Isoleucine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Leucine	0.0300	0.0150	0.0000	0.0000	0.0359	0.0167
AS_Phenylalanin_to_Tyrosine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Saccharopine_to_Lysine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Serine_to_Cysteine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Serine_to_Glycine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Serine_to_Methionine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Serine_to_Pyruvate	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Threonine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Tryptophan_to_Tryptamine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
AS_Valine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
ATP-energy_to_ATP-metabolism	0.0585	0.0293	0.0567	0.0192	-0.0852	-0.0396
DNA-extern_to_DNA-intern	0.0103	0.0051	0.0766	0.0260	0.0692	0.0322

DNA_to_DNA-blocked	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FA_Deg_C16_to_Acetyl-CoA	0.0593	0.0297	0.0690	0.0234	0.0532	0.0248
FA_Syn_Acetyl-CoA_to_C16	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
GBAP-extern_to_GBAP	0.2765	0.1385	0.3861	0.1311	0.3234	0.1504
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	-0.4361	-0.2184	-0.9255	-0.3142	-0.5350	-0.2489
Glyc_2-phospho-D-glycerate-hydro-lyase	0.4361	0.2184	0.9255	0.3142	0.5350	0.2489
Glyc_6-phospho-beta-glucosidase	0.1375	0.0688	0.3708	0.1259	0.3314	0.1542
Glyc_6-phosphofructokinase	0.2378	0.1191	0.4819	0.1636	0.2821	0.1313
Glyc_acetaldehyde-dehydrogenase_NAD+	0.0340	0.0170	-0.2046	-0.0695	-0.0912	-0.0424
Glyc_Actetate-CoA-ligase	0.1130	0.0566	-0.1279	-0.0434	-0.0246	-0.0115
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	-0.0790	-0.0396	0.0781	0.0265	-0.0665	-0.0310
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	0.1043	0.0522	0.3279	0.1113	0.1451	0.0675
Glyc_ATP-alpha-D-glucokinase	-0.0553	-0.0277	0.3141	0.1066	0.1424	0.0662
Glyc_ATP-beta-D-glucokinase	0.0553	0.0277	-0.3141	-0.1066	-0.1424	-0.0662
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	0.1138	0.0570	0.1348	0.0458	0.1224	0.0570
Glyc_D-Glucose-1-epimerase	0.0553	0.0277	-0.3141	-0.1066	-0.1424	-0.0662
Glyc_D-Glucose-1-epimerase-ketol-isomerase	-0.2180	-0.1092	-0.4628	-0.1571	-0.2675	-0.1244
Glyc_dihydrolipoamide-dehydrogenase	0.1580	0.0791	0.1532	0.0520	0.2928	0.1362
Glyc_fructose-bisphosphat-aldolase	0.2180	0.1092	0.4628	0.1571	0.2675	0.1244
Glyc_fructose-bisphosphatase	0.0198	0.0099	0.0192	0.0065	0.0146	0.0068
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	0.3160	0.1582	0.3065	0.1040	0.2662	0.1238
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	0.1201	0.0601	0.6191	0.2102	0.2688	0.1251
Glyc_lipoic_acetyltransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
Glyc_phosphoglycerate-kinase	-0.4361	-0.2184	-0.9255	-0.3142	-0.5350	-0.2489
Glyc_PTS-permease1	0.0806	0.0404	0.0919	0.0312	-0.0639	-0.0297
Glyc_PTS-permease2	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
Glyc_pyruvate_dehydrogenase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
Glyc_Succinate-CoA-ligase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
N-acylneuraminate-9-phosphatase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
OP_complex1	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
OP_complex2	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
OP_complex3	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
OP_complex4	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
OP_complex5	0.0427	0.0214	0.0322	0.0109	0.0067	0.0031

PurM_5-Hydroxyisourate-amidohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_5-nucleotidase_AMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_5-nucleotidase_CMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_5-nucleotidase_dAMP	0.0387	0.0194	0.0306	0.0104	0.0938	0.0436
PurM_5-nucleotidase_dCMP	0.0458	0.0229	0.0467	0.0159	0.1011	0.0471
PurM_5-nucleotidase_dGMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_5-nucleotidase_dTMP	0.0300	0.0150	0.0000	0.0000	0.0393	0.0183
PurM_5-nucleotidase_GMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_5-nucleotidase_IMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_5-nucleotidase_UMP	0.0790	0.0396	0.0766	0.0260	0.1597	0.0743
PurM_5-nucleotidase_XMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_adenylate-kinase_AMP	0.1801	0.0902	0.2819	0.0957	0.3267	0.1520
PurM_adenylate-kinase_dAMP	0.0577	0.0289	0.0605	0.0205	0.0632	0.0294
PurM_adenylosuccinate-lyase	0.0300	0.0150	0.0291	0.0099	0.0240	0.0111
PurM_adenylosuccinate-lyase2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_adenylylsulfate-kinase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ADP-ribose-ribophosphohydrolase	0.0198	0.0099	0.0192	0.0065	0.0146	0.0068
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_AIR-carboxylase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_allantoinase	0.0474	0.0237	0.1073	0.0364	0.0932	0.0433
PurM_AMP-pyrophosphorylase2	0.0569	0.0285	0.0674	0.0229	0.0612	0.0285
PurM_ATP-phosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_CDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dADP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dCDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dGDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dIDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dTDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_dUDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_GMP-guanylate-kinase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_GMP_guanylate-kinase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_GTP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_IDP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ATP_UTP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310

PurM_carbamate-kinase_ATP	-0.0055	-0.0028	-0.0329	-0.0112	-0.0087	-0.0040
PurM_D-Ribose-1.5-phosphomutase	0.0095	0.0047	0.0000	0.0000	0.0639	0.0297
PurM_deoxyadenosine-kinase_ATP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_deoxycytidine-kinase_ATP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_deoxycytidine-kinase_ATP2	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_dGTP-diphosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_dITP-diphosphohydrolase	0.0300	0.0150	0.1548	0.0525	0.0313	0.0145
PurM_DNA-directed-RNA-polyermase_ATP	0.1580	0.0791	0.0000	0.0000	0.0000	0.0000
PurM_DNA-directed-RNA-polyermase_CTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_DNA-directed-RNA-polyermase_GTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_DNA-directed-RNA-polyermase_UTP	0.0569	0.0285	0.0674	0.0229	0.0612	0.0285
PurM_GDP-reductase	0.1825	0.0914	0.1686	0.0572	0.0998	0.0464
PurM_GMP-pyrophosphorylase2	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_GTP-diphosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_GTP-pyrophosphokinase	0.0174	0.0087	0.0766	0.0260	0.1371	0.0638
PurM_IMP-cyclohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_IMP-dehydrogenase	0.0980	0.0491	0.0881	0.0299	0.0838	0.0390
PurM_IMP-pyrophosphorylase	0.4645	0.2326	0.4597	0.1561	0.2994	0.1393
PurM_IMP_L-aspartate-ligase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_ITP-diphosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_metaphosphatase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_nucleoside-diphosphate-phosphotransferase_ATP	0.5688	0.2848	0.4122	0.1399	0.5536	0.2576
PurM_nucleotide-phosphatase_Adenine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_nucleotide-phosphatase_Deoxyadenosine	0.0261	0.0131	-0.0299	-0.0101	-0.0266	-0.0124
PurM_nucleotide-phosphatase_Deoxyguanosine	-0.0790	-0.0396	-0.0766	-0.0260	-0.0665	-0.0310
PurM_nucleotide-phosphatase_Deoxyinosine	-0.0790	-0.0396	-0.0766	-0.0260	-0.0665	-0.0310
PurM_nucleotide-phosphatase_Deoxyuridine	0.1051	0.0526	0.1019	0.0346	0.0885	0.0412
PurM_nucleotide-phosphatase_Guanosine	0.0790	0.0396	0.0766	0.0260	0.0306	0.0142
PurM_nucleotide-phosphatase_Inosine	-0.3855	-0.1931	-0.3831	-0.1301	-0.2329	-0.1083
PurM_nucleotide-phosphatase_Xanthosine	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_PRPP-synthetase	0.0292	0.0146	0.0192	0.0065	0.0785	0.0365
PurM_pyruvate-phosphotransferase_ATP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_pyruvate-phosphotransferase_dATP	0.0458	0.0229	0.0475	0.0161	0.0106	0.0050
PurM_pyruvate-phosphotransferase_dGTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310

PurM_pyruvate-phosphotransferase_GTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_SAICAR-synthetase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_thioredoxin-oxidoreductase_dADP	0.1580	0.0791	0.1532	0.0520	0.2928	0.1362
PurM_thioredoxin-oxidoreductase_dATP	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
PurM_thioredoxin-oxidoreductase_dCDP	0.0435	0.0218	0.0437	0.0148	0.0566	0.0263
PurM_thioredoxin-oxidoreductase_dCTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_thioredoxin-oxidoreductase_dGDP	0.0126	0.0063	0.0176	0.0060	0.0260	0.0121
PurM_thioredoxin-oxidoreductase_dGTP	0.0095	0.0047	0.0000	0.0000	0.0240	0.0111
PurM_thioredoxin-oxidoreductase_dUDP	0.0213	0.0107	0.0161	0.0055	0.0033	0.0015
PurM_thioredoxin-oxidoreductase_dUTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_urea-amidohydrolase	0.0790	0.0396	0.0766	0.0260	0.1464	0.0681
PurM_UTP-diphosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.1910	0.0888
PurM_xanthosine-phosphoribosyltransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_XMP-ligase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_XMP-pyrophosphorylase	-0.0261	-0.0131	0.0299	0.0101	0.0266	0.0124
PurM_XMP_L-glutamine-amide-ligase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PurM_XTP-diphosphohydrolase	0.0450	0.0225	0.0414	0.0140	0.0000	0.0000
PyrM_2.3-cyclic-nucleotidase_CMP	0.0198	0.0099	0.0192	0.0065	0.0186	0.0087
PyrM_2.3-cyclic-nucleotidase_UMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_AMP-pyrophosphorylase	0.1011	0.0506	0.0858	0.0291	0.0719	0.0334
PyrM_aspartate-carbamoyltransferase	0.0300	0.0150	0.0000	0.0000	0.0013	0.0006
PyrM_ATP_dTDP_thymidylate-kinase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_ATP_dUDP_thymidylate-kinase	-0.0261	-0.0131	0.0299	0.0101	0.0266	0.0124
PyrM_CO2_L-glutamine-amido-ligase	0.0356	0.0178	0.0329	0.0112	0.0100	0.0046
PyrM_CTP-synthase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidilate-kinase_CTP	0.0790	0.0396	0.0383	0.0130	0.0665	0.0310
PyrM_cytidilate-kinase_dCMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-aminohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-kinase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-kinase_ATP	0.0324	0.0162	0.0207	0.0070	0.0845	0.0393
PyrM_cytidine-kinase_dATP	0.0853	0.0427	0.0421	0.0143	0.0346	0.0161
PyrM_cytidine-kinase_dCTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-kinase_dGTP	0.1011	0.0506	0.0858	0.0291	0.0719	0.0334
PyrM_cytidine-kinase_dTTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310

PyrM_cytidine-kinase_dUTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-kinase_GTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-kinase_ITP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_cytidine-ribohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_dCMP-aminohydrolase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_deoxyadenosine-phosphorylase	-0.0664	-0.0332	-0.0161	-0.0055	0.0539	0.0251
PyrM_Deoxycytidine-aminohydrolase	-0.0593	-0.0297	0.0000	0.0000	0.0612	0.0285
PyrM_Deoxycytidine-deaminase	0.0261	0.0131	-0.0299	-0.0101	-0.0266	-0.0124
PyrM_deoxyguanosine-phosphorylase	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
PyrM_deoxyinosine-phosphorylase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_deoxyuridine-phosphorylase	-0.0593	-0.0297	-0.0552	-0.0187	0.0126	0.0059
PyrM_dihydroorotase	-0.0790	-0.0396	-0.0766	-0.0260	-0.0665	-0.0310
PyrM_dihydroorotate-oxidase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_dUMP-phosphotransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_dUTP-diphosphatase	0.0419	0.0210	0.0391	0.0133	0.0180	0.0084
PyrM_dUTP-diphosphohydrolase	0.0790	0.0396	0.0766	0.0260	0.1783	0.0830
PyrM_GMP-pyrophosphorylase	-0.0514	-0.0257	-0.0506	-0.0172	-0.0439	-0.0204
PyrM_nucleoside-phosphate-kinase_ATP	0.0790	0.0396	-0.0437	-0.0148	-0.0393	-0.0183
PyrM_nucleoside-phosphate-kinase_ATP2	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_nucleoside-triphosphate-adenylate-kinase	-0.0261	-0.0131	0.0299	0.0101	0.0266	0.0124
PyrM_OMP-decarboxylase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_orotate-phosphoribosyltransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_pyrimidine-nucleoside-phosphorylase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_thioredoxin-reductase	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
PyrM_thymidilate-synthase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_thymidine-kinase_dTMP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_thymidine-kinase_dUMP	-0.0790	-0.0396	-0.0766	-0.0260	-0.0665	-0.0310
PyrM_thymidine-phosphorylase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_UMP-pyrophosphorylase	-0.0687	-0.0344	-0.0299	-0.0101	-0.0240	-0.0111
PyrM_uridine-kinase_ATP	0.0300	0.0150	0.0000	0.0000	0.0759	0.0353
PyrM_uridine-kinase_dATP	0.0790	0.0396	0.0360	0.0122	0.0299	0.0139
PyrM_uridine-kinase_dCTP	0.0593	0.0297	0.0575	0.0195	0.0479	0.0223
PyrM_uridine-kinase_dGTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_uridine-kinase_dTTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310

PyrM_uridine-kinase_dUTP	0.0790	0.0396	0.0766	0.0260	0.0233	0.0108
PyrM_uridine-kinase_GTP	0.0790	0.0396	0.0766	0.0260	0.1876	0.0873
PyrM_uridine-kinase_ITP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_uridine-kinase_UTP	0.1185	0.0593	0.1149	0.0390	0.0998	0.0464
PyrM_uridine-phosphorylase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
PyrM_uridine-ribohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_UTP_L-glutamine-amido-ligase	0.0198	0.0099	0.0192	0.0065	0.0146	0.0068
SERP0290-zinc-transport_efflux	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0291-zinc-transporter_import	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0292-iron-dicitrate-transporter_import	0.0790	0.0396	0.0414	0.0140	0.0286	0.0133
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	0.0340	0.0170	-0.2046	-0.0695	-0.0912	-0.0424
SERP0653-PurM_FGAM-synthethase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0655-PurM_amidophosphoribosyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0656-PurM_AIR_synthetase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0657-PurM_GAR-formyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0658-PurM_AICAR-formyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0659-PurM_phosphoribosylamine-glycine-ligase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0686-spermidine/putrescine-transport_import	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0687-spermidine/putrescine-transport_import	0.0126	0.0063	0.0176	0.0060	0.0353	0.0164
SERP0688-spermidine/putrescine-transport_import	0.0245	0.0123	0.0253	0.0086	0.0326	0.0152
SERP0765-Uracil-permease-transport_import	0.1936	0.0969	0.1854	0.0629	0.1697	0.0789
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	0.0790	0.0396	0.0766	0.0260	0.0260	0.0121
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP0841-PurM_PNPase_ADP	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
SERP0841-PurM_PNPase_GDP	0.0529	0.0265	0.0513	0.0174	0.0446	0.0207
SERP1403-MultiDrug-transport_efflux	0.0988	0.0495	0.0843	0.0286	0.0798	0.0371
SERP1802-cobalt/nickel-transport_efflux	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP1803-cobalt/nickel-transport_efflux	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP1944-MultiDrug-transport_efflux	0.0988	0.0495	0.2406	0.0817	0.1903	0.0885
SERP1951-lipoprotein-transport_efflux/import	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP1952-macrolide-transport_efflux	0.0790	0.0396	0.0766	0.0260	0.1530	0.0712
SERP1997-formate/nitrite-transport_efflux/import	0.1161	0.0582	0.1724	0.0585	0.2163	0.1006

SERP2060-glyerol-transport_import	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP2156-Glyc_L-lactate-dehydrogenase	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
SERP2179-choline/betaine/carnitine-transp_efflux	0.1059	0.0530	0.3080	0.1046	0.2528	0.1176
SERP2186-PurM_ATP_sulfate-adenylyltransferase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP2283-phopsphonate-transport_import	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
SERP2289-MultiDrug-transport_efflux	0.0790	0.0396	0.0613	0.0208	0.0532	0.0248
TCA_citrate-hydro-lyase	-0.2489	-0.1246	-0.4068	-0.1381	-0.3081	-0.1433
TCA_citrate-hydroxymutase	-0.0758	-0.0380	-0.0751	-0.0255	-0.0645	-0.0300
TCA_citrate_synthase	0.3247	0.1626	0.4819	0.1636	0.3726	0.1734
TCA_fumarate-hydratase	0.0758	0.0380	0.0751	0.0255	0.0645	0.0300
TCA_isocitrate-hydro-lyase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
TCA_lipoic-transsuccinylase	-0.2370	-0.1187	-0.2298	-0.0780	-0.1996	-0.0929
TCA_Oxidoreductase	0.1580	0.0791	0.1532	0.0520	0.1331	0.0619
TCA_oxoglutarate-dehydrogenase-complex1	0.2370	0.1187	0.2298	0.0780	0.1996	0.0929
TCA_oxoglutarate-dehydrogenase-complex2	0.2370	0.1187	0.2298	0.0780	0.1996	0.0929
TCA_oxoglutarate-synthase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310
TCA_PEP-carboxylase	-0.7189	-0.3600	-1.2029	-0.4084	-0.7452	-0.3467
TCA_Pyruvate_CO2-ligase	-0.0356	-0.0178	-0.0329	-0.0112	-0.0100	-0.0046
TCA_pyruvate_dehydrogenase	0.0790	0.0396	0.0766	0.0260	0.0665	0.0310

Table S VI.1.21: Calculated enzyme activities of *S. epidermidis* RP62A.

S. EPIDERMIDIS	0.00 µM	0.00 µM	0.16 µM	0.16 µM	1.25 µM	1.25 µM
Name	Raw flux	Normalized flux	Raw flux	Normalized flux	Raw flux	Normalized flux
ADP-energy_to_ADP-metabolism	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
AMP-energy_to_AMP-metabolism	-0.0293	-0.0124	-0.0293	-0.0124	-0.0191	-0.0085
AS_Acetyl-CoA_to_L-Leucine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Acetyl-CoA_to_L-Valine	0.0395	0.0167	0.0395	0.0167	0.0494	0.0219
AS_Alanine_to_Pyruvate	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Aspartate_to_Alanine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Aspartate_to_Arginine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Aspartate_to_Asparagine	0.0791	0.0334	0.0791	0.0334	0.1449	0.0643
AS_Aspartate_to_beta-Alanine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Aspartate_to_Homoserine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Glutamate_to_Glutamine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Glutamate_to_Proline	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Histidine_to_Glutamate	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Homoserine_to_Threonine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Isoleucine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Leucine	0.0285	0.0120	0.0285	0.0120	0.0586	0.0260
AS_Phenylalanin_to_Tyrosine	0.0198	0.0084	0.0198	0.0084	0.0165	0.0073
AS_Saccharopine_to_Lysine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Serine_to_Cysteine	0.0522	0.0221	0.0522	0.0221	0.0171	0.0076
AS_Serine_to_Glycine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Serine_to_Methionine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Serine_to_Pyruvate	0.0791	0.0334	0.0791	0.0334	0.0290	0.0129
AS_Threonine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Tryptophan_to_Tryptamine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
AS_Valine	0.0380	0.0161	0.0380	0.0161	0.0975	0.0433
ATP-energy_to_ATP-metabolism	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
DNA-extern_to_DNA-intern	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
DNA_to_DNA-blocked	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FA_Deg_C16_to_Acetyl-CoA	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
FA_Syn_Acetyl-CoA_to_C16	0.0198	0.0084	0.0198	0.0084	0.0165	0.0073

GBAP-extern_to_GBAP	0.2594	0.1097	0.2594	0.1097	0.3615	0.1605
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	-0.2151	-0.0910	-0.2151	-0.0910	-0.1831	-0.0813
Glyc_2-phospho-D-glycerate-hydro-lyase	0.2151	0.0910	0.2151	0.0910	0.1831	0.0813
Glyc_6-phospho-beta-glucosidase	0.0285	0.0120	0.0285	0.0120	0.0257	0.0114
Glyc_6-phosphofructokinase	0.1273	0.0538	0.1273	0.0538	0.1080	0.0479
Glyc_acetaldehyde-dehydrogenase_NAD+	-0.0221	-0.0094	-0.0221	-0.0094	-0.2799	-0.1243
Glyc_Actetate-CoA-ligase	0.0300	0.0127	0.0300	0.0127	-0.2627	-0.1167
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	-0.7639	-0.3230	-0.7639	-0.3230	-0.6862	-0.3047
Glyc_ATP-alpha-D-glucokinase	-0.7639	-0.3230	-0.7639	-0.3230	-0.6862	-0.3047
Glyc_ATP-beta-D-glucokinase	0.7639	0.3230	0.7639	0.3230	0.6862	0.3047
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	0.8714	0.3685	0.8714	0.3685	0.7777	0.3453
Glyc_D-Glucose-1-epimerase	0.7639	0.3230	0.7639	0.3230	0.6862	0.3047
Glyc_D-Glucose-1-epimerase-ketol-isomerase	-0.1075	-0.0455	-0.1075	-0.0455	-0.0915	-0.0406
Glyc_dihydrolipoamide-dehydrogenase	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
Glyc_fructose-bisphosphat-aldolase	0.1075	0.0455	0.1075	0.0455	0.0915	0.0406
Glyc_fructose-bisphosphatase	0.0198	0.0084	0.0198	0.0084	0.0165	0.0073
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	0.0569	0.0241	0.0569	0.0241	0.0514	0.0228
Glyc_lipoic_acetyltransferase	0.0720	0.0304	0.0720	0.0304	0.0658	0.0292
Glyc_phosphoglycerate-kinase	-0.2151	-0.0910	-0.2151	-0.0910	-0.1831	-0.0813
Glyc_PTS-permease1	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
Glyc_PTS-permease2	0.0593	0.0251	0.0593	0.0251	0.0738	0.0327
Glyc_pyruvate_dehydrogenase	0.0380	0.0161	0.0380	0.0161	0.1054	0.0468
Glyc_Succinate-CoA-ligase	0.0395	0.0167	0.0395	0.0167	0.0494	0.0219
OP_complex1	0.0474	0.0201	0.0474	0.0201	0.0283	0.0126
OP_complex2	0.0380	0.0161	0.0380	0.0161	0.0112	0.0050
OP_complex3	0.0854	0.0361	0.0854	0.0361	0.0395	0.0175
OP_complex4	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
OP_complex5	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PurM_5-nucleotidase_AMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_CMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292

PurM_5-nucleotidase_dAMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_dCMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_dGMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_dTMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_GMP	0.0380	0.0161	0.0380	0.0161	0.0362	0.0161
PurM_5-nucleotidase_IMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_UMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_5-nucleotidase_XMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_adenylate-kinase_AMP	-0.2238	-0.0946	-0.2238	-0.0946	-0.2114	-0.0939
PurM_adenylate-kinase_dAMP	0.0727	0.0308	0.0727	0.0308	0.0606	0.0269
PurM_adenylosuccinate-lyase	-0.0514	-0.0217	-0.0514	-0.0217	-0.0606	-0.0269
PurM_adenylosuccinate-lyase2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_adenylylsulfate-kinase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ADP-ribose-ribophosphohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_AIR-carboxylase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_AMP-pyrophosphorylase	0.0727	0.0308	0.0727	0.0308	0.0606	0.0269
PurM_AMP-pyrophosphorylase2	0.0854	0.0361	0.0854	0.0361	0.0711	0.0316
PurM_ATP-phosphohydrolase	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PurM_ATP_CDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dADP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dCDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dGDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dIDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dTDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_dUDP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_GMP-guanylate-kinase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_GMP_guanylate-kinase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_GTP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ATP_IDP-phosphotransferase	0.0554	0.0234	0.0554	0.0234	-0.0441	-0.0196
PurM_ATP_UTP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_carbamate-kinase_ATP	-0.0467	-0.0197	-0.0467	-0.0197	0.0059	0.0026
PurM_D-Ribose-1.5-phosphomutase	0.0150	0.0064	0.0150	0.0064	0.0000	0.0000

PurM_deoxyadenosine-kinase_ATP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_deoxycytidine-kinase_ATP	0.0150	0.0064	0.0150	0.0064	0.0000	0.0000
PurM_deoxycytidine-kinase_ATP2	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_dGTP-diphosphohydrolase	0.0380	0.0161	0.0380	0.0161	0.0316	0.0140
PurM_dITP-diphosphohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_DNA-directed-RNA-polyermase_CTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_DNA-directed-RNA-polyermase_GTP	0.0285	0.0120	0.0285	0.0120	0.0981	0.0436
PurM_DNA-directed-RNA-polyermase_UTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_DNA-directed-RNA-polymerase_ATP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_GDP-reductase	0.2088	0.0883	0.2088	0.0883	0.1317	0.0585
PurM_GMP-pyrophosphorylase	0.0577	0.0244	0.0577	0.0244	0.0441	0.0196
PurM_GMP-pyrophosphorylase2	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_GTP-diphosphohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_GTP-pyrophosphokinase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_IMP-cyclohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_IMP-dehydrogenase	0.0988	0.0418	0.0988	0.0418	0.1238	0.0550
PurM_IMP-pyrophosphorylase	0.4523	0.1913	0.4523	0.1913	0.3556	0.1579
PurM_IMP_L-aspartate-ligase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_ITP-diphosphohydrolase	0.0237	0.0100	0.0237	0.0100	0.0316	0.0140
PurM_metaphosphatase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_nucleoside-diphosphate-phosphotransferase_ATP	-0.0759	-0.0321	-0.0759	-0.0321	0.0593	0.0263
PurM_nucleotide-phosphatase_Adenine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_nucleotide-phosphatase_Deoxyadenosine	-0.0419	-0.0177	-0.0419	-0.0177	-0.0349	-0.0155
PurM_nucleotide-phosphatase_Deoxyguanosine	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
PurM_nucleotide-phosphatase_Deoxyinosine	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
PurM_nucleotide-phosphatase_Deoxyuridine	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
PurM_nucleotide-phosphatase_Guanosine	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_nucleotide-phosphatase_Inosine	-0.3732	-0.1578	-0.3732	-0.1578	-0.2897	-0.1286
PurM_nucleotide-phosphatase_Xanthosine	0.0791	0.0334	0.0791	0.0334	0.0257	0.0114
PurM_PRPP-synthetase	0.0941	0.0398	0.0941	0.0398	0.0658	0.0292
PurM_pyruvate-phosphotransferase_ATP	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PurM_pyruvate-phosphotransferase_dATP	0.0791	0.0334	0.0791	0.0334	0.1515	0.0672
PurM_pyruvate-phosphotransferase_dGTP	0.0411	0.0174	0.0411	0.0174	0.0547	0.0243
PurM_pyruvate-phosphotransferase_GTP	0.0277	0.0117	0.0277	0.0117	0.0053	0.0023

PurM_SAICAR-synthetase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PurM_thioredoxin-oxidoreductase_dATP	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PurM_thioredoxin-oxidoreductase_dCDP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_thioredoxin-oxidoreductase_dCTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_thioredoxin-oxidoreductase_dGDP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_thioredoxin-oxidoreductase_dGTP	0.0150	0.0064	0.0150	0.0064	0.0000	0.0000
PurM_thioredoxin-oxidoreductase_dUDP	0.0324	0.0137	0.0324	0.0137	0.0270	0.0120
PurM_thioredoxin-oxidoreductase_dUTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_thioredoxin-oxidoreductased_dADP	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PurM_urea-amidohydrolase	0.0791	0.0334	0.0791	0.0334	0.1449	0.0643
PurM_UTP-diphosphohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_xanthosine-phosphoribosyltransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_XMP-pyrophosphorylase	0.0419	0.0177	0.0419	0.0177	0.0349	0.0155
PurM_XMP_L-glutamine-amide-ligase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PurM_XTP-diphosphohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_2.3-cyclic-nucleotidase_CMP	0.0198	0.0084	0.0198	0.0084	0.0184	0.0082
PyrM_2.3-cyclic-nucleotidase_UMP	0.0759	0.0321	0.0759	0.0321	0.0632	0.0281
PyrM_aspartate-carbamoyltransferase	0.0324	0.0137	0.0324	0.0137	0.0718	0.0319
PyrM_ATP_dTDP_thymidylate-kinase	-0.0411	-0.0174	-0.0411	-0.0174	-0.0342	-0.0152
PyrM_ATP_dUDP_thymidylate-kinase	0.0419	0.0177	0.0419	0.0177	0.0349	0.0155
PyrM_CO2_L-glutamine-amido-ligase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_CTP-synthase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_cytidilate-kinase_CTP	0.0830	0.0351	0.0830	0.0351	0.0731	0.0325
PyrM_cytidilate-kinase_dCMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_cytidine-aminohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_cytidine-kinase_ATP	0.0791	0.0334	0.0791	0.0334	0.1449	0.0643
PyrM_cytidine-kinase_dATP	0.0443	0.0187	0.0443	0.0187	0.0369	0.0164
PyrM_cytidine-kinase_dCTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_cytidine-kinase_dGTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_cytidine-kinase_dTTP	0.0791	0.0334	0.0791	0.0334	0.1357	0.0602
PyrM_cytidine-kinase_dUTP	0.0380	0.0161	0.0380	0.0161	0.0658	0.0292
PyrM_cytidine-kinase_GTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292

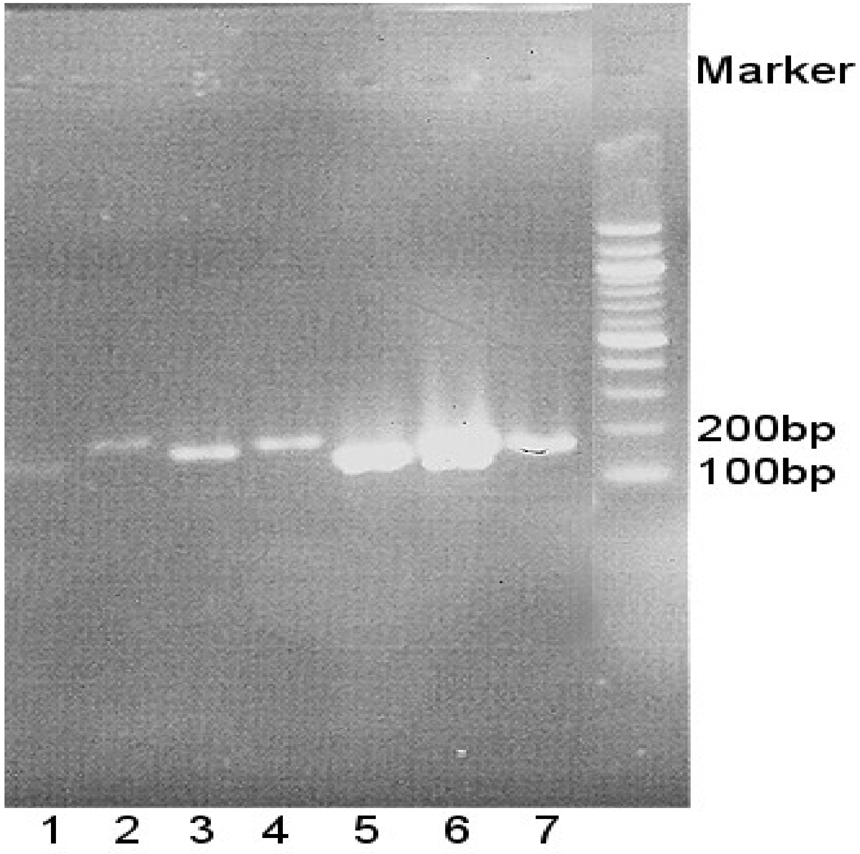
PyrM_cytidine-kinase_ITP	0.0198	0.0084	0.0198	0.0084	0.0184	0.0082
PyrM_cytidine-kinase_UTP	0.0791	0.0334	0.0791	0.0334	0.1765	0.0784
PyrM_cytidine-ribohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_dCMP-aminohydrolase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_deoxyadenosine-phosphorylase	0.0419	0.0177	0.0419	0.0177	0.0349	0.0155
PyrM_Deoxycytidine-aminohydrolase	0.0419	0.0177	0.0419	0.0177	0.0349	0.0155
PyrM_Deoxycytidine-deaminase	-0.0419	-0.0177	-0.0419	-0.0177	-0.0349	-0.0155
PyrM_deoxyguanosine-phosphorylase	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PyrM_deoxyinosine-phosphorylase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_deoxyuridine-phosphorylase	-0.0261	-0.0110	-0.0261	-0.0110	-0.0217	-0.0096
PyrM_dihydroorotase	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
PyrM_dihydroorotate-oxidase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_dUMP-phosphotransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_dUTP-diphosphatase	0.0435	0.0184	0.0435	0.0184	0.0184	0.0082
PyrM_dUTP-diphosphohydrolase	0.0285	0.0120	0.0285	0.0120	0.0007	0.0003
PyrM_nucleoside-phosphate-kinase_ATP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_nucleoside-phosphate-kinase_ATP2	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_nucleoside-triphosphate-adenylate-kinase	0.0625	0.0264	0.0625	0.0264	0.0520	0.0231
PyrM_OMP-decarboxylase	0.0791	0.0334	0.0791	0.0334	0.1890	0.0839
PyrM_orotate-phosphoribosyltransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_pyrimidine-nucleoside-phosphorylase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_thioredoxin-reductase	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
PyrM_thymidilate-synthase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_thymidine-kinase_dTMP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_thymidine-kinase_dUMP	0.1052	0.0445	0.1052	0.0445	0.0876	0.0389
PyrM_thymidine-phosphorylase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_UMP-pyrophosphorylase	-0.1060	-0.0448	-0.1060	-0.0448	-0.1146	-0.0509
PyrM_uridine-kinase_ATP	0.0285	0.0120	0.0285	0.0120	0.0507	0.0225
PyrM_uridine-kinase_dATP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_uridine-kinase_dCTP	0.0593	0.0251	0.0593	0.0251	0.0474	0.0211
PyrM_uridine-kinase_dGTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_uridine-kinase_dTTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_uridine-kinase_dUTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292

PyrM_uridine-kinase_GTP	0.0791	0.0334	0.0791	0.0334	0.0323	0.0143
PyrM_uridine-kinase_ITP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
PyrM_uridine-kinase_UTP	0.1384	0.0585	0.1384	0.0585	0.0738	0.0327
PyrM_uridine-phosphorylase	0.0720	0.0304	0.0720	0.0304	0.0665	0.0295
PyrM_uridine-ribohydrolase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PyrM_UTP_L-glutamine-amido-ligase	0.0403	0.0171	0.0403	0.0171	0.1040	0.0462
SERP0290-zinc-transport_efflux	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP0291-zinc-transporter_import	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP0292-iron-dicitrate-transporter_import	0.0791	0.0334	0.0791	0.0334	0.2022	0.0898
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	-0.0221	-0.0094	-0.0221	-0.0094	-0.2799	-0.1243
SERP0653-PurM_FGAM-synthethase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0655-PurM_amidophosphoribosyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0656-PurM_AIR_synthetase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0657-PurM_GAR-formyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0658-PurM_AICAR-formyltransferase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0659-PurM_phosphoribosylamine-glycine-ligase	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SERP0686-spermidine/putrescine-transport_import	0.1581	0.0669	0.1581	0.0669	0.2594	0.1152
SERP0687-spermidine/putrescine-transport_import	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP0688-spermidine/putrescine-transport_import	0.0277	0.0117	0.0277	0.0117	0.0454	0.0202
SERP0765-Uracil-permease-transport_import	0.1605	0.0679	0.1605	0.0679	0.1771	0.0786
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	0.0791	0.0334	0.0791	0.0334	0.1725	0.0766
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	0.0530	0.0224	0.0530	0.0224	0.0441	0.0196
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	0.1107	0.0468	0.1107	0.0468	0.0922	0.0409
SERP0841-PurM_PNPase_ADP	0.1581	0.0669	0.1581	0.0669	0.1317	0.0585
SERP0841-PurM_PNPase_GDP	0.0285	0.0120	0.0285	0.0120	0.0112	0.0050
SERP1403-MultiDrug-transport_efflux	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP1802-cobalt/nickel-transport_efflux	0.0727	0.0308	0.0727	0.0308	0.0632	0.0281
SERP1803-cobalt/nickel-transport_efflux	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP1944-MultiDrug-transport_efflux	0.1170	0.0495	0.1170	0.0495	0.2430	0.1079
SERP1951-lipoprotein-transport_efflux/import	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP1952-macrolide-transport_efflux	0.0791	0.0334	0.0791	0.0334	0.1363	0.0605
SERP1997-formate/nitrite-transport_efflux/import	0.1297	0.0548	0.1297	0.0548	0.0711	0.0316
SERP2060-glyerol-transport_import	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292

SERP2156-Glyc_L-lactate-dehydrogenase	-0.1581	-0.0669	-0.1581	-0.0669	0.1317	0.0585
SERP2179-choline/betaine/carnitine-transp_efflux	0.1961	0.0829	0.1961	0.0829	0.1449	0.0643
SERP2186-PurM_ATP_sulfate-adenylyltransferase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP2283-phopsphonate-transport_import	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
SERP2289-MultiDrug-transport_efflux	0.0633	0.0268	0.0633	0.0268	0.0527	0.0234
TCA_citrate-hydro-lyase	0.2222	0.0940	0.2222	0.0940	-0.0988	-0.0439
TCA_citrate-hydroxymutase	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
TCA_citrate_synthase	-0.1431	-0.0605	-0.1431	-0.0605	0.1646	0.0731
TCA_fumarate-hydratase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
TCA_isocitrate-hydro-lyase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
TCA_lipoic-transsuccinylase	-0.1676	-0.0709	-0.1676	-0.0709	-0.2278	-0.1012
TCA_Oxidoreductase	0.0886	0.0375	0.0886	0.0375	0.1620	0.0719
TCA_oxoglutarate-dehydrogenase-complex1	0.1676	0.0709	0.1676	0.0709	0.2278	0.1012
TCA_oxoglutarate-dehydrogenase-complex2	0.1676	0.0709	0.1676	0.0709	0.2278	0.1012
TCA_oxoglutarate-synthase	0.0791	0.0334	0.0791	0.0334	0.0658	0.0292
TCA_PEP-carboxylase	-0.5211	-0.2204	-0.5211	-0.2204	-0.5261	-0.2336
TCA_Pyruvate_CO2-ligase	-0.0791	-0.0334	-0.0791	-0.0334	-0.0658	-0.0292
TCA_pyruvate_dehydrogenase	0.0380	0.0161	0.0380	0.0161	0.1054	0.0468
TCA_succinate-dehydrogenase	0.0419	0.0177	0.0419	0.0177	0.0349	0.0155

9: PCR results

Figure S VI.1.6: Results for PCR detection of *in silico* predicted additional enzymes for *S. epidermidis*[1].



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[1] Lanes 1-7: *S. epidermidis* (1 = nucleoside-triphosphate diphosphatase, 2 = adenosinetriphosphatase, 3 = deoxycytidine kinase, 4 = 5'-nucleotidase, 5 = xanthine phosphoribosyltransferase, 6 = thymidine phosphorylase, 7 = epoxyadenosine kinase). Lanes 8-13: *C. albicans*.

10: Mode of action: Complex 1&3 of the oxidative phosphorylation

Figure S VI.1.7: Mode of action of complex 1 of the oxidative phosphorylation.

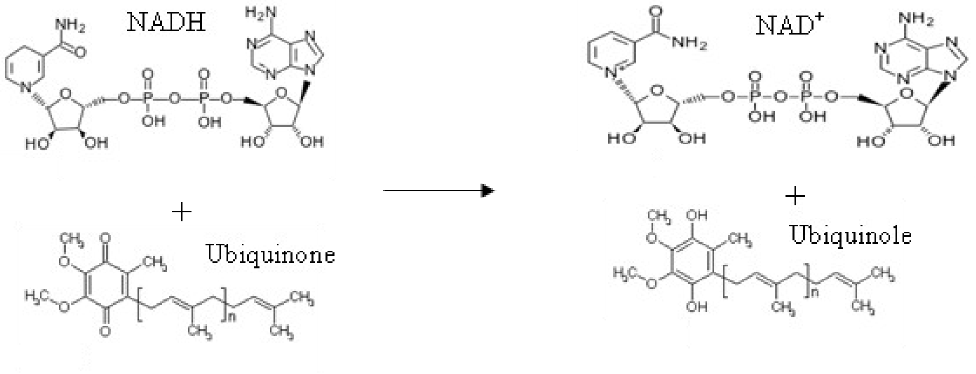
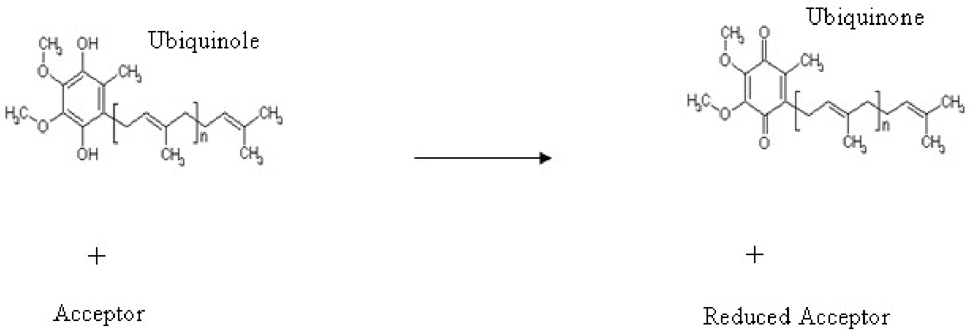


Figure S VI.1.8: Mode of action of complex 3 of the oxidative phosphorylation.



2. Daten der Simulationen des Naphtyhlisochinolinium IQ-238

1) Enzymes found by iterative sequence analysis:
   1. Table S VI.2.1: List of enzymes used to build metabolic webs found to be not part of KEGG data.
2) Full list of enzymes of YANAsquare modes:
   1. Table S VI.2.2: List of enzmyes used to build metabolic web for *S. aureus USA 300.*
   2. Table S VI.2.3: List of enzmyes used to build metabolic web for *S. epidermidis RP62A*.
3) Gene expression data gathered by Ohlsen et al:
   1. Table S VI.2.4: Gene expression data of S. epidermidis RP62A with GB-AP-238 added.
4) Extreme modes calculated by YANAsquare models:
   1. Table S VI.2.5: Extreme modes of *S. aureus USA300* calculated.
   2. Table S VI.2.6: Extreme modes of *S. epidermidis RP62A* calculated.

1: Enzymes found by iterative sequence search

Table S VI.2.1: List of enzymes used to build metabolic webs found to be not part of KEGG data[1].

S. epidermidis RP62A

EC- Number	Enzymename	Query Sequence: Brenda/NCBI	Hit: exPASY/NCBI	e- Value	Bit- Score
3.6.1.19	nucleoside-triphosphate diphosphatase	Q9BY32	Q5HQ23	8.7e-16	177
3.6.1.3	adenosinetriphosphatase	A2QUY7	Q5HME0	7.3e-51	508
2.7.1.74	deoxycytidine kinase	P27707	Q5HRJ1	1.2e-10	136
3.1.3.5	5'-nucleotidase	Q2YUP8	Q5HKQ5	1.5e-19	244
2.4.2.22	xanthine phosphoribosyltransferase	Q04IV9	Q5HRX4	4.2e-48	486
2.4.2.4	thymidine phosphorylase	Q301G5	Q5HM85	2.4e-116	1126
2.7.1.76	epoxyadenosine kinase	Q48VP1	Q5HRJ0	2.5e-27	286

S. aureus USA300

EC- Number	Enzymename	Query Sequence: Brenda/NCBI	Hit: exPASY/NCBI	e- Value	Bit- Score
2.4.2.3	uridine phosphorylase	P12758	ref|NC_007793.1	2,00E-022	100
3.2.2.3	uridine nucleosidase	Q88S31	ref|NC_007793.1	3,00E-048	186
2.7.4.4	uridine-cytidine kinase	ref|NP_036606.2	ref|NC_007793.1	9,00E-042	163
2.7.4.10	nucleoside-triphosphate-adenylate kinase	Q9UIJ7	ref|NC_007793.1	2,00E-043	169
3.6.1.19	nucleoside-triphosphate diphosphatase	Q9BY32	ref|NC_007793.1	3,00E-012	65
2.7.7.6	DNA-directed RNA polymerase	Q2FER5	ref|NC_007793.1	1,00E-159	553
3.2.2.8	riboyslpyrimidine nucleosidase	A7ZNY5	ref|NC_007793.1	3,00E-060	225
2.7.1.74	deoxycytidine kinase	P27707	ref|NC_007793.1	3,00E-008	52
3.5.4.14	deoxycytidine deaminase	O74047	ref|NC_007793.1	5,00E-021	94
3.5.2.2	dihydropyrimidinase	A2UD01	ref|NC_007793.1	4,00E-024	106
4.2.1.70	pseudouridylate synthase	A5ISF5	ref|NC_007793.1|	1,00E-168	583
2.4.2.4	thymidine phosphorylase	A5IUT1	ref|NC_007793.1	0	716

[1] Enzymes added through iterative sequence analysis to the enzymelist derived from KEGG.

2: Full list of enzymes of YANAsquare modes

Table S VI.2.2: List of enzmyes used to build metabolic web for *S. aureus USA300* [1].

Enzyme name	reversible?	Reaction equation
ADP-energy_to_ADP-metabolism	true	ADP-energy = ADP-metabolism
AMP-energy_to_AMP-metabolism	true	AMP-energy = AMP-metabolism
AS_Acetyl-CoA_to_L-Leucine	false	Acetyl-CoA + L-Glutamate + NAD+ = CO2 + L-Leucine + NADH + Oxo-Glutarate
AS_Acetyl-CoA_to_L-Valine	true	Acetyl-CoA + L-Glutamate = CoA-SH + Oxo-Glutarate
AS_Alanine_to_Pyruvate	true	Pyruvate + beta_Alanine = L-Alanine + Malonate_semi_aldehyde
AS_Aspartate_to_Alanine	false	L-Aspartate = CO2 + L-Alanine
AS_Aspartate_to_Arginine	false	ATP-energy + L-Aspartate = ADP-energy + Fumarate + L-Arginine
AS_Aspartate_to_Asparagine	false	ATP-energy + L-Aspartate + L-Glutamine = ADP-energy + L-Asparagine + L-Glutamate + Orthophosphate
AS_Aspartate_to_beta-Alanine	false	L-Aspartate = CO2 + beta_Alanine
AS_Aspartate_to_Homoserine	true	ATP-energy + L-Aspartate + 2 NADPH = ADP-energy + Homoserine + 2 NADP+ + Phosphate
AS_Glutamate_to_Glutamine	false	ATP-energy + L-Glutamate + NH3 = ADP-energy + L-Glutamine + Phosphate
AS_Glutamate_to_Proline	false	ATP-energy + L-Glutamate + 2 NADPH = ADP-energy + L-Proline + 2 NADP+ + 2 Phosphate
AS_Histidine_to_Glutamate	false	2 H2O + L-Histidine + THF = Formamido-THF + L-Glutamate + NH3
AS_Homoserine_to_Threonine	false	ATP-energy + H2O + Homoserine = ADP-energy + L-Threonine + Phosphate
AS_Isoleucine	false	ATP-energy + Isoleucine_ext = ADP-energy + iso-Leucine
AS_Leucine	false	ATP-energy + Leucine-ext = ADP-energy + L-Leucine
AS_Phenylalanin_to_Tyrosine	false	L-Phenylalanine + NADPH + O2 = H2O + L-Tyrosine + NADP+
AS_Saccharopine_to_Lysine	true	H2O + NAD+ + Saccharopine = L-Lysine + NADH + Oxo-Glutarate
AS_Serine_to_Cysteine	false	Acetyl-CoA + H2S + L-Serine = Acetate + CoA-SH + L-Cysteine
AS_Serine_to_Glycine	true	L-Serine + THF = 5-10-Methylene-THF + H2O + L-Glycine
AS_Serine_to_Methionine	false	5-10-Methylene-THF + L-Serine = L-Methionine + NH3 + Pyruvate + THF
AS_Serine_to_Pyruvate	false	L-Serine = NADPH + Pyruvate
AS_Threonine	false	ATP-energy + Threonine_ext = ADP-energy + L-Threonine

AS_Tryptophan_to_Tryptamine	false	L-Tryptophan = CO2 + Tryptamine
AS_Valine	false	ATP-energy + Valine-ext = ADP-energy + L-Valine
ATP-energy_to_ATP-metabolism	true	ATP-energy = ATP-metabolism
DNA-extern_to_DNA-intern	false	DNA-extern = DNA
DNA_to_DNA-blocked	false	DNA + IQ-143 = DNA_blocked + IQ-143_used
FA_Deg_C16_to_Acetyl-CoA	false	C16 + 6 FAD + 6 NAD+ = 6 Acetyl-CoA + 6 CoA-SH + 6 FADH2 + 6 NADH
FA_Syn_Acetyl-CoA_to_C16	false	6 Acetyl-CoA + 6 NADPH = 6 ACP + C16 + 6 CO2 + 6 H2O + 6 NADP+
IQ-143-extern_to_IQ-143	false	IQ-143_extern = IQ-143
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	true	2-Phospho-D-glycerate = 3-Phospho-D-glycerate
Glyc_2-phospho-D-glycerate-hydro-lyase	true	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
Glyc_6-phospho-beta-glucosidase	true	H2O + Salicin6-phosphate = Salicylalcohol + beta-D-Glucose6-phosphate
Glyc_6-phosphofructokinase	true	ATP-energy + beta-D-Fructose6-phosphate = ADP-energy + beta-D-Fructose16-bisphosphate
Glyc_acetaldehyde-dehydrogenase_NAD+	true	Acetaldehyde + H2O + NAD+ = Acetate + H+ + NADH
Glyc_Actetate-CoA-ligase	true	ATP-energy + Acetate + CoA = ADP-energy + Acetyl-CoA + Pyrophosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	true	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	true	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_ATP-alpha-D-glucokinase	true	ATP-energy + alpha-D-Glucose = ADP-energy + alpha-D-Glucose6-phosphate
Glyc_ATP-beta-D-glucokinase	true	ATP-energy + beta-D-Glucose = ADP-metabolism + beta-D-Glucose6-phosphate
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	true	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_D-Glucose-1-epimerase	true	alpha-D-Glucose = beta-D-Glucose
Glyc_D-Glucose-1-epimerase-ketol-isomerase	true	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal = Glyceronephosphate
Glyc_dihydrolipoamide-dehydrogenase	false	EnzymeN6-(dihydrolipoyl)lysine + NAD+ = EnzymeN6-(lipoyl)lysine + H+ + NADH
Glyc_fructose-bisphosphat-aldolase	true	beta-D-Fructose16-bisphosphate = (2R)-2-Hydroxy-3-(phosphonooxy)-propanal + Glyceronephosphate
Glyc_fructose-bisphosphatase	false	H2O + beta-D-Fructose16-bisphosphate = Orthophosphate + beta-D-Fructose6-phosphate
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NADP+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADPH
Glyc_lipoic_acetyltransferase	true	Acetyl-CoA + EnzymeN6-(dihydrolipoyl)lysine = CoA + Dihydrolipoyllysine-residueacetyltransferaseS-

		acetyldihydrolipoyllysine
Glyc_phosphoglycerate-kinase	true	3-Phospho-D-glycerate + ATP-energy = 3-Phospho-D-glyceroylphosphate + ADP-energy
Glyc_PTS-permease1	true	D-Glucose + ProteinN(pi)-phospho-L-histidine = Proteinhistidine + alpha-D-Glucose6-phosphate
Glyc_PTS-permease2	true	Arbutin + ProteinN(pi)-phospho-L-histidine = Arbutin6-phosphate + Proteinhistidine
Glyc_pyruvate_dehydrogenase	false	Pyruvate + Thiamindiphosphate = 2-(alpha-Hydroxyethyl)thiaminediphosphate + CO2
Glyc_Succinate-CoA-ligase	true	ATP-energy + CoA + Succinate = ADP-energy + Orthophosphate + Succinyl-CoA
N-acylneuraminate-9-phosphatase	true	H2O + alpha-D-ribose-5P = AMP-metabolism + alpha-D-Ribose1-phosphate
OP_complex1	false	2 H+ + NADH + Ubichinon = 4 H+_ext + NAD+ + Ubihydrochinon
OP_complex2	false	4 H+ + Succinate + Ubichinon = Fumarate + Ubihydrochinon
OP_complex3	false	2 H+ + Ubihydrochinon + cytochrome_BC = 4 H+_ext + Ubichinon + cytochrome_C
OP_complex4	false	2 H+ + O- + cytochrome_C = 2 H+_ext + H2O
OP_complex5	false	ADP-energy + 3 H+_ext + Phosphate = ATP-energy + 3 H+ + H2O
PurM_5-Hydroxyisourate-amidohydrolase	false	5-Hydroxyisourate + H2O = (S)(+)-Allantoin
PurM_5-nucleotidase_AMP	false	AMP-metabolism + H2O = Adenosine + Orthophosphate
PurM_5-nucleotidase_CMP	false	CMP + H2O = Cytidine + Orthophosphate
PurM_5-nucleotidase_dAMP	false	H2O + dAMP = Deoxyadenosine + Orthophosphate
PurM_5-nucleotidase_dCMP	false	H2O + dCMP = Deoxycytidine + Orthophosphate
PurM_5-nucleotidase_dGMP	false	H2O + dGMP = Deoxyguanosine + Orthophosphate
PurM_5-nucleotidase_dTMP	false	H2O + dTMP = Orthophosphate + Thymidine
PurM_5-nucleotidase_GMP	false	GMP + H2O = Guanosine + Orthophosphate
PurM_5-nucleotidase_IMP	false	H2O + IMP = Inosine + Orthophosphate
PurM_5-nucleotidase_UMP	false	H2O + UMP = Orthophosphate + Uridine
PurM_5-nucleotidase_XMP	false	H2O + Xanthosine5-phosphate = Orthophosphate + Xanthosine
PurM_adenylate-kinase_AMP	true	AMP-metabolism + ATP-energy = 2 ADP-metabolism
PurM_adenylate-kinase_dAMP	true	ATP-energy + dAMP = ADP-energy + dADP
PurM_adenylosuccinate-lyase	true	N6-(12-Dicarboxyethyl)-AMP = AMP-metabolism + Fumarate
PurM_adenylosuccinate-lyase2	true	1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole = 1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Fumarate

PurM_adenylylsulfate-kinase	true	ATP-energy + Adenylylsulfate = 3-phosphoadenylylsulfate + ADP-energy
PurM_ADP-ribose-ribophosphohydrolase	false	ADP-ribose + H2O = AMP-metabolism + D-Ribose5-phosphate
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	true	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Pyrophosphate = 5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate
PurM_AIR-carboxylase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate = Aminoimidazoleribotide + CO2
PurM_allantoinase	false	Allantoate + H2O = Allantoine
PurM_AMP-pyrophosphorylase2	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_ATP-phosphohydrolase	false	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
PurM_ATP_CDP-phosphotransferase	true	ATP-energy + CDP = ADP-energy + CTP
PurM_ATP_dADP-phosphotransferase	true	ATP-energy + dADP = ADP-energy + dATP
PurM_ATP_dCDP-phosphotransferase	true	ATP-energy + dCDP = ADP-energy + dCTP
PurM_ATP_dGDP-phosphotransferase	true	ATP-energy + dGDP = ADP-energy + dGTP
PurM_ATP_dIDP-phosphotransferase	true	ATP-energy + dIDP = ADP-energy + dITP
PurM_ATP_dTDP-phosphotransferase	true	ATP-energy + dTDP = ADP-energy + dTTP
PurM_ATP_dUDP-phosphotransferase	true	ATP-energy + dUDP = ADP-energy + dUTP
PurM_ATP_GMP-guanylate-kinase	true	ATP-energy + GMP = ADP-energy + GDP
PurM_ATP_GMP_guanylate-kinase	true	ATP-energy + dGMP = ADP-energy + dGDP
PurM_ATP_GTP-phosphotransferase	true	ATP-energy + GDP = ADP-energy + GTP
PurM_ATP_IDP-phosphotransferase	true	ATP-energy + IDP = ADP-energy + ITP
PurM_ATP_UTP-phosphotransferase	true	ATP-energy + UDP = ADP-energy + UTP
PurM_carbamate-kinase_ATP	true	ATP-energy + CO2 + NH3 = ADP-energy + Carbamoylphosphate
PurM_D-Ribose-1,5-phosphomutase	false	alpha-D-Ribose1-phosphate = D-Ribose5-phosphate
PurM_deoxyadenosine-kinase_ATP	false	ATP-energy + Deoxyadenosine = ADP-energy + dAMP
PurM_deoxycytidine-kinase_ATP	false	ATP-energy + Adenosine = ADP-energy + AMP-metabolism
PurM_deoxycytidine-kinase_ATP2	false	ATP-energy + Deoxycytidine = ADP-energy + dCMP
PurM_dGTP-diphosphohydrolase	false	H2O + dGTP = Pyrophosphate + dGMP
PurM_dITP-diphosphohydrolase	false	H2O + dITP = 2-Deoxyinosine-5-phosphate + Pyrophosphate
PurM_DNA-directed-RNA-polyermase_ATP	false	ATP-metabolism + RNA = Pyrophosphate + RNA-A

PurM_DNA-directed-RNA-polyermase_CTP	false	CTP + RNA = Pyrophosphate + RNA-C
PurM_DNA-directed-RNA-polyermase_GTP	false	GTP + RNA = Pyrophosphate + RNA-G
PurM_DNA-directed-RNA-polyermase_UTP	false	RNA + UTP = Pyrophosphate + RNA-U
PurM_GDP-reductase	false	GMP + H+-intern + NADPH = IMP + NADP+ + NH3
PurM_GMP-pyrophosphorylase2	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PurM_GTP-diphosphohydrolase	false	GTP + H2O = GMP + Pyrophosphate
PurM_GTP-pyrophosphokinase	false	ATP-energy + GTP = ADP-energy + Guanosine3-diphosphate5-triphosphate
PurM_IMP-cyclohydrolase	true	H2O + IMP = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide
PurM_IMP-dehydrogenase	false	H2O + IMP + NAD+ = H+-intern + NADH + Xanthosine5-phosphate
PurM_IMP-pyrophosphorylase	true	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
PurM_IMP_L-aspartate-ligase	true	GTP + IMP + L-Aspartate = GDP + N6-(12-Dicarboxyethyl)-AMP + Orthophosphate
PurM_ITP-diphosphohydrolase	false	H2O + ITP = IMP + Pyrophosphate
PurM_metaphosphatase	true	Guanosine3-diphosphate5-triphosphate + H2O = Guanosine_3',5'-bis(diphosphate) + Orthophosphate
PurM_nucleoside-diphosphate-phosphotransferase_ATP	true	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
PurM_nucleotide-phosphatase_Adenine	true	Adenosine + Orthophosphate = Adenine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Deoxyadenosine	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PurM_nucleotide-phosphatase_Deoxyguanosine	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PurM_nucleotide-phosphatase_Deoxyinosine	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
PurM_nucleotide-phosphatase_Deoxyuridine	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PurM_nucleotide-phosphatase_Guanosine	true	Guanosine + Orthophosphate = Guanine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Inosine	true	Inosine + Orthophosphate = Hypoxanthine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Xanthosine	true	Orthophosphate + Xanthosine = Xanthine + alpha-D-Ribose1-phosphate
PurM_PRPP-synthetase	true	ATP-energy + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy
PurM_pyruvate-phosphotransferase_ATP	false	ATP-metabolism + Pyruvate = ADP-metabolism + Phosphoenolpyruvate
PurM_pyruvate-phosphotransferase_dATP	false	Pyruvate + dATP = Phosphoenolpyruvate + dADP
PurM_pyruvate-phosphotransferase_dGTP	false	Pyruvate + dGTP = Phosphoenolpyruvate + dGDP
PurM_pyruvate-phosphotransferase_GTP	false	GTP + Pyruvate = GDP + Phosphoenolpyruvate
PurM_SAICAR-synthetase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate + ATP-metabolism + L-Aspartate = 1-(5-

		Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole + ADP-metabolism + Orthophosphate
PurM_thioredoxin-oxidoreductase_dADP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dATP	false	ATP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dCDP	false	CDP + Thioredoxin = H2O + Oxidizedthioredoxin + dCDP
PurM_thioredoxin-oxidoreductase_dCTP	false	CTP + Thioredoxin = Oxidizedthioredoxin + dCTP
PurM_thioredoxin-oxidoreductase_dGDP	false	GDP + Thioredoxin = H2O + Oxidizedthioredoxin + dGDP
PurM_thioredoxin-oxidoreductase_dGTP	false	GTP + Thioredoxin = H2O + Oxidizedthioredoxin + dGTP
PurM_thioredoxin-oxidoreductase_dUDP	false	Thioredoxin + UDP = H2O + Oxidizedthioredoxin + dUDP
PurM_thioredoxin-oxidoreductase_dUTP	false	Thioredoxin + UTP = Oxidizedthioredoxin + dUTP
PurM_urea-amidohydrolase	false	H2O + Urea = CO2 + 2 NH3
PurM_UTP-diphosphohydrolase	false	H2O + UTP = Pyrophosphate + UMP
PurM_xanthosine-phosphoribosyltransferase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP-ligase	false	ATP-energy + NH3 + Xanthosine5-phosphate = ADP-energy + GMP + Pyrophosphate
PurM_XMP-pyrophosphorylase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP_L-glutamine-amide-ligase	false	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = ADP-energy + GMP + L-Glutamate + Pyrophosphate
PurM_XTP-diphosphohydrolase	false	H2O + XTP = Pyrophosphate + Xanthosine5-phosphate
PyrM_2,3-cyclic-nucleotidase_CMP	false	23-CyclicCMP + H2O = 3-CMP
PyrM_2,3-cyclic-nucleotidase_UMP	false	23-CyclicUMP + H2O = 3-UMP
PyrM_AMP-pyrophosphorylase	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PyrM_aspartate-carbamoyltransferase	false	Carbamoylphosphate + L-Aspartate = N-Carbamoyl-L-aspartate + Orthophosphate
PyrM_ATP_dTDP_thymidylate-kinase	true	ATP-energy + dTMP = ADP-energy + dTDP
PyrM_ATP_dUDP_thymidylate-kinase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_CO2_L-glutamine-amido-ligase	false	2 ATP-energy + H2O + HCO3- + L-Glutamine = 2 ADP-energy + Carbamoylphosphate + L-Glutamate + Orthophosphate
PyrM_CTP-synthase	false	ATP-energy + NH3 + UTP = ADP-energy + CTP + Orthophosphate
PyrM_cytidilate-kinase_CTP	true	ATP-energy + CMP = ADP-energy + CDP
PyrM_cytidilate-kinase_dCMP	true	ATP-energy + dCMP = ADP-energy + dCDP
PyrM_cytidine-aminohydrolase	true	Cytidine + H2O = NH3 + Uridine

PyrM_cytidine-kinase	false	Cytidine + UTP = CMP + UDP
PyrM_cytidine-kinase_ATP	false	ATP-energy + Cytidine = ADP-energy + CMP
PyrM_cytidine-kinase_dATP	false	Cytidine + dATP = CMP + dADP
PyrM_cytidine-kinase_dCTP	false	Cytidine + dCTP-ex = CMP + dCDP-ex
PyrM_cytidine-kinase_dGTP	false	Cytidine + dGTP = CMP + dGDP
PyrM_cytidine-kinase_dTTP	false	Cytidine + dTTP-ex = CMP + dTDP-ex
PyrM_cytidine-kinase_dUTP	false	Cytidine + dUTP-ex = CMP + dUDP-ex
PyrM_cytidine-kinase_GTP	false	Cytidine + GTP = CMP + GDP
PyrM_cytidine-kinase_ITP	false	Cytidine + ITP = CMP + IDP
PyrM_cytidine-ribohydrolase	false	Cytidine + H2O = Cytosine + D-Ribose
PyrM_dCMP-aminohydrolase	true	H2O + dCMP = NH3 + dUMP
PyrM_deoxyadenosine-phosphorylase	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PyrM_Deoxycytidine-aminohydrolase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_Deoxycytidine-deaminase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_deoxyguanosine-phosphorylase	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PyrM_deoxyinosine-phosphorylase	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Inosine
PyrM_deoxyuridine-phosphorylase	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PyrM_dihydroorotase	true	(S)-Dihydroorotate + H2O = N-Carbamoyl-L-aspartate
PyrM_dihydroorotate-oxidase	true	(S)-Dihydroorotate + Oxygen = H2O2 + Orotate
PyrM_dUMP-phosphotransferase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_dUTP-diphosphatase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_dUTP-diphosphohydrolase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_GMP-pyrophosphorylase	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PyrM_nucleoside-phosphate-kinase_ATP	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-phosphate-kinase_ATP2	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-triphosphate-adenylate-kinase	true	ATP-energy + UTP = ADP-energy + UDP
PyrM_OMP-decarboxylase	false	Orotidine5-phosphate = CO2 + UMP
PyrM_orotate-phosphoribosyltransferase	true	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate

PyrM_pyrimidine-nucleoside-phosphorylase	true	Cytidine + Orthophosphate = Cytosine + alpha-D-Ribose1-phosphate
PyrM_thioredoxin-reductase	false	H+ + NADPH + Oxidizedthioredoxin = NADP+ + Thioredoxin
PyrM_thymidilate-synthase	false	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
PyrM_thymidine-kinase_dTMP	true	ATP-energy + Thymidine = ADP-energy + dTMP
PyrM_thymidine-kinase_dUMP	true	ATP-energy + Deoxyuridine = ADP-energy + dUMP
PyrM_thymidine-phosphorylase	true	Orthophosphate + Thymidine = 2-Deoxy-D-ribose1-phosphate + Thymine
PyrM_UMP-pyrophosphorylase	true	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil
PyrM_uridine-kinase_ATP	false	ATP-energy + Uridine = ADP-energy + UMP
PyrM_uridine-kinase_dATP	false	Uridine + dATP = UMP + dADP
PyrM_uridine-kinase_dCTP	false	Uridine + dCTP-ex = UMP + dCDP-ex
PyrM_uridine-kinase_dGTP	false	Uridine + dGTP = UMP + dGDP
PyrM_uridine-kinase_dTTP	false	Uridine + dTTP-ex = UMP + dTDP-ex
PyrM_uridine-kinase_dUTP	false	Uridine + dUTP-ex = UMP + dUDP-ex
PyrM_uridine-kinase_GTP	false	GTP + Uridine = GDP + UMP
PyrM_uridine-kinase_ITP	false	ITP + Uridine = IDP + UMP
PyrM_uridine-kinase_UTP	false	UTP + Uridine = UDP + UMP
PyrM_uridine-phosphorylase	true	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
PyrM_uridine-ribohydrolase	false	H2O + Uridine = D-Ribose + Uracil
PyrM_UTP_L-glutamine-amido-ligase	false	ATP-energy + H2O + L-Glutamine + UTP = ADP-energy + CTP + L-Glutamate + Orthophosphate
SERP0290-zinc-transport_efflux	false	ATP-energy + H2O + Zn2+-intern = ADP-energy + Pyrophosphate + Zn2+-extern
SERP0291-zinc-transporter_import	false	ATP-energy + H2O + Zn2+-extern = ADP-energy + Pyrophosphate + Zn2+-intern
SERP0292-iron-dicitrate-transporter_import	false	ATP-energy + H2O + ferric-dicitrate_extern = ADP-energy + Pyrophosphate + ferric_dicitrate_intern
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	true	Ethanol + NAD+ = Acetaldehyde + H+ + NADH
SERP0653-PurM_FGAM-synthethase	false	5-Phosphoribosyl-N-formylglycinamide + ATP-metabolism + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ADP-metabolism + L-Glutamate + Orthophosphate
SERP0655-PurM_amidophosphoribosyltransferase	false	5-Phosphoribosylamine + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O + L-Glutamine
SERP0656-PurM_AIR_synthetase	false	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-metabolism = ADP-metabolism + Aminoimidazoleribotide + Orthophosphate

SERP0657-PurM_GAR-formyltransferase	false	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide = 5-Phosphoribosyl-N-formylglycinamide + Tetrahydrofolate
SERP0658-PurM_AICAR-formyltransferase	false	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + 10-Formyltetrahydrofolate = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide + Tetrahydrofolate
SERP0659-PurM_phosphoribosylamine-glycine-ligase	false	5-Phosphoribosylamine + ATP-metabolism + Glycine = 5-Phosphoribosylglycinamide + ADP-metabolism + Orthophosphate
SERP0686-spermidine/putrescine-transport_import	false	ATP-metabolism + H2O + putrescine_extern + spermidine_extern = ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0687-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0688-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0765-Uracil-permease-transport_import	false	H+-extern + uracil_extern = H+-intern + uracil_intern
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	false	DNA + dATP = DNA-A + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	false	DNA + dCTP = DNA-C + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	false	DNA + dGTP = DNA-G + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	false	DNA + dTTP = DNA-T + Pyrophosphate
SERP0841-PurM_PNPase_ADP	false	ADP-metabolism + RNA = Orthophosphate + RNA-A
SERP0841-PurM_PNPase_GDP	false	GDP + RNA = Orthophosphate + RNA-G
SERP1403-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143_extern + Pyrophosphate
SERP1802-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1803-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1944-MultiDrug-transport_efflux	false	IQ-143 + H+-intern = IQ-143_extern + H+-extern
SERP1951-lipoprotein-transport_efflux/import	true	ATP-energy + H2O + lipoprotein_extern = ADP-energy + Pyrophosphate + lipoprotein_intern
SERP1952-macrolide-transport_efflux	false	ATP-energy + H2O + macrolide_intern = ADP-energy + Pyrophosphate + macrolide_extern
SERP1997-formate/nitrite-transport_efflux/import	false	H+-intern + formate_internal + nitrite_external = H+-extern + formate_extern + nitrite_intern
SERP2060-glyerol-transport_import	false	ATP-energy + H2O + glycerol-3-phosphate_extern = ADP-energy + Pyrophosphate + glycerol-3-phosphate_intern
SERP2156-Glyc_L-lactate-dehydrogenase	true	(S)-Lactate + NAD+ = H+ + NADH + Pyruvate

SERP2179-choline/betaine/carnitine-transp_efflux	false	H+-extern + betaine_intern + carnitine-extern + choline-extern = H+-intern + betaine-extern + carnitine-intern + choline-intern
SERP2186-PurM_ATP_sulfate-adenylyltransferase	false	ATP-energy + Sulfate = Adenylylsulfate + Pyrophosphate
SERP2283-phopsphonate-transport_import	false	ATP-energy + H2O + phosphonate_extern = ADP-energy + Pyrophosphate + phosphonate_intern
SERP2289-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143_extern + Pyrophosphate
TCA_citrate-hydro-lyase	true	Citrate = H2O + cis-Aconitate
TCA_citrate-hydroxymutase	true	Citrate = Isocitrate
TCA_citrate_synthase	true	Citrate + CoA = Acetyl-CoA + H2O + Oxaloacetate
TCA_fumarate-hydratase	true	(S)-Malate = Fumarate + H2O
TCA_isocitrate-hydro-lyase	true	Isocitrate = H2O + cis-Aconitate
TCA_lipoic-transsuccinylase	true	EnzymeN6-(dihydrolipoyl)lysine + Succinyl-CoA = CoA + Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine
TCA_Oxidoreductase	false	Isocitrate + NAD+ = 2-Oxoglutarate + CO2 + H+ + NADH
TCA_oxoglutarate-dehydrogenase-complex1	true	2-Oxoglutarate + Thiamindiphosphate = 3-Carboxy-1-hydroxypropyl-ThPP + CO2
TCA_oxoglutarate-dehydrogenase-complex2	true	3-Carboxy-1-hydroxypropyl-ThPP + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine + Thiamindiphosphate
TCA_oxoglutarate-synthase	false	CO2 + Reducedferredoxin + Succinyl-CoA = 2-Oxoglutarate + CoA + Oxidizedferredoxin
TCA_PEP-carboxylase	true	ATP-energy + Oxaloacetate = ADP-energy + CO2 + Phosphoenolpyruvate
TCA_Pyruvate_CO2-ligase	true	ATP-energy + HCO3- + Pyruvate = ADP-energy + Orthophosphate + Oxaloacetate
TCA_pyruvate_dehydrogenase	false	2-(alpha-Hydroxyethyl)thiaminediphosphate + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine + Thiamindiphosphate

[1] List of enzymes used to build the metabolic web of *S. aureus USA 300*. This list is composed of data derived from KEGG and own annotations. Abbreviations: AS: Amino acids; FA: fatty acid synthesis and degradation; Glyc: Glycolysis and Pentose Phosphate Pathways; OP: Oxidative phosphorylation; PurM: Purine Metabolism; PyrM: Pyrimidine Metabolism; TCA: Citric acid Cycle; SERP: Enzymes measured by gene expression micro array (see point IV, supplementary materials).

Table S VI.2.3: List of enzmyes used to build metabolic web for *S. epidermidis RP62A* [1].

Enzyme name	reversible?	Reaction equation
ADP-energy_to_ADP-metabolism	true	ADP-energy = ADP-metabolism
AMP-energy_to_AMP-metabolism	true	AMP-energy = AMP-metabolism
AS_Acetyl-CoA_to_L-Leucine	false	Acetyl-CoA + L-Glutamate + NAD+ = CO2 + L-Leucine + NADH + Oxo-Glutarate
AS_Acetyl-CoA_to_L-Valine	true	Acetyl-CoA + L-Glutamate = CoA-SH + Oxo-Glutarate
AS_Alanine_to_Pyruvate	true	Pyruvate + beta_Alanine = L-Alanine + Malonate_semi_aldehyde
AS_Aspartate_to_Alanine	false	L-Aspartate = CO2 + L-Alanine
AS_Aspartate_to_Arginine	false	ATP-energy + L-Aspartate = ADP-energy + Fumarate + L-Arginine
AS_Aspartate_to_Asparagine	false	ATP-energy + L-Aspartate + L-Glutamine = ADP-energy + L-Asparagine + L-Glutamate + Orthophosphate
AS_Aspartate_to_beta-Alanine	false	L-Aspartate = CO2 + beta_Alanine
AS_Aspartate_to_Homoserine	true	ATP-energy + L-Aspartate + 2 NADPH = ADP-energy + Homoserine + 2 NADP+ + Phosphate
AS_Glutamate_to_Glutamine	false	ATP-energy + L-Glutamate + NH3 = ADP-energy + L-Glutamine + Phosphate
AS_Glutamate_to_Proline	false	ATP-energy + L-Glutamate + 2 NADPH = ADP-energy + L-Proline + 2 NADP+ + 2 Phosphate
AS_Histidine_to_Glutamate	false	2 H2O + L-Histidine + THF = Formamido-THF + L-Glutamate + NH3
AS_Homoserine_to_Threonine	false	ATP-energy + H2O + Homoserine = ADP-energy + L-Threonine + Phosphate
AS_Isoleucine	false	ATP-energy + Isoleucine_ext = ADP-energy + iso-Leucine
AS_Leucine	false	ATP-energy + Leucine-ext = ADP-energy + L-Leucine
AS_Phenylalanin_to_Tyrosine	false	L-Phenylalanine + NADPH + O2 = H2O + L-Tyrosine + NADP+
AS_Saccharopine_to_Lysine	true	H2O + NAD+ + Saccharopine = L-Lysine + NADH + Oxo-Glutarate
AS_Serine_to_Cysteine	false	Acetyl-CoA + H2S + L-Serine = Acetate + CoA-SH + L-Cysteine
AS_Serine_to_Glycine	true	L-Serine + THF = 5-10-Methylene-THF + H2O + L-Glycine
AS_Serine_to_Methionine	false	5-10-Methylene-THF + L-Serine = L-Methionine + NH3 + Pyruvate + THF
AS_Serine_to_Pyruvate	false	L-Serine = NADPH + Pyruvate
AS_Threonine	false	ATP-energy + Threonine_ext = ADP-energy + L-Threonine
AS_Tryptophan_to_Tryptamine	false	L-Tryptophan = CO2 + Tryptamine
AS_Valine	false	ATP-energy + Valine-ext = ADP-energy + L-Valine

ATP-energy_to_ATP-metabolism	true	ATP-energy = ATP-metabolism
DNA-extern_to_DNA-intern	false	DNA-extern = DNA
DNA_to_DNA-blocked	false	DNA + IQ-143 = DNA_blocked + IQ-143_used
FA_Deg_C16_to_Acetyl-CoA	false	C16 + 6 FAD + 6 NAD+ = 6 Acetyl-CoA + 6 CoA-SH + 6 FADH2 + 6 NADH
FA_Syn_Acetyl-CoA_to_C16	false	6 Acetyl-CoA + 6 NADPH = 6 ACP + C16 + 6 CO2 + 6 H2O + 6 NADP+
IQ-143-extern_to_IQ-143	false	IQ-143-extern = IQ-143
Glyc_2-Phospho-D-glycerate-2.3-phosphomutase	true	2-Phospho-D-glycerate = 3-Phospho-D-glycerate
Glyc_2-phospho-D-glycerate-hydro-lyase	true	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
Glyc_6-phospho-beta-glucosidase	true	H2O + Salicin6-phosphate = Salicylalcohol + beta-D-Glucose6-phosphate
Glyc_6-phosphofructokinase	true	ATP-energy + beta-D-Fructose6-phosphate = ADP-energy + beta-D-Fructose16-bisphosphate
Glyc_acetaldehyde-dehydrogenase_NAD+	true	Acetaldehyde + H2O + NAD+ = Acetate + H+ + NADH
Glyc_Actetate-CoA-ligase	true	ATP-energy + Acetate + CoA = ADP-energy + Acetyl-CoA + Pyrophosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase	true	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2	true	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_ATP-alpha-D-glucokinase	true	ATP-metabolism + alpha-D-Glucose = ADP-metabolism + alpha-D-Glucose6-phosphate
Glyc_ATP-beta-D-glucokinase	true	ATP-energy + beta-D-Glucose = ADP-metabolism + beta-D-Glucose6-phosphate
Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase	true	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Glyc_D-Glucose-1-epimerase	true	alpha-D-Glucose = beta-D-Glucose
Glyc_D-Glucose-1-epimerase-ketol-isomerase	true	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal = Glyceronephosphate
Glyc_dihydrolipoamide-dehydrogenase	false	EnzymeN6-(dihydrolipoyl)lysine + NAD+ = EnzymeN6-(lipoyl)lysine + H+ + NADH
Glyc_fructose-bisphosphat-aldolase	true	beta-D-Fructose16-bisphosphate = (2R)-2-Hydroxy-3-(phosphonooxy)-propanal + Glyceronephosphate
Glyc_fructose-bisphosphatase	false	H2O + beta-D-Fructose16-bisphosphate = Orthophosphate + beta-D-Fructose6-phosphate
Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+	false	(2R)-2-Hydroxy-3-(phosphonooxy)-propanal + NADP+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADPH
Glyc_lipoic_acetyltransferase	true	Acetyl-CoA + EnzymeN6-(dihydrolipoyl)lysine = CoA + Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine
Glyc_phosphoglycerate-kinase	true	3-Phospho-D-glycerate + ATP-energy = 3-Phospho-D-glyceroylphosphate + ADP-energy

Glyc_PTS-permease1	true	D-Glucose + ProteinN(pi)-phospho-L-histidine = Proteinhistidine + alpha-D-Glucose6-phosphate
Glyc_PTS-permease2	true	Arbutin + ProteinN(pi)-phospho-L-histidine = Arbutin6-phosphate + Proteinhistidine
Glyc_pyruvate_dehydrogenase	false	Pyruvate + Thiamindiphosphate = 2-(alpha-Hydroxyethyl)thiaminediphosphate + CO2
Glyc_Succinate-CoA-ligase	true	ATP-energy + CoA + Succinate = ADP-energy + Orthophosphate + Succinyl-CoA
OP_complex1	false	2 H+ + NADH + Ubichinon = 4 H+_ext + NAD+ + Ubihydrochinon
OP_complex2	false	4 H+ + Succinate + Ubichinon = Fumarate + Ubihydrochinon
OP_complex3	false	2 H+ + Ubihydrochinon + cytochrome_BC = 4 H+_ext + Ubichinon + cytochrome_C
OP_complex4	false	2 H+ + O- + cytochrome_C = 2 H+_ext + H2O
OP_complex5	false	ADP-energy + 3 H+_ext + Phosphate = ATP-energy + 3 H+ + H2O
PurM_5-nucleotidase_AMP	false	AMP-metabolism + H2O = Adenosine + Orthophosphate
PurM_5-nucleotidase_CMP	false	CMP + H2O = Cytidine + Orthophosphate
PurM_5-nucleotidase_dAMP	false	H2O + dAMP = Deoxyadenosine + Orthophosphate
PurM_5-nucleotidase_dCMP	false	H2O + dCMP = Deoxycytidine + Orthophosphate
PurM_5-nucleotidase_dGMP	false	H2O + dGMP = Deoxyguanosine + Orthophosphate
PurM_5-nucleotidase_dTMP	false	H2O + dTMP = Orthophosphate + Thymidine
PurM_5-nucleotidase_GMP	false	GMP + H2O = Guanosine + Orthophosphate
PurM_5-nucleotidase_IMP	false	H2O + IMP = Inosine + Orthophosphate
PurM_5-nucleotidase_UMP	false	H2O + UMP = Orthophosphate + Uridine
PurM_5-nucleotidase_XMP	false	H2O + Xanthosine5-phosphate = Orthophosphate + Xanthosine
PurM_adenylate-kinase_AMP	true	AMP-metabolism + ATP-energy = 2 ADP-metabolism
PurM_adenylate-kinase_dAMP	true	ATP-energy + dAMP = ADP-energy + dADP
PurM_adenylosuccinate-lyase	true	N6-(12-Dicarboxyethyl)-AMP = AMP-metabolism + Fumarate
PurM_adenylosuccinate-lyase2	true	1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole = 1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Fumarate
PurM_adenylylsulfate-kinase	true	ATP-energy + Adenylylsulfate = 3-phosphoadenylylsulfate + ADP-energy
PurM_ADP-ribose-ribophosphohydrolase	false	ADP-ribose + H2O = AMP-metabolism + D-Ribose5-phosphate
PurM_AICAR-pyrophosphate-phosphoribosyltransferase	true	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + Pyrophosphate = 5-Amino-4-imidazolecarboxyamide + 5-Phospho-alpha-D-ribose1-diphosphate
PurM_AIR-carboxylase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate = Aminoimidazoleribotide + CO2

PurM_AMP-pyrophosphorylase	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_AMP-pyrophosphorylase2	true	AMP-metabolism + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Adenine
PurM_ATP-phosphohydrolase	false	ATP-metabolism + H2O = ADP-metabolism + Orthophosphate
PurM_ATP_CDP-phosphotransferase	true	ATP-energy + CDP = ADP-energy + CTP
PurM_ATP_dADP-phosphotransferase	true	ATP-energy + dADP = ADP-energy + dATP
PurM_ATP_dCDP-phosphotransferase	true	ATP-energy + dCDP = ADP-energy + dCTP
PurM_ATP_dGDP-phosphotransferase	true	ATP-energy + dGDP = ADP-energy + dGTP
PurM_ATP_dIDP-phosphotransferase	true	ATP-energy + dIDP = ADP-energy + dITP
PurM_ATP_dTDP-phosphotransferase	true	ATP-energy + dTDP = ADP-energy + dTTP
PurM_ATP_dUDP-phosphotransferase	true	ATP-energy + dUDP = ADP-energy + dUTP
PurM_ATP_GMP-guanylate-kinase	true	ATP-energy + GMP = ADP-energy + GDP
PurM_ATP_GMP_guanylate-kinase	true	ATP-energy + dGMP = ADP-energy + dGDP
PurM_ATP_GTP-phosphotransferase	true	ATP-energy + GDP = ADP-energy + GTP
PurM_ATP_IDP-phosphotransferase	true	ATP-energy + IDP = ADP-energy + ITP
PurM_ATP_UTP-phosphotransferase	true	ATP-energy + UDP = ADP-energy + UTP
PurM_carbamate-kinase_ATP	true	ATP-energy + CO2 + NH3 = ADP-energy + Carbamoylphosphate
PurM_D-Ribose-1,5-phosphomutase	false	alpha-D-Ribose1-phosphate = D-Ribose5-phosphate
PurM_deoxyadenosine-kinase_ATP	false	ATP-energy + Deoxyadenosine = ADP-energy + dAMP
PurM_deoxycytidine-kinase_ATP	false	ATP-energy + Adenosine = ADP-energy + AMP-metabolism
PurM_deoxycytidine-kinase_ATP2	false	ATP-energy + Deoxycytidine = ADP-energy + dCMP
PurM_dGTP-diphosphohydrolase	false	H2O + dGTP = Pyrophosphate + dGMP
PurM_dITP-diphosphohydrolase	false	H2O + dITP = 2-Deoxyinosine-5-phosphate + Pyrophosphate
PurM_DNA-directed-RNA-polyermase_CTP	false	CTP + RNA = Pyrophosphate + RNA-C
PurM_DNA-directed-RNA-polyermase_GTP	false	GTP + RNA = Pyrophosphate + RNA-G
PurM_DNA-directed-RNA-polyermase_UTP	false	RNA + UTP = Pyrophosphate + RNA-U
PurM_DNA-directed-RNA-polymerase_ATP	false	ATP-metabolism + RNA = Pyrophosphate + RNA-A
PurM_GDP-reductase	false	GMP + H+-intern + NADPH = IMP + NADP+ + NH3
PurM_GMP-pyrophosphorylase	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine

PurM_GMP-pyrophosphorylase2	true	GMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Guanine
PurM_GTP-diphosphohydrolase	false	GTP + H2O = GMP + Pyrophosphate
PurM_GTP-pyrophosphokinase	false	ATP-energy + GTP = ADP-energy + Guanosine3-diphosphate5-triphosphate
PurM_IMP-cyclohydrolase	true	H2O + IMP = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide
PurM_IMP-dehydrogenase	false	H2O + IMP + NAD+ = H+-intern + NADH + Xanthosine5-phosphate
PurM_IMP-pyrophosphorylase	true	IMP + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Hypoxanthine
PurM_IMP_L-aspartate-ligase	true	GTP + IMP + L-Aspartate = GDP + N6-(12-Dicarboxyethyl)-AMP + Orthophosphate
PurM_ITP-diphosphohydrolase	false	H2O + ITP = IMP + Pyrophosphate
PurM_metaphosphatase	true	Guanosine3-diphosphate5-triphosphate + H2O = Guanosine_3',5'-bis(diphosphate) + Orthophosphate
PurM_nucleoside-diphosphate-phosphotransferase_ATP	true	ADP-metabolism + ATP-energy = ADP-energy + ATP-metabolism
PurM_nucleotide-phosphatase_Adenine	true	Adenosine + Orthophosphate = Adenine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Deoxyadenosine	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PurM_nucleotide-phosphatase_Deoxyguanosine	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PurM_nucleotide-phosphatase_Deoxyinosine	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Hypoxanthine
PurM_nucleotide-phosphatase_Deoxyuridine	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PurM_nucleotide-phosphatase_Guanosine	true	Guanosine + Orthophosphate = Guanine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Inosine	true	Inosine + Orthophosphate = Hypoxanthine + alpha-D-Ribose1-phosphate
PurM_nucleotide-phosphatase_Xanthosine	true	Orthophosphate + Xanthosine = Xanthine + alpha-D-Ribose1-phosphate
PurM_PRPP-synthetase	true	ATP-energy + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + ADP-energy
PurM_pyruvate-phosphotransferase_ATP	false	ATP-metabolism + Pyruvate = ADP-metabolism + Phosphoenolpyruvate
PurM_pyruvate-phosphotransferase_dATP	false	Pyruvate + dATP = Phosphoenolpyruvate + dADP
PurM_pyruvate-phosphotransferase_dGTP	false	Pyruvate + dGTP = Phosphoenolpyruvate + dGDP
PurM_pyruvate-phosphotransferase_GTP	false	GTP + Pyruvate = GDP + Phosphoenolpyruvate
PurM_SAICAR-synthetase	true	1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate + ATP-metabolism + L-Aspartate = 1-(5-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole + ADP-metabolism + Orthophosphate
PurM_thioredoxin-oxidoreductase_dATP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_thioredoxin-oxidoreductase_dCDP	false	CDP + Thioredoxin = H2O + Oxidizedthioredoxin + dCDP
PurM_thioredoxin-oxidoreductase_dCTP	false	CTP + Thioredoxin = Oxidizedthioredoxin + dCTP

PurM_thioredoxin-oxidoreductase_dGDP	false	GDP + Thioredoxin = H2O + Oxidizedferredoxin + dGDP
PurM_thioredoxin-oxidoreductase_dGTP	false	GTP + Thioredoxin = H2O + Oxidizedthioredoxin + dGTP
PurM_thioredoxin-oxidoreductase_dUDP	false	Thioredoxin + UDP = H2O + Oxidizedthioredoxin + dUDP
PurM_thioredoxin-oxidoreductase_dUTP	false	Thioredoxin + UTP = Oxidizedthioredoxin + dUTP
PurM_thioredoxin-oxidoreductased_dADP	false	ADP-metabolism + Thioredoxin = H2O + Oxidizedthioredoxin + dADP
PurM_urea-amidohydrolase	false	H2O + Urea = CO2 + 2 NH3
PurM_UTP-diphosphohydrolase	false	H2O + UTP = Pyrophosphate + UMP
PurM_xanthosine-phosphoribosyltransferase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP-pyrophosphorylase	true	Pyrophosphate + Xanthosine5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Xanthine
PurM_XMP_L-glutamine-amide-ligase	false	ATP-energy + H2O + L-Glutamine + Xanthosine5-phosphate = ADP-energy + GMP + L-Glutamate + Pyrophosphate
PurM_XTP-diphosphohydrolase	false	H2O + XTP = Pyrophosphate + Xanthosine5-phosphate
PyrM_2,3-cyclic-nucleotidase_CMP	false	23-CyclicCMP + H2O = 3-CMP
PyrM_2,3-cyclic-nucleotidase_UMP	false	23-CyclicUMP + H2O = 3-UMP
PyrM_aspartate-carbamoyltransferase	false	Carbamoylphosphate + L-Aspartate = N-Carbamoyl-L-aspartate + Orthophosphate
PyrM_ATP_dTDP_thymidylate-kinase	true	ATP-energy + dTMP = ADP-energy + dTDP
PyrM_ATP_dUDP_thymidylate-kinase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_CO2_L-glutamine-amido-ligase	false	2 ATP-energy + H2O + HCO3- + L-Glutamine = 2 ADP-energy + Carbamoylphosphate + L-Glutamate + Orthophosphate
PyrM_CTP-synthase	false	ATP-energy + NH3 + UTP = ADP-energy + CTP + Orthophosphate
PyrM_cytidilate-kinase_CTP	true	ATP-energy + CMP = ADP-energy + CDP
PyrM_cytidilate-kinase_dCMP	true	ATP-energy + dCMP = ADP-energy + dCDP
PyrM_cytidine-aminohydrolase	true	Cytidine + H2O = NH3 + Uridine
PyrM_cytidine-kinase_ATP	false	ATP-energy + Cytidine = ADP-energy + CMP
PyrM_cytidine-kinase_dATP	false	Cytidine + dATP = CMP + dADP
PyrM_cytidine-kinase_dCTP	false	Cytidine + dCTP-ex = CMP + dCDP-ex
PyrM_cytidine-kinase_dGTP	false	Cytidine + dGTP = CMP + dGDP
PyrM_cytidine-kinase_dTTP	false	Cytidine + dTTP-ex = CMP + dTDP-ex
PyrM_cytidine-kinase_dUTP	false	Cytidine + dUTP-ex = CMP + dUDP-ex

PyrM_cytidine-kinase_GTP	false	Cytidine + GTP = CMP + GDP
PyrM_cytidine-kinase_ITP	false	Cytidine + ITP = CMP + IDP
PyrM_cytidine-kinase_UTP	false	Cytidine + UTP = CMP + UDP
PyrM_cytidine-ribohydrolase	false	Cytidine + H2O = Cytosine + D-Ribose
PyrM_dCMP-aminohydrolase	true	H2O + dCMP = NH3 + dUMP
PyrM_deoxyadenosine-phosphorylase	true	Deoxyadenosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Adenine
PyrM_Deoxycytidine-aminohydrolase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_Deoxycytidine-deaminase	true	Deoxycytidine + H2O = Deoxyuridine + NH3
PyrM_deoxyguanosine-phosphorylase	true	Deoxyguanosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Guanine
PyrM_deoxyinosine-phosphorylase	true	Deoxyinosine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Inosine
PyrM_deoxyuridine-phosphorylase	true	Deoxyuridine + Orthophosphate = 2-Deoxy-D-ribose1-phosphate + Uracil
PyrM_dihydroorotase	true	(S)-Dihydroorotate + H2O = N-Carbamoyl-L-aspartate
PyrM_dihydroorotate-oxidase	true	(S)-Dihydroorotate + Oxygen = H2O2 + Orotate
PyrM_dUMP-phosphotransferase	true	ATP-energy + dUMP = ADP-energy + dUDP
PyrM_dUTP-diphosphatase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_dUTP-diphosphohydrolase	false	H2O + dUTP = Pyrophosphate + dUMP
PyrM_nucleoside-phosphate-kinase_ATP	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-phosphate-kinase_ATP2	true	ATP-energy + UMP = ADP-energy + UDP
PyrM_nucleoside-triphosphate-adenylate-kinase	true	ATP-energy + UTP = ADP-energy + UDP
PyrM_OMP-decarboxylase	false	Orotidine5-phosphate = CO2 + UMP
PyrM_orotate-phosphoribosyltransferase	true	Orotidine5-phosphate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + Orotate
PyrM_pyrimidine-nucleoside-phosphorylase	true	Cytidine + Orthophosphate = Cytosine + alpha-D-Ribose1-phosphate
PyrM_thioredoxin-reductase	false	H+ + NADPH + Oxidizedthioredoxin = NADP+ + Thioredoxin
PyrM_thymidilate-synthase	false	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
PyrM_thymidine-kinase_dTMP	true	ATP-energy + Thymidine = ADP-energy + dTMP
PyrM_thymidine-kinase_dUMP	true	ATP-energy + Deoxyuridine = ADP-energy + dUMP
PyrM_thymidine-phosphorylase	true	Orthophosphate + Thymidine = 2-Deoxy-D-ribose1-phosphate + Thymine
PyrM_UMP-pyrophosphorylase	true	Pyrophosphate + UMP = 5-Phospho-alpha-D-ribose1-diphosphate + Uracil

PyrM_uridine-kinase_ATP	false	ATP-energy + Uridine = ADP-energy + UMP
PyrM_uridine-kinase_dATP	false	Uridine + dATP = UMP + dADP
PyrM_uridine-kinase_dCTP	false	Uridine + dCTP-ex = UMP + dCDP-ex
PyrM_uridine-kinase_dGTP	false	Uridine + dGTP = UMP + dGDP
PyrM_uridine-kinase_dTTP	false	Uridine + dTTP-ex = UMP + dTDP-ex
PyrM_uridine-kinase_dUTP	false	Uridine + dUTP-ex = UMP + dUDP-ex
PyrM_uridine-kinase_GTP	false	GTP + Uridine = GDP + UMP
PyrM_uridine-kinase_ITP	false	ITP + Uridine = IDP + UMP
PyrM_uridine-kinase_UTP	false	UTP + Uridine = UDP + UMP
PyrM_uridine-phosphorylase	true	Orthophosphate + Uridine = Uracil + alpha-D-Ribose1-phosphate
PyrM_uridine-ribohydrolase	false	H2O + Uridine = D-Ribose + Uracil
PyrM_UTP_L-glutamine-amido-ligase	false	ATP-energy + H2O + L-Glutamine + UTP = ADP-energy + CTP + L-Glutamate + Orthophosphate
SERP0290-zinc-transport_efflux	false	ATP-energy + H2O + Zn2+-intern = ADP-energy + Pyrophosphate + Zn2+-extern
SERP0291-zinc-transporter_import	false	ATP-energy + H2O + Zn2+-extern = ADP-energy + Pyrophosphate + Zn2+-intern
SERP0292-iron-dicitrate-transporter_import	false	ATP-energy + H2O + ferric-dicitrate_extern = ADP-energy + Pyrophosphate + ferric_dicitrate_intern
SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	true	Ethanol + NAD+ = Acetaldehyde + H+ + NADH
SERP0653-PurM_FGAM-synthethase	false	5-Phosphoribosyl-N-formylglycinamide + ATP-metabolism + H2O + L-Glutamine = 2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ADP-metabolism + L-Glutamate + Orthophosphate
SERP0655-PurM_amidophosphoribosyltransferase	false	5-Phosphoribosylamine + L-Glutamate + Pyrophosphate = 5-Phospho-alpha-D-ribose1-diphosphate + H2O + L-Glutamine
SERP0656-PurM_AIR_synthetase	false	2-(Formamido)-N1-(5-phosphoribosyl)acetamidine + ATP-metabolism = ADP-metabolism + Aminoimidazoleribotide + Orthophosphate
SERP0657-PurM_GAR-formyltransferase	false	10-Formyltetrahydrofolate + 5-Phosphoribosylglycinamide = 5-Phosphoribosyl-N-formylglycinamide + Tetrahydrofolate
SERP0658-PurM_AICAR-formyltransferase	false	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide + 10-Formyltetrahydrofolate = 1-(5-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide + Tetrahydrofolate
SERP0659-PurM_phosphoribosylamine-glycine-ligase	false	5-Phosphoribosylamine + ATP-metabolism + Glycine = 5-Phosphoribosylglycinamide + ADP-metabolism + Orthophosphate
SERP0686-spermidine/putrescine-transport_import	false	ATP-metabolism + H2O + putrescine_extern + spermidine_extern = ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern

SERP0687-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0688-spermidine/putrescine-transport_import	false	2 ATP-metabolism + 2 H2O + putrescine_extern + spermidine_extern = 2 ADP-metabolism + 2 Pyrophosphate + putrescine_intern + spermidine_intern
SERP0765-Uracil-permease-transport_import	false	H+-extern + uracil_extern = H+-intern + uracil_intern
SERP0831-PurM_DNA-directed-DNA-polymerase_dATP	false	DNA + dATP = DNA-A + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP	false	DNA + dCTP = DNA-C + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP	false	DNA + dGTP = DNA-G + Pyrophosphate
SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP	false	DNA + dTTP = DNA-T + Pyrophosphate
SERP0841-PurM_PNPase_ADP	false	ADP-metabolism + RNA = Orthophosphate + RNA-A
SERP0841-PurM_PNPase_GDP	false	GDP + RNA = Orthophosphate + RNA-G
SERP1403-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143-extern + Pyrophosphate
SERP1802-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1803-cobalt/nickel-transport_efflux	false	2 ATP-energy + 2 H2O + cobalt-intern + nickel-intern = 2 ADP-energy + 2 Pyrophosphate + cobalt-extern + nickel-extern
SERP1944-MultiDrug-transport_efflux	false	IQ-143 + H+-intern = IQ-143-extern + H+-extern
SERP1951-lipoprotein-transport_efflux/import	true	ATP-energy + H2O + lipoprotein_extern = ADP-energy + Pyrophosphate + lipoprotein_intern
SERP1952-macrolide-transport_efflux	false	ATP-energy + H2O + macrolide_intern = ADP-energy + Pyrophosphate + macrolide_extern
SERP1997-formate/nitrite-transport_efflux/import	false	H+-intern + formate_internal + nitrite_external = H+-extern + formate_extern + nitrite_intern
SERP2060-glyerol-transport_import	false	ATP-energy + H2O + glycerol-3-phosphate_extern = ADP-energy + Pyrophosphate + glycerol-3-phosphate_intern
SERP2156-Glyc_L-lactate-dehydrogenase	true	(S)-Lactate + NAD+ = H+ + NADH + Pyruvate
SERP2179-choline/betaine/carnitine-transp_efflux	false	H+-extern + betaine_intern + carnitine-extern + choline-extern = H+-intern + betaine-extern + carnitine-intern + choline-intern
SERP2186-PurM_ATP_sulfate-adenylyltransferase	false	ATP-energy + Sulfate = Adenylylsulfate + Pyrophosphate
SERP2283-phopsphonate-transport_import	false	ATP-energy + H2O + phosphonate_extern = ADP-energy + Pyrophosphate + phosphonate_intern
SERP2289-MultiDrug-transport_efflux	false	ATP-energy + IQ-143 + H2O = ADP-energy + IQ-143-extern + Pyrophosphate
TCA_citrate-hydro-lyase	true	Citrate = H2O + cis-Aconitate
TCA_citrate-hydroxymutase	true	Citrate = Isocitrate

TCA_citrate_synthase	true	Citrate + CoA = Acetyl-CoA + H2O + Oxaloacetate
TCA_fumarate-hydratase	true	(S)-Malate = Fumarate + H2O
TCA_isocitrate-hydro-lyase	true	Isocitrate = H2O + cis-Aconitate
TCA_lipoic-transsuccinylase	true	EnzymeN6-(dihydrolipoyl)lysine + Succinyl-CoA = CoA + Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine
TCA_Oxidoreductase	false	Isocitrate + NAD+ = 2-Oxoglutarate + CO2 + H+ + NADH
TCA_oxoglutarate-dehydrogenase-complex1	true	2-Oxoglutarate + Thiamindiphosphate = 3-Carboxy-1-hydroxypropyl-ThPP + CO2
TCA_oxoglutarate-dehydrogenase-complex2	true	3-Carboxy-1-hydroxypropyl-ThPP + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residuesuccinyltransferaseS-succinyldihydrolipoyllysine + Thiamindiphosphate
TCA_oxoglutarate-synthase	false	CO2 + Reducedferredoxin + Succinyl-CoA = 2-Oxoglutarate + CoA + Oxidizedferredoxin
TCA_PEP-carboxylase	true	ATP-energy + Oxaloacetate = ADP-energy + CO2 + Phosphoenolpyruvate
TCA_Pyruvate_CO2-ligase	true	ATP-energy + HCO3- + Pyruvate = ADP-energy + Orthophosphate + Oxaloacetate
TCA_pyruvate_dehydrogenase	false	2-(alpha-Hydroxyethyl)thiaminediphosphate + EnzymeN6-(lipoyl)lysine = Dihydrolipoyllysine-residueacetyltransferaseS-acetyldihydrolipoyllysine + Thiamindiphosphate
TCA_succinate-dehydrogenase	true	Acceptor + Succinate = Fumarate + Reducedacceptor

[1] List of enzymes used to build the metabolic web of *S. epidermidis RP62A*. This list is composed of data derived from KEGG and own annotations.

Abbreviations: AS: Amino acids; FA: fatty acid synthesis and degradation; Glyc: Glycolysis and Pentose Phosphate Pathways; OP: Oxidative phosphorylation; PurM: Purine Metabolism; PyrM: Pyrimidine Metabolism; TCA: Citric acid Cycle; SERP: Enzymes measured by gene expression micro array (see point IV, supplementary materials).

3: Gene expression data gathered by Ohlsen et al.

Table S VI.2.4: Gene expression data of S. epidermidis RP62A with GB-AP-238 added.

EC/TC- Number of model	**Gene**	**COGs**	**Average of Fold-Change (WT w GB-AP-238 vs WT w/o GB-AP-238)**	**Description**	**Average of p-value (WT w GB-AP-238 vs WT w/o GB-AP-238)2**
	aacA	J	3,40	N-acetyltransferase	0,0065
	accA	I	2,97	acetyl-CoA carboxylase carboxyltransferase subunit alpha	0,0008
	accC	I	3,35	acetyl-CoA carboxylase biotin carboxylase subunit	0,0025
	acsA	I	-20,26	acetyl-CoA synthetase	0,0002
	acuA	-	-6,37	hypothetical protein	0,0001
	acuC	BQ	-3,61	acetoin utilization protein	0,0021
	aldA	C	-6,58	hypothetical protein	0,0000
	ampA	E	-3,32	cytosol aminopeptidase	0,0002
	araB	C	-3,87	ribulokinase	0,0087
	arg	E	-5,21	arginase	0,0019
	arsR2	K	3,80	arsenical resistance operon repressor 2	0,0009
	atl	G	3,38	autolysin, N-acetylmuramyl-L-alanine amidase and endo-b-N-acetylglucosaminidas	0,0009
	betA	E	18,02	choline dehydrogenase	0,0003
	betB	C	33,81	betaine aldehyde dehydrogenase	0,0000
	bglA	G	-3,34	6-phospho-beta-glucosidase	0,0057
	braB	E	9,78	branched-chain amino acid carrier protein	0,0002
	brnQ2	E	6,54	branched-chain amino acid transport system II carrier protein	0,0006
	bsaA	O	-3,51	glutathione peroxidase	0,0005
	butA	IQR	-5,29	acetoin reductase	0,0015
	cap5K	-	3,97	capsular polysaccharide synthesis protein Cap5K	0,0182
	capE	MG	3,82	capsular polysaccharide synthesis enzyme Cap8E	0,0098
	capG	M	3,59	capsular polysaccharide synthesis enzyme Cap5G	0,0076
	capH	R	3,34	capsular polysaccharide synthesis enzyme Cap5H	0,0003

	capI	M	2,99	capsular polysaccharide synthesis enzyme Cap5I	0,0034
	capJ	M	3,37	capsular polysaccharide synthesis enzyme Cap5J	0,0012
	capK	-	3,88	capsular polysaccharide synthesis enzyme Cap5K	0,0068
	capL	M	3,75	capsular polysaccharide synthesis enzyme Cap5L	0,0061
	capM	M	3,21	capsular polysaccharide synthesis enzyme Cap5M	0,0026
	capN	MG	3,27	capsular polysaccharide synthesis enzyme Cap5N	0,0015
	capO	M	3,05	capsular polysaccharide synthesis enzyme Cap8O	0,0071
	carB	EF	-3,97	carbamoyl phosphate synthase large subunit	0,0044
	cdsA	I	8,26	phosphatidate cytidylyltransferase	0,0001
2.3.3.1 – TCA-citrate-synthase	***citZ***	C	-3,04	citrate synthase	0,0007
	clfA	M	3,23	clumping factor A	0,0008
	clfB	M	3,96	clumping factor B	0,0054
	clpB	O	-3,36	putative ATPase subunit of an ATP-dependent protease	0,0017
	cspB	K	3,16	cold shock protein cspB	0,0114
	cudA	C	9,31	putative betaine aldehyde dehydrogenase	0,0007
	cudB	E	27,06	choline dehydrogenase	0,0000
2.A.15 – SERP 2179	***cudT***	M	14,33	choline transporter	0,0000
	cysE	E	-3,46	hypothetical protein	0,0002
	cysM	E	3,54	hypothetical protein	0,0022
	ddh	CHR	-3,86	D-lactate dehydrogenase	0,0032
2.4.2.1 – PurM nucleotide phosphatase, SERP0655-PurM amidophosphoribosyltransferase ,	***deoD***	F	-3,74	purine nucleoside phosphorylase	0,0014
	dhoM	E	3,09	homoserine dehydrogenase	0,0016
	dltA	Q	3,13	D-alanine--poly(phosphoribitol) ligase subunit 1	0,0012
	dltB	M	2,98	DltB membrane protein	0,0028
	dnaG	L	4,13	DNA primase	0,0031
	drp35	G	-3,60	Drp35	0,0012
	est	R	5,09	putative carboxylesterase	0,0002
	eutD	C	-3,06	phosphotransacetylase	0,0008

4.1.2.13 – Glyc-fructose-bisphosphate-aldolase	***fbaA***	G	-4,33	fructose-bisphosphate aldolase	0,0001
3.1.3.11 – Glyc-fructose-bisphosphatase	***fbp***	G	-3,64	fructose-bisphosphatase	0,0016
1.2.7.3 – TCA-oxoglutarate-synthase	***fer***	C	6,04	ferredoxin	0,0003
	fhs	F	-7,48	formate--tetrahydrofolate ligase	0,0021
	fhuB	P	3,34	ferrichrome transport permease	0,0005
	fhuG	P	2,99	ferrichrome transport permease	0,0035
	fnb	-	3,30	fibrinogen-binding protein	0,0010
	fnbA	-	3,49	fibronectin-binding protein precursor	0,0016
	fnbB	-	20,23	hypothetical protein	0,0007
	folD	H	-4,12	methylenetetrahydrofolate dehydrogenase/methenyltetrahydrofolate cyclohydrolase	0,0002
	frr	J	3,76	ribosome recycling factor	0,0092
4.2.1.2 – TCA-fumarate-hydratase	***fumC***	C	-9,53	fumarate hydratase	0,0028
	galM	G	6,06	aldose 1-epimerase	0,0001
1.2.1.12, 1.2.1.13 – Glyc-glyceraldehyde-3-phospho-dehydrogenase(NAD+/NADP+)	***gapB***	G	-3,00	glyceraldehyde 3-phosphate dehydrogenase 2	0,0007
	gapR	K	3,75	glycolytic operon regulator	0,0013
	gbsA	C	23,22	glycine betaine aldehyde dehydrogenase gbsA	0,0001
	geh	R	-3,12	glycerol ester hydrolase	0,0080
	gid	J	4,27	tRNA (uracil-5-)-methyltransferase Gid	0,0040
	gidA	D	8,19	tRNA uridine 5-carboxymethylaminomethyl modification enzyme GidA	0,0000
	gidB	M	7,74	16S rRNA methyltransferase GidB	0,0001
	glcA	G	3,00	hypothetical protein	0,0073
	glmS	M	-3,56	glucosamine--fructose-6-phosphate aminotransferase	0,0012
	glnA	E	-4,18	glutamine synthetase	0,0068
	glpD	C	-3,80	aerobic glycerol-3-phosphate dehydrogenase	0,0033
	glpQ	C	-3,25	glycerophosphoryl diester phosphodiesterase	0,0048
	gltT	C	3,08	proton/sodium-glutamate	0,0005

			symport protein	
gntK	G	-12,30	gluconokinase	0,0004
gntP	GE	-5,43	gluconate permease	0,0009
gntR	K	-12,12	gluconate operon transcriptional repressor	0,0002
groEL	O	-3,90	chaperonin GroEL	0,0022
groES	O	-3,95	co-chaperonin GroES	0,0032
gsaB	H	-3,40	glutamate-1-semialdehyde aminotransferase	0,0030
gudB	E	-3,29	NAD-specific glutamate dehydrogenase	0,0003
hemN	H	8,87	coproporphyrinogen III oxidase	0,0001
hisZ	E	5,88	ATP phosphoribosyltransferase regulatory subunit	0,0005
hlb	R	4,08	truncated beta-hemplysin	0,0025
hlgA	-	-10,78	gamma-hemolysin chain II precursor	0,0000
hlgC	-	-4,38	gamma-hemolysin component C	0,0028
hom	E	3,10	homoserine dehydrogenase	0,0010
hutH	E	-7,96	histidine ammonia-lyase	0,0002
hutI	Q	-35,32	imidazolonepropionase	0,0011
hutU	E	-98,52	urocanate hydratase	0,0000
icaA	M	3,34	N-glycosyltransferase PgaC	0,0007
ileS	J	-3,17	isoleucyl-tRNA synthetase	0,0058
infB	J	4,33	translation initiation factor IF-2	0,0001
isaA	M	11,76	immunodominant antigen A	0,0006
isaB	-	-3,10	immunodominant antigen B	0,0139
isdA	M	-3,84	cell surface protein	0,0011
ispD	I	-7,91	2-C-methyl-D-erythritol 4-phosphate cytidylyltransferase	0,0002
lacA	G	-9,48	galactose-6-phosphate isomerase subunit LacA	0,0002
lacB	G	-6,33	galactose-6-phosphate isomerase subunit LacB	0,0003
lacC	G	-5,43	tagatose-6-phosphate kinase	0,0008
lacD	G	-5,62	tagatose 1,6-diphosphate aldolase	0,0012
lacF	G	-13,60	PTS system, lactose-specific IIA component	0,0069
lip	R	-3,51	triacylglycerol lipase precursor	0,0054
lspA	MU	3,82	lipoprotein signal peptidase	0,0016
luxS	T	-3,55	S-ribosylhomocysteinase	0,0014
malR	K	-3,21	maltose operon transcriptional	0,0007

			repressor	
menE	IQ	-3,40	O-succinylbenzoic acid-CoA ligase	0,0002
metB	E	3,18	cystathionine gamma-synthase	0,0009
metK	H	5,60	S-adenosylmethionine synthetase	0,0008
mnmA	J	3,38	tRNA-specific 2-thiouridylase MnmA	0,0015
modA	P	-3,49	molybdate-binding protein	0,0005
mscL	M	3,94	large-conductance mechanosensitive channel	0,0002
msmX	G	-20,52	multiple sugar-binding transport ATP-binding protein	0,0006
murQ	R	-4,57	N-acetylmuramic acid-6-phosphate etherase	0,0014
MW1296	-	8,85	putative transposase	0,0087
MW1906	S	5,80	portal protein	0,0001
nanA	EM	-13,92	N-acetylneuraminate lyase	0,0003
ndhF	CP	-9,15	NADH dehydrogenase subunit 5	0,0004
nrdF	F	3,35	ribonucleotide-diphosphate reductase subunit beta	0,0000
nrgA	P	-7,00	probabale ammonium transporter	0,0011
nuc	L	0,15	thermonuclease	0,0011
nupC	F	-3,10	pyrimidine nucleoside transport protein	0,0003
nusA	K	4,01	transcription elongation factor NusA	0,0009
obgE	R	4,72	GTPase ObgE	0,0004
opp-1A	E	-3,89	oligopeptide transporter substrate binding protein	0,0001
opp-2B	EP	4,97	oligopeptide transporter permease	0,0004
opp-2C	EP	5,96	oligopeptide transporter permease	0,0000
opp-2D	EP	5,37	oligopeptide transport ATPase	0,0008
oppB	EP	-5,70	oligopeptide transport system permease protein	0,0007
oppD	EP	-3,21	hypothetical protein	0,0007
opuCA	E	4,58	glycine betaine/carnitine/choline ABC transporter opuCA	0,0014
opuCB	E	4,59	glycine betaine/carnitine/choline ABC transporter opuCB	0,0015

	opuCC	M	3,59	glycine betaine/carnitine/choline ABC transporter opuCC	0,0003
	opuCD	E	3,96	glycine betaine/carnitine/choline ABC transporter opuCD	0,0013
	opuD	M	4,20	glycine betaine transporter	0,0016
	pbp2	M	4,41	penicillin-binding protein 2	0,0014
	pbp4	M	6,49	penicillin binding protein 4	0,0001
	pbuX	F	3,75	xanthine permease	0,0024
	pckA	C	-3,62	phosphoenolpyruvate carboxykinase	0,0018
1.2.4.1 – Glyc/TCA-pyruvate-dehydrogenase	**pdhA**	C	-3,54	pyruvate dehydrogenase E1 component alpha subunit	0,0002
2.4.2.2 – PurM_GMP-pyrophosphorylase, PyrM_pyrimidine-nucleoside-phosphorylase	**pdp**	F	-4,68	pyrimidine-nucleoside phosphorylase	0,0003
2.7.1.11 – Glyc-6-phosphofructokinase	**pfkA**	G	-3,54	6-phosphofructokinase	0,0010
	pflB	C	-3,25	formate acetyltransferase	0,0068
5.3.1.9 – Glyc_alpha/beta-D-Glucose-6-phosphate-ketol-isomerase	**pgi**	G	-4,41	glucose-6-phosphate isomerase	0,0069
	phoB	P	5,65	alkaline phosphatase III precursor	0,0090
	plsX	I	2,99	putative glycerol-3-phosphate acyltransferase PlsX	0,0011
2.7.7.7 – SERP0831	**polC**	L	3,72	DNA polymerase III PolC	0,0049
	potA	E	11,35	hypothetical protein	0,0003
	potB	E	13,68	hypothetical protein	0,0007
	potC	E	12,53	hypothetical protein	0,0007
	potD	E	11,83	hypothetical protein	0,0005
	proP	G	3,66	proline/betaine transporter	0,0047
	proS	J	5,35	prolyl-tRNA synthetase	0,0005
4.3.2.2 PurM_adenylosuccinate-lyase	**purB**	F	-3,22	adenylosuccinate lyase	0,0002
6.3.5.3 – SERP0653-PurM_FGAM-synthethase	**purL**	F	-3,52	phosphoribosylformylglycinamidine synthase II	0,0043
	purQ	F	-4,04	phosphoribosylformylglycinamidine synthase I	0,0064
6.4.1.1 – TCA_Pyruvate_CO2-ligase	**pycA**	C	-3,01	pyruvate carboxylase	0,0018
2.4.2.10 – PyrM_orotate-phosphoribosyltransferase	**pyrE**	F	-6,60	orotate phosphoribosyltransferase	0,0022

4.1.1.23 – PyrM_OMP-decarboxylase	**pyrF**	F	-5,77	orotidine 5'-phosphate decarboxylase	0,0006
	queA	J	5,23	S-adenosylmethionine:tRNA ribosyltransferase-isomerase	0,0002
	rbfA	J	3,19	ribosome-binding factor A	0,0073
	rbgA	R	3,21	ribosomal biogenesis GTPase	0,0020
	recQ	L	3,09	DNA helicase	0,0028
	recU	R	4,79	Holliday junction-specific endonuclease	0,0001
	recX	R	-3,09	recombination regulator RecX	0,0027
	ribA	H	5,79	riboflavin biosynthesis protein	0,0005
	ribB	H	6,38	riboflavin synthase subunit alpha	0,0002
	ribD	H	5,36	riboflavin specific deaminase	0,0009
	rimM	J	8,74	16S rRNA-processing protein RimM	0,0005
	rnhB	L	3,01	ribonuclease HII	0,0045
	rnpA	J	16,11	ribonuclease P	0,0002
	rnr	K	5,65	ribonuclease R	0,0017
	rocA	C	-14,41	1-pyrroline-5-carboxylate dehydrogenase	0,0023
	rocD	E	-8,49	ornithine--oxo-acid transaminase	0,0006
	rocF	E	-5,91	arginase	0,0004
	rplA	J	6,60	50S ribosomal protein L1	0,0004
	rplB	J	3,09	50S ribosomal protein L2	0,0035
	rplC	J	3,50	50S ribosomal protein L3	0,0026
	rplD	J	3,12	50S ribosomal protein L4	0,0054
	rplJ	J	3,31	50S ribosomal protein L10	0,0166
	rplK	J	3,24	50S ribosomal protein L11	0,0041
	rplL	J	4,21	50S ribosomal protein L7/L12	0,0101
	rplS	J	5,19	50S ribosomal protein L19	0,0016
	rplT	J	8,23	50S ribosomal protein L20	0,0005
	rplU	J	4,19	50S ribosomal protein L21	0,0138
	rplW	J	3,24	50S ribosomal protein L23	0,0081
	rpmA	J	5,37	50S ribosomal protein L27	0,0008
	rpmE2	J	5,22	50S ribosomal protein L31 type B	0,0032
	rpmH	-	11,38	50S ribosomal protein L34	0,0026
	rpmI	J	3,88	50S ribosomal protein L35	0,0040
2.7.7.6 – PurM_DNA-directed-RNA-polyermase	**rpoB**	K	4,19	DNA-directed RNA polymerase subunit beta	0,0004
2.7.7.6 – PurM_DNA-directed-	**rpoE**	K	3,02	DNA-directed RNA polymerase	0,0015

RNA-polyermase				subunit delta	
	rpsB	J	3,41	30S ribosomal protein S2	0,0053
	rpsC	J	3,44	30S ribosomal protein S3	0,0035
	rpsD	J	6,02	30S ribosomal protein S4	0,0002
	rpsF	J	3,40	30S ribosomal protein S6	0,0079
	rpsI	J	3,35	30S ribosomal protein S9	0,0003
	rpsK	J	2,99	30S ribosomal protein S11	0,0130
	rpsP	J	6,69	30S ribosomal protein S16	0,0087
	rpsR	J	8,27	30S ribosomal protein S18	0,0018
	rpsU	J	3,58	30S ribosomal protein S21	0,0111
	ruvA	L	4,79	Holliday junction DNA helicase RuvA	0,0014
	ruvB	L	5,03	Holliday junction DNA helicase RuvB	0,0003
	SA0345	E	-3,51	bifunctional homocysteine S-methyltransferase/5,10-methylenetetrahydrofolate reductase protein	0,0018
	SA0433	G	3,66	alpha-glucosidase	0,0046
	SA0477	H	-13,62	pyridoxal biosynthesis lyase PdxS	0,0000
	SA0478	H	-10,13	glutamine amidotransferase subunit PdxT	0,0005
	SA0508	H	-4,38	2-amino-3-ketobutyrate coenzyme A ligase	0,0059
	SA0528	G	-3,10	hypothetical protein	0,0022
	SA0537	H	-3,63	phosphomethylpyrimidine kinase	0,0003
	SA0541	E	4,04	hypothetical protein	0,0012
	SA0544	S	-3,33	putative heme peroxidase	0,0025
	SA0581	CP	3,36	putative monovalent cation/H+ antiporter subunit D	0,0017
	SA0582	P	4,08	putative monovalent cation/H+ antiporter subunit E	0,0018
	SA0583	P	4,09	putative monovalent cation/H+ antiporter subunit F	0,0018
	SA0584	P	4,54	putative monovalent cation/H+ antiporter subunit G	0,0005
	SA0683	R	5,46	7-cyano-7-deazaguanine reductase	0,0002
	SA0746	L	-4,18	staphylococcal nuclease	0,0004
	SA1071	Q	2,99	fatty acid biosynthesis transcriptional regulator	0,0092

	SA1163	E	3,39	aspartate kinase	0,0052
	SA1406	S	3,01	16S ribosomal RNA methyltransferase RsmE	0,0028
	SA1537	H	6,20	thiamine biosynthesis protein ThiI	0,0016
	SA1572	E	-3,60	dipeptidase PepV	0,0000
	SA1725	-	-4,17	staphopain, cysteine proteinase	0,0006
	SA1729	H	-6,07	nicotinate phosphoribosyltransferase	0,0000
	SA1756	-	3,70	truncated amidase	0,0017
	SA1757	-	3,55	truncated amidase	0,0005
	SA1759	-	5,50	lytic enzyme	0,0170
	SA1765	-	7,50	hypothetical protein	0,0006
	SA1792	L	10,65	single-strand DNA-binding protein	0,0003
	SA1893	U	2,96	lipoprotein precursor	0,0004
	SA1939	F	-3,40	deoxyribose-phosphate aldolase	0,0014
	SA1999	K	-3,23	NAD-dependent deacetylase	0,0017
	SA2098	CHR	-3,15	glycerate dehydrogenase	0,0013
	SA2155	R	-4,72	malate:quinone oxidoreductase	0,0016
	SA2346	CHR	-4,26	D-lactate dehydrogenase	0,0034
1.1.1.27 – SERP2156-Glyc_L-lactate-dehydrogenase	**SA2395**	C	-9,53	L-lactate dehydrogenase	0,0000
	SAB0204	G,COG2190G	-5,36	PTS system transport protein	0,0044
	SAB0344	K	-6,42	pathogenicity island protein	0,0010
	SAB0534	E	3,94	amino acid transporter	0,0002
	SAB0968	E	11,57	spermidine/putrescine-binding periplasmic protein precursor	0,0006
	SAB1124	M	3,87	zinc metalloprotease	0,0006
	SAB1186	E	3,20	homoserine dehydrogenase	0,0024
	SAB1348c	-	3,65	lipoprotein	0,0065
	SAB1796c	O	-3,38	bacterioferritin comigratory protein	0,0006
	SAB2048c	GEPR	11,04	multidrug resistance protein	0,0000
	SAB2388	V	-16,80	ABC transporter	0,0002
	SACOL0024	F	-3,91	5'-nucleotidase family protein	0,0010
	SACOL0062	S	3,07	hypothetical protein	0,0005
	SACOL0067	J	3,03	hypothetical protein	0,0005
	SACOL0087	-	14,50	hypothetical protein	0,0001
	SACOL0122	GEPR	4,02	tetracycline resistance protein, putative	0,0003
	SACOL0181	-	-3,09	hypothetical protein	0,0006
	SACOL0182	-	-5,76	hypothetical protein	0,0068

	SACOL0183	-	-4,01	hypothetical protein	0,0017
	SACOL0192	G	-18,87	maltose ABC transporter, ATP-binding protein, putative	0,0000
	SACOL0193	G	-15,97	maltose ABC transporter, maltose-binding protein, putative	0,0001
	SACOL0194	G	-8,04	maltose ABC transporter, permease protein	0,0015
	SACOL0195	G	-7,18	maltose ABC transporter, permease protein	0,0000
	SACOL0196	R	-4,43	Gfo/Idh/MocA family oxidoreductase	0,0044
	SACOL0197	R	-4,12	Gfo/Idh/MocA family oxidoreductase	0,0018
	SACOL0198	G	-3,12	hypothetical protein	0,0002
	SACOL0199	S	9,23	hypothetical protein	0,0022
	SACOL0211	I	-4,89	acetyl-CoA acetyltransferase	0,0016
	SACOL0214	IQ	-6,03	long-chain-fatty-acid--CoA ligase, putative	0,0004
1.1.1.1 – SERP0389-Glyc_Ethanol_NAD+-oxidoreductase	**SACOL0237**	ER	-6,02	alcohol dehydrogenase, zinc-containing	0,0018
	SACOL0269	-	3,54	hypothetical protein	0,0077
	SACOL0366	-	5,65	prophage L54a, terminase, small subunit, putative	0,0029
	SACOL0384	-	9,76	hypothetical protein	0,0020
	SACOL0385	-	3,79	hypothetical protein	0,0095
	SACOL0386	-	3,37	hypothetical protein	0,0015
	SACOL0387	-	5,64	hypothetical protein	0,0034
	SACOL0467	MG	-3,14	hypothetical protein	0,0021
	SACOL0490	-	-3,14	hypothetical protein	0,0032
	SACOL0495	S	-6,20	hypothetical protein	0,0001
	SACOL0501	R	7,63	sodium-dependent transporter, putative	0,0006
	SACOL0553	D	4,06	hypothetical protein	0,0000
	SACOL0619	R	-3,93	HAD superfamily hydrolase	0,0098
	SACOL0633	S	-3,31	putative heme peroxidase	0,0000
	SACOL0684	P	3,96	putative monovalent cation/H+ antiporter subunit E	0,0005
	SACOL0686	P	4,65	putative monovalent cation/H+ antiporter subunit G	0,0007
	SACOL0689	P	-8,81	ABC transporter, permease protein	0,0006

SACOL0725	K	2,98	AraC family transcriptional regulator	0,0120
SACOL0755	-	6,22	hypothetical protein	0,0000
SACOL0770	O	6,56	radical activating enzyme family protein	0,0000
SACOL0778	M	4,55	sulfatase family protein	0,0004
SACOL0820	M,COG3942R	8,30	LysM domain-containing protein	0,0011
SACOL0846	K	5,23	VacB/RNase II family exoribonuclease	0,0001
SACOL0884	P	4,65	ABC transporter, substrate-binding protein	0,0016
SACOL0919	-	26,21	hypothetical protein	0,0003
SACOL0930	S	-3,13	hypothetical protein	0,0001
SACOL1003	OTN	4,15	adaptor protein	0,0003
SACOL1034	H	-2,95	lipoate-protein ligase A family protein	0,0001
SACOL1059	G	5,87	hypothetical protein	0,0009
SACOL1107	K	10,67	Cro/CI family transcriptional regulator	0,0002
SACOL1110	E	13,05	spermidine/putrescine ABC transporter, permease protein	0,0003
SACOL1111	E	13,26	spermidine/putrescine ABC transporter, spermidine/putrescine-binding protein	0,0002
SACOL1120	-	-3,38	hypothetical protein	0,0005
SACOL1299	IQR	3,08	acetoacetyl-CoA reductase, putative	0,0012
SACOL1338	-	5,49	hypothetical protein	0,0029
SACOL1444	P	5,99	hypothetical protein	0,0001
SACOL1445	R	4,87	CbbQ/NirQ/NorQ/GpvN family protein	0,0011
SACOL1488	-	4,58	hypothetical protein	0,0001
SACOL1501	S	4,38	hypothetical protein	0,0056
SACOL1502	S	3,26	hypothetical protein	0,0054
SACOL1584	-	-4,36	hypothetical protein	0,0101
SACOL1600	NU	9,98	competence protein ComGB, putative	0,0043
SACOL1620	S	-3,34	hypothetical protein	0,0018
SACOL1633	J	4,45	hypothetical protein	0,0012
SACOL1677	E	3,09	aminotransferase, class V	0,0002
SACOL1763	R	5,97	hypothetical protein	0,0003

	SACOL1766	-	3,67	hypothetical protein	0,0000
	SACOL1771	O	-4,01	OsmC/Ohr family protein	0,0004
	SACOL1777	O	-3,62	serine protease HtrA, putative	0,0026
	SACOL1810	R	3,09	hypothetical protein	0,0143
	SACOL1825	G	6,50	N-acetylmuramoyl-L-alanine amidase	0,0004
	SACOL1828	-	5,36	hypothetical protein	0,0050
	SACOL1833	D	4,24	crcB family protein	0,0084
	SACOL1857	-	3,82	hypothetical protein	0,0009
	SACOL1865	E	4,53	serine protease splE	0,0002
	SACOL1903	S	5,13	hypothetical protein	0,0013
	SACOL1904	K	7,76	transcriptional regulator, putative	0,0001
	SACOL1924	V	5,04	toxin exporting ABC transporter, permease/ATP-binding protein, putative	0,0008
	SACOL1952	P	3,06	ferritins family protein	0,0160
	SACOL2082	U	3,33	hypothetical protein	0,0006
	SACOL2088	-	3,23	sceD protein, putative	0,0040
	SACOL2142	-	-3,47	SAP domain-containing protein	0,0004
	SACOL2156	D	-3,85	ATP-binding Mrp/Nbp35 family protein	0,0005
	SACOL2158	-	5,69	hypothetical protein	0,0020
	SACOL2163	C	-3,39	hypothetical protein	0,0177
	SACOL2164	S	3,25	hypothetical protein	0,0070
	SACOL2257	GEPR	3,72	drug transporter, putative	0,0109
	SACOL2291	R	12,56	staphyloxanthin biosynthesis protein	0,0004
	SACOL2322	R	-3,11	M20/M25/M40 family peptidase	0,0019
	SACOL2363	C	3,55	L-lactate permease	0,0052
SERP1944	**SACOL2413**	GEPR	3,64	EmrB/QacA family drug resistance transporter	0,0102
	SACOL2435	G	-3,71	glycerate kinase	0,0023
	SACOL2454	-	6,49	hypothetical protein	0,0068
	SACOL2518	S	-3,90	hypothetical protein	0,0017
	SACOL2520	S	6,92	hypothetical protein	0,0005
	SACOL2525	V	-17,47	ABC transporter, ATP-binding protein	0,0002
	SACOL2631	R	6,18	hypothetical protein	0,0013
	SAOUHSC_00032	-	5,10	hypothetical protein	0,0000
	SAOUHSC_00108	-	8,25	hypothetical protein	0,0003
	SAOUHSC_00194	-	-3,15	hypothetical protein	0,0040
	SAOUHSC_00811	R	3,06	hypothetical protein	0,0034

SAOUHSC_01230	-	7,52	hypothetical protein	0,0060
SAOUHSC_01381	-	3,46	hypothetical protein	0,0007
SAOUHSC_01658	L	4,71	endonuclease IV	0,0002
SAOUHSC_02044	-	-3,99	hypothetical protein	0,0005
SAOUHSC_02090	R	3,77	hypothetical protein	0,0033
SAOUHSC_02294	-	4,01	hypothetical protein	0,0027
SAOUHSC_02416	-	3,04	hypothetical protein	0,0016
SAOUHSC_02802	-	5,54	fibronectin binding protein B, putative	0,0060
SAOUHSC_A01041	-	6,11	hypothetical protein	0,0102
SAOUHSC_A01079	-	3,34	hypothetical protein	0,0001
SAOUHSC_A02483	-	3,11	hypothetical protein	0,0049
SAOUHSC_A02811	-	3,21	hypothetical protein	0,0011
sarA	-	3,67	staphylococcal accessory regulator A	0,0048
sarZ	K	-3,01	staphylococcal accessory protein Z	0,0029
SAS0128	MG	3,50	capsular polysaccharide synthesis enzyme	0,0035
SAS0248	K	-3,62	LacI family regulatory protein	0,0018
SAS044	R	-3,12	4-oxalocrotonate tautomerase	0,0041
SAS046/SAS046 []	-	4,42	SAS046/SAS046 []	0,0044
SAS0542	E	3,40	putative amino acid permease	0,0002
SAS0546	S	-3,33	putative heme peroxidase	0,0001
SAS0717	J	-4,74	S30EA family ribosomal protein	0,0003
SAS0813	R	10,03	putative transporter protein	0,0061
SAS0984	E	-5,08	glutamyl endopeptidase precursor	0,0002
SAS0988	G	3,56	bifunctional autolysin precursor	0,0064
SAS1028	C	-3,12	putative pyruvate dehydrogenase E1 component, alpha subunit	0,0151
SAS1205	J	3,32	putative tRNA pseudouridine synthase B	0,0087
SAS1637	T	-4,82	putative universal stress protein	0,0003
SAS1707	D	4,42	CrcB-like protein	0,0000
SAS1712	C	-3,38	phosphoenolpyruvate carboxykinase	0,0130
SAS1887	-	-3,45	putative capsid protein	0,0125
SAS1889	S	6,81	putative portal protein	0,0030
SAS1904	L	-23,88	putative single-strand DNA-binding protein	0,0167
SAS2225	K	-9,06	LysR family regulatory protein	0,0001

SAS2340	E	4,17	putative glycine betaine/carnitine/choline transport ATP-binding protein	0,0014
sasH	F	-4,42	putative 5'-nucleotidase	0,0004
SAUSA300_0267	L	5,41	transposase	0,0010
SAV0465	R	6,53	N-acetylmuramoyl-L-alanine amidase	0,0013
SAV1409	R	4,64	nitric-oxide reductase	0,0002
SAV1785	L	5,01	putative transposase	0,0014
SAV1786	-	4,47	putative transposase	0,0029
sbcC	L	4,35	exonuclease SbcC	0,0001
scdA	D	3,01	cell wall biosynthesis protein ScdA	0,0040
sdrD	M	-3,07	Ser-Asp rich fibrinogen-binding, bone sialoprotein-binding protein	0,0046
secA	U	3,06	preprotein translocase subunit SecA	0,0007
secG	U	2,99	preprotein translocase subunit SecG	0,0000
serS	J	-10,29	seryl-tRNA synthetase	0,0001
sigA	K	3,37	RNA polymerase sigma factor RpoD	0,0018
smbA	F	4,58	uridylate kinase	0,0018
smc	D	2,99	chromosome segregation SMC protein	0,0069
smpB	O	7,41	SsrA-binding protein	0,0003
spa	R	-16,45	immunoglobulin G binding protein A precursor	0,0105
splA	E	-31,82	serine protease SplA	0,0160
splB	E	6,17	serine protease SplB	0,0000
splC	E	4,32	serine protease SplC	0,0017
splD	E	4,61	serine protease SplD	0,0004
splE	E	4,05	serine protease splE	0,0018
splF	E	4,34	serine protease SplF	0,0024
spoIIIE	D	3,74	hypothetical protein	0,0027
spsA	U	4,01	type-I signal peptidase	0,0011
spsB	U	4,48	type-1 signal peptidase 1B	0,0032
ssaA	R	26,17	secretory antigen precursor	0,0001
sspA	E	-4,55	serine protease; V8 protease; glutamyl endopeptidase	0,0003
tgt	J	4,98	queuine tRNA-ribosyltransferase	0,0000

	thrB	E	3,14	homoserine kinase	0,0101
	thrC	E	3,09	threonine synthase	0,0002
	tnp	L	7,86	putative transposase	0,0005
	trmD	J	15,32	tRNA-(guanine-N1)-mehtyltransferase	0,0000
	trmE	R	13,15	tRNA modification GTPase TrmE	0,0000
	trpC	E	-3,05	indole-3-glycerol-phosphate synthase	0,0051
	trpG	EH	-6,22	anthranilate synthase component II	0,0015
	tsf	J	3,55	elongation factor Ts	0,0006
	tst	-	-5,15	toxic shock syndrome toxin-1	0,0005
	tyrS	J	-3,02	tyrosyl-tRNA synthetase	0,0000
2.7.1.48 – PyrM_uridine-kinase, PyrM_cytidine-kinase,	**udk**	F	3,73	uridine kinase	0,0072
	uhpT	G	-6,45	sugar phosphate antiporter	0,0015
	ulaA	S	-5,38	ascorbate-specific PTS system enzyme IIC	0,0048
	uppS	I	4,35	undecaprenyl pyrophosphate synthetase	0,0008
	veg	S	3,20	hypothetical protein	0,0141
	vraD	V	-3,46	hypothetical protein	0,0004
2.4.2.22 – PurM_xanthosine-phosphoribosyltransferase	**xprT**	F	4,16	xanthine phosphoribosyltransferase	0,0035
	ywpF		-4,14	hypothetical protein	0,01

4: Extreme modes calculated by our YANAsquare models:

Table S VI.2.5: Extreme Modes of *S. aureus USA300* without GB-AP-238[1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	-0,65	1	true	1	(1 PyrM_GMP-pyrophosphorylase)
4	1,00	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
5	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
6	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
7	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
8	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
9	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
10	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
11	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
12	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
13	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
14	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
15	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
16	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
17	0,96	1	true	1	(1 TCA_fumarate-hydratase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
21	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
22	1,00	1	true	1	(1 AS_Serine_to_Glycine)
23	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
24	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)

25	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
26	1,00	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
27	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)
28	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
29	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
30	-1,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
31	1,00	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
32	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
33	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
34	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
35	0,96	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
36	1,00	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
38	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
39	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
40	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
41	1,00	1	true	1	(1 Glyc_Succinate-CoA-ligase)
42	1,00	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
43	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
44	1,00	1	true	1	(1 PurM_metaphosphatase)
45	1,00	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
46	1,00	1	true	1	(1 Glyc_PTS-permease2)
47	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
48	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)
49	-0,87	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
50	-0,33	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
51	-0,33	1	true	1	(1 PurM_XMP-pyrophosphorylase)

52	-0,33	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
53	-0,33	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
54	-0,33	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
55	0,73	1	true	1	(1 PurM_adenylate-kinase_dAMP)
56	0,72	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
57	1,28	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PyrM_AMP-pyrophosphorylase)
58	-0,50	10	true	6	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP)
59	0,37	6	true	4	(-1 AMP-energy_to_AMP-metabolism) (2 ATP-energy_to_ATP-metabolism) (-1 PurM_adenylate-kinase_AMP) (-2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
60	0,38	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
61	0,72	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP)
62	0,51	12	true	7	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_6-phospho-beta-glucosidase) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_D-Glucose-1-epimerase) (2 Glyc_PTS-permease1) (-1 PurM_adenylate-kinase_AMP)
63	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
64	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
65	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
67	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
68	1,00	2	false	2	(1 PurM_ATP-phosphohydrolase) (1 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
69	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
70	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
71	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
72	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
73	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
74	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
75	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)
76	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)

77	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
78	0,53	1	false	1	(1 PyrM_dUTP-diphosphatase)
79	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
80	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
81	1,28	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
82	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
83	1,00	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
84	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
85	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
86	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
87	1,00	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
90	0,13	1	false	1	(1 DNA-extern_to_DNA-intern)
91	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
92	0,67	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
93	0,38	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
94	0,16	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
95	1,00	1	false	1	(1 PurM_ITP-diphosphohydrolase)
96	0,31	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0688-spermidine/putrescine-transport_import)
97	0,58	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
98	1,00	2	false	2	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0686-spermidine/putrescine-transport_import)
99	1,00	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)

100	0,38	1	false	1	(1 PurM_dITP-diphosphohydrolase)
101	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
102	0,58	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
103	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
104	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
105	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
106	1,00	1	false	1	(1 AS_Valine)
107	0,49	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
108	1,00	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
109	0,72	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
110	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
111	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
112	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
113	1,00	1	false	1	(1 AS_Serine_to_Methionine)
114	1,00	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,12	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
117	0,12	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
118	1,00	1	false	1	(1 PyrM_cytidine-kinase)
119	0,38	1	false	1	(1 AS_Leucine)
120	0,38	48	false	20	(1 AMP-energy_to_AMP-metabolism) (-4 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (4 Glyc_2-phospho-D-glycerate-hydro-lyase) (2 Glyc_6-phospho-beta-glucosidase) (2 Glyc_6-phosphofructokinase) (-2 Glyc_acetaldehyde-dehydrogenase_NAD+) (-2 Glyc_Actetate-CoA-ligase) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_D-Glucose-1-epimerase) (-2 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (2 Glyc_fructose-bisphosphat-aldolase) (4 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-4 Glyc_phosphoglycerate-kinase) (1 PurM_adenylate-kinase_AMP) (-2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-2 TCA_citrate-hydro-lyase) (2 TCA_citrate_synthase) (-4 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,22	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)

123	1,00	1	false	1	(1 PyrM_CTP-synthase)
124	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,50	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	0,60	1	false	1	(1 PurM_allantoinase)
131	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
132	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
133	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
134	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
135	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
136	1,00	1	false	1	(1 AS_Isoleucine)
137	0,55	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
138	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
139	0,38	1	false	1	(1 PurM_5-nucleotidase_dTMP)
140	0,12	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,38	1	false	1	(1 PyrM_uridine-kinase_ATP)
142	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
143	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
144	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
145	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
146	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
147	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dADP)
148	0,60	1	false	1	(1 AS_Aspartate_to_Asparagine)
149	0,41	1	false	1	(1 PyrM_cytidine-kinase_ATP)

150	0,81	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
151	0,64	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
152	1,00	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)
153	1,00	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
154	0,57	1	false	1	(1 PurM_XTP-diphosphohydrolase)
155	0,45	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
156	1,00	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
157	1,00	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
158	0,22	1	false	1	(1 PurM_GTP-pyrophosphokinase)
159	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
160	1,00	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
161	0,27	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
162	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
163	1,00	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
164	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (2 PurM_thioredoxin-oxidoreductase_dATP)
165	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
166	0,25	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
167	1,25	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
168	1,00	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
169	0,25	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
170	1,00	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
171	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
172	1,00	6	false	4	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_DNA-directed-RNA-polyermase_ATP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)

173	0,50	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
174	0,49	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
175	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
176	1,00	1	false	1	(1 PurM_5-nucleotidase_GMP)
177	1,00	1	false	1	(1 PyrM_cytidine-kinase_ITP)
178	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
179	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
180	0,75	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
181	1,00	3	false	3	(1 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 PurM_pyruvate-phosphotransferase_ATP) (-1 TCA_PEP-carboxylase)
182	1,00	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
183	0,16	3	false	2	(2 PurM_nucleoside-diphosphate-phosphotransferase_ATP) (1 SERP0687-spermidine/putrescine-transport_import)
184	0,27	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
185	1,00	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
186	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
187	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
188	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
189	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
190	1,04	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
191	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
192	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	1,00	1	false	1	(1 PurM_XMP-ligase)
196	1,08	1	false	1	(1 PyrM_cytidine-kinase_dATP)
197	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
198	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. aureus USA300* without GB-AP-238.

Table S VI.2.6: Extreme Modes of *S. epidermidis RP62A* without GB-AP-238 [1]:

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	1,00	1	true	1	(1 AS_Alanine_to_Pyruvate)
2	1,00	1	true	1	(1 PyrM_dCMP-aminohydrolase)
3	0,70	1	true	1	(1 PurM_ATP_IDP-phosphotransferase)
4	1,00	1	true	1	(1 PyrM_cytidilate-kinase_dCMP)
5	1,00	1	true	1	(1 PyrM_dUMP-phosphotransferase)
6	1,00	1	true	1	(1 PurM_ATP_GMP-guanylate-kinase)
7	1,00	1	true	1	(1 PyrM_cytidine-aminohydrolase)
8	1,00	1	true	1	(1 PurM_ATP_UTP-phosphotransferase)
9	1,00	1	true	1	(1 PurM_ATP_GTP-phosphotransferase)
10	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyguanosine) (1 PyrM_deoxyguanosine-phosphorylase)
11	1,00	2	true	2	(-1 PyrM_dihydroorotase) (1 PyrM_dihydroorotate-oxidase)
12	1,00	1	true	1	(1 PurM_ATP_dIDP-phosphotransferase)
13	1,00	1	true	1	(1 PyrM_thymidine-kinase_dTMP)
14	1,00	1	true	1	(1 PurM_xanthosine-phosphoribosyltransferase)
15	1,00	1	true	1	(1 PurM_ATP_dUDP-phosphotransferase)
16	1,00	1	true	1	(1 TCA_fumarate-hydratase)
17	0,91	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_uridine-phosphorylase)
18	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Guanosine) (-1 PurM_nucleotide-phosphatase_Inosine)
19	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_nucleotide-phosphatase_Xanthosine)
20	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Deoxyinosine) (1 PyrM_deoxyinosine-phosphorylase)
21	1,00	1	true	1	(1 AS_Serine_to_Glycine)
22	1,00	1	true	1	(1 SERP1951-lipoprotein-transport_efflux/import)
23	1,00	1	true	1	(1 PurM_GMP-pyrophosphorylase2)
24	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP)
25	-0,52	1	true	1	(1 PyrM_ATP_dTDP_thymidylate-kinase)
26	1,00	1	true	1	(1 PurM_ATP_dTDP-phosphotransferase)

27	1,00	1	true	1	(1 PurM_ATP_GMP_guanylate-kinase)
28	1,00	1	true	1	(1 PyrM_nucleoside-phosphate-kinase_ATP2)
29	1,00	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyuridine) (1 PyrM_deoxyuridine-phosphorylase)
30	-1,33	2	true	2	(1 PyrM_deoxyuridine-phosphorylase) (-1 PyrM_thymidine-kinase_dUMP)
31	1,00	1	true	1	(1 PurM_ATP_dGDP-phosphotransferase)
32	1,00	1	true	1	(1 AS_Aspartate_to_Homoserine)
33	1,00	1	true	1	(1 PurM_ATP_dADP-phosphotransferase)
34	1,00	2	true	2	(1 TCA_citrate-hydro-lyase) (-1 TCA_citrate-hydroxymutase)
35	0,91	3	true	3	(1 Glyc_lipoic_acetyltransferase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
36	-1,00	7	true	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 SERP2156-Glyc_L-lactate-dehydrogenase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
37	1,00	1	true	1	(1 PurM_ATP_CDP-phosphotransferase)
38	1,00	1	true	1	(1 AS_Saccharopine_to_Lysine)
39	1,00	1	true	1	(1 PurM_IMP_L-aspartate-ligase)
40	0,50	1	true	1	(1 Glyc_Succinate-CoA-ligase)
41	0,50	3	true	3	(1 AS_Acetyl-CoA_to_L-Valine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
42	1,00	1	true	1	(1 PyrM_orotate-phosphoribosyltransferase)
43	1,00	1	true	1	(1 PurM_metaphosphatase)
44	1,05	1	true	1	(1 PyrM_cytidilate-kinase_CTP)
45	0,73	1	true	1	(1 PurM_GMP-pyrophosphorylase)
46	1,00	3	true	3	(1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase)
47	1,00	6	true	6	(1 ATP-energy_to_ATP-metabolism) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (1 Glyc_ATP-alpha-D-glucokinase) (-1 Glyc_ATP-beta-D-glucokinase) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase)
48	0,75	1	true	1	(1 Glyc_PTS-permease2)
49	1,00	4	true	4	(-1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_PTS-permease1)
50	1,00	1	true	1	(1 PyrM_thymidine-phosphorylase)
51	1,00	1	true	1	(1 PurM_ATP_dCDP-phosphotransferase)

52	-1,34	1	true	1	(1 PyrM_UMP-pyrophosphorylase)
53	0,79	1	true	1	(1 PyrM_nucleoside-triphosphate-adenylate-kinase)
54	0,53	1	true	1	(1 PurM_XMP-pyrophosphorylase)
55	0,53	1	true	1	(1 TCA_succinate-dehydrogenase)
56	0,53	2	true	2	(1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_Deoxycytidine-deaminase)
57	0,53	2	true	2	(-1 PurM_nucleotide-phosphatase_Deoxyadenosine) (1 PyrM_deoxyadenosine-phosphorylase)
58	0,53	1	true	1	(1 PyrM_ATP_dUDP_thymidylate-kinase)
59	0,92	1	true	1	(1 PurM_adenylate-kinase_dAMP)
60	1,08	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase2)
61	-0,65	2	true	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylosuccinate-lyase)
62	0,92	2	true	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_AMP-pyrophosphorylase)
63	-0,48	14	true	8	(1 AMP-energy_to_AMP-metabolism) (2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (2 Glyc_ATP-alpha-D-glucokinase) (-2 Glyc_ATP-beta-D-glucokinase) (-2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-2 Glyc_D-Glucose-1-epimerase) (1 PurM_adenylate-kinase_AMP) (2 PurM_nucleoside-diphosphate-phosphotransferase_ATP)
64	1,00	1	true	1	(1 PurM_adenylylsulfate-kinase)
65	1,00	4	true	3	(2 ADP-energy_to_ADP-metabolism) (-1 AMP-energy_to_AMP-metabolism) (-1 PurM_adenylate-kinase_AMP)
66	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Adenine) (-1 PurM_nucleotide-phosphatase_Inosine)
67	1,00	3	true	3	(1 PurM_IMP-pyrophosphorylase) (-1 PurM_nucleotide-phosphatase_Inosine) (1 PyrM_pyrimidine-nucleoside-phosphorylase)
68	1,00	1	true	1	(1 TCA_isocitrate-hydro-lyase)
69	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_ATP-phosphohydrolase)
70	1,00	2	false	2	(1 AMP-energy_to_AMP-metabolism) (1 PurM_5-nucleotidase_AMP)
71	1,00	1	false	1	(1 PyrM_uridine-kinase_dGTP)
72	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 SERP0841-PurM_PNPase_ADP)
73	1,00	1	false	1	(1 PurM_5-nucleotidase_XMP)
74	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dATP)
75	1,00	1	false	1	(1 PyrM_uridine-kinase_dTTP)
76	1,00	1	false	1	(1 PyrM_cytidine-kinase_dCTP)

77	1,00	1	false	1	(1 SERP1952-macrolide-transport_efflux)
78	1,00	2	false	2	(1 PurM_deoxyadenosine-kinase_ATP) (-1 PyrM_deoxyadenosine-phosphorylase)
79	0,55	1	false	1	(1 PyrM_dUTP-diphosphatase)
80	1,00	1	false	1	(1 AS_Aspartate_to_beta-Alanine)
81	1,00	1	false	1	(1 SERP1803-cobalt/nickel-transport_efflux)
82	1,00	1	false	1	(1 PyrM_cytidine-kinase_dGTP)
83	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUTP)
84	1,00	1	false	1	(1 SERP0292-iron-dicitrate-transporter_import)
85	0,25	2	false	2	(1 Glyc_6-phosphofructokinase) (1 Glyc_fructose-bisphosphatase)
86	1,00	1	false	1	(1 PurM_XMP_L-glutamine-amide-ligase)
87	1,00	1	false	1	(1 AS_Aspartate_to_Arginine)
88	1,00	7	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (2 PyrM_thioredoxin-reductase) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
89	1,00	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NAD+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
90	0,96	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_UMP)
91	1,00	1	false	1	(1 DNA-extern_to_DNA-intern)
92	0,67	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dCTP)
93	0,36	1	false	1	(1 SERP0841-PurM_PNPase_GDP)
94	0,41	2	false	2	(1 PurM_carbamate-kinase_ATP) (1 PyrM_aspartate-carbamoyltransferase)
95	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGDP)
96	0,30	1	false	1	(1 PurM_ITP-diphosphohydrolase)
97	0,35	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0688-spermidine/putrescine-transport_import)
98	1,00	3	false	3	(1 PurM_5-nucleotidase_dCMP) (1 PyrM_Deoxycytidine-aminohydrolase) (1 PyrM_deoxyuridine-phosphorylase)
99	1,00	14	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1

					PurM_adenylate-kinase_AMP) (2 SERP0686-spermidine/putrescine-transport_import)
100	0,36	1	false	1	(1 PyrM_dUTP-diphosphohydrolase)
101	1,00	1	false	1	(1 PurM_dITP-diphosphohydrolase)
102	0,35	2	false	2	(1 PurM_pyruvate-phosphotransferase_GTP) (-1 TCA_PEP-carboxylase)
103	1,00	2	false	2	(1 PurM_pyruvate-phosphotransferase_dATP) (-1 TCA_PEP-carboxylase)
104	1,00	1	false	1	(1 PurM_5-nucleotidase_UMP)
105	1,00	1	false	1	(1 SERP2283-phopsphonate-transport_import)
106	1,00	2	false	2	(1 PurM_GDP-reductase) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
107	0,48	1	false	1	(1 AS_Valine)
108	1,00	2	false	2	(1 PurM_5-nucleotidase_dAMP) (1 PyrM_deoxyadenosine-phosphorylase)
109	0,92	1	false	1	(1 SERP1802-cobalt/nickel-transport_efflux)
110	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_UTP)
111	1,00	4	false	4	(-1 TCA_lipoic-transsuccinylase) (1 TCA_oxoglutarate-dehydrogenase-complex1) (1 TCA_oxoglutarate-dehydrogenase-complex2) (1 TCA_oxoglutarate-synthase)
112	1,00	1	false	1	(1 PyrM_cytidine-kinase_dTTP)
113	1,00	1	false	1	(1 PurM_UTP-diphosphohydrolase)
114	1,00	1	false	1	(1 AS_Serine_to_Methionine)
115	1,00	2	false	2	(1 PurM_5-nucleotidase_dGMP) (1 PyrM_deoxyguanosine-phosphorylase)
116	0,19	2	false	2	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_deoxycytidine-kinase_ATP)
117	0,19	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dGTP)
118	1,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP1944-MultiDrug-transport_efflux) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
119	0,36	1	false	1	(1 AS_Leucine)
120	0,36	20	false	15	(-2 Glyc_2-Phospho-D-glycerate-2.3-phosphomutase) (2 Glyc_2-phospho-D-glycerate-hydro-lyase) (1 Glyc_6-phospho-beta-glucosidase) (1 Glyc_6-phosphofructokinase) (-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (-1 Glyc_D-Glucose-1-epimerase-ketol-isomerase) (1 Glyc_fructose-bisphosphat-aldolase) (2 Glyc_glyceraldehyde-3-P-dehydrogenase_NADP+) (-2 Glyc_phosphoglycerate-kinase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_PEP-carboxylase)
121	0,25	1	false	1	(1 PyrM_2,3-cyclic-nucleotidase_CMP)
122	0,48	2	false	2	(1 SERP1997-formate/nitrite-transport_efflux/import) (1 SERP2179-choline/betaine/carnitine-transp_efflux)
123	1,00	1	false	1	(1 PyrM_CTP-synthase)

124	0,80	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP2289-MultiDrug-transport_efflux)
125	1,00	1	false	1	(1 AS_Glutamate_to_Proline)
126	0,75	1	false	1	(1 PyrM_uridine-kinase_dCTP)
127	1,75	1	false	1	(1 PyrM_uridine-kinase_UTP)
128	1,00	3	false	3	(1 PurM_deoxycytidine-kinase_ATP2) (-1 PyrM_Deoxycytidine-aminohydrolase) (-1 PyrM_deoxyuridine-phosphorylase)
129	1,00	1	false	1	(1 AS_Threonine)
130	1,40	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dTTP)
131	1,00	1	false	1	(1 PurM_GTP-diphosphohydrolase)
132	1,00	1	false	1	(1 PyrM_uridine-kinase_dATP)
133	1,00	1	false	1	(1 AS_Serine_to_Pyruvate)
134	1,00	2	false	2	(1 SERP0290-zinc-transport_efflux) (1 SERP0291-zinc-transporter_import)
135	1,00	1	false	1	(1 AS_Isoleucine)
136	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCDP)
137	0,52	2	false	2	(1 PurM_pyruvate-phosphotransferase_dGTP) (-1 TCA_PEP-carboxylase)
138	1,00	1	false	1	(1 PurM_5-nucleotidase_dTMP)
139	0,36	1	false	1	(1 PyrM_uridine-kinase_ATP)
140	0,19	4	false	4	(1 PurM_D-Ribose-1,5-phosphomutase) (-1 PurM_IMP-pyrophosphorylase) (1 PurM_nucleotide-phosphatase_Inosine) (1 PurM_PRPP-synthetase)
141	0,36	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_GTP)
142	1,00	7	false	6	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (2 Glyc_dihydrolipoamide-dehydrogenase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
143	1,00	1	false	1	(1 PyrM_OMP-decarboxylase)
144	1,00	1	false	1	(1 AS_Glutamate_to_Glutamine)
145	1,00	1	false	1	(1 PurM_urea-amidohydrolase)
146	1,00	1	false	1	(1 AS_Aspartate_to_Asparagine)
147	1,00	1	false	1	(1 PyrM_cytidine-kinase_ATP)
148	0,64	2	false	2	(1 PurM_GDP-reductase) (1 SERP0765-Uracil-permease-transport_import)
149	0,48	3	false	3	(1 IQ-143-extern_to_IQ-) (1 SERP0765-Uracil-permease-transport_import) (1 SERP1944-MultiDrug-transport_efflux)
150	0,91	2	false	2	(1 SERP0765-Uracil-permease-transport_import) (1 SERP1997-formate/nitrite-transport_efflux/import)

151	0,56	13	false	9	(-1 Glyc_acetaldehyde-dehydrogenase_NAD+) (-1 Glyc_Actetate-CoA-ligase) (-1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase) (-2 TCA_lipoic-transsuccinylase) (2 TCA_Oxidoreductase) (2 TCA_oxoglutarate-dehydrogenase-complex1) (2 TCA_oxoglutarate-dehydrogenase-complex2)
152	1,00	1	false	1	(1 PurM_XTP-diphosphohydrolase)
153	1,00	3	false	3	(-1 PurM_carbamate-kinase_ATP) (1 PyrM_CO2_L-glutamine-amido-ligase) (-1 TCA_Pyruvate_CO2-ligase)
154	0,60	12	false	7	(2 Glyc_acetaldehyde-dehydrogenase_NAD+) (2 Glyc_Actetate-CoA-ligase) (1 OP_complex1) (1 OP_complex3) (2 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (2 TCA_citrate-hydro-lyase) (-2 TCA_citrate_synthase)
155	0,48	17	false	7	(3 Glyc_acetaldehyde-dehydrogenase_NAD+) (3 Glyc_Actetate-CoA-ligase) (1 OP_complex2) (1 OP_complex3) (3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (3 TCA_citrate-hydro-lyase) (-3 TCA_citrate_synthase)
156	1,00	1	false	1	(1 PurM_GTP-pyrophosphokinase)
157	1,00	6	false	6	(1 Glyc_acetaldehyde-dehydrogenase_NAD+) (1 Glyc_Actetate-CoA-ligase) (1 OP_complex4) (1 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (1 TCA_citrate-hydro-lyase) (-1 TCA_citrate_synthase)
158	0,48	2	false	2	(1 Glyc_pyruvate_dehydrogenase) (1 TCA_pyruvate_dehydrogenase)
159	1,00	17	false	6	(-3 Glyc_acetaldehyde-dehydrogenase_NAD+) (-3 Glyc_Actetate-CoA-ligase) (2 OP_complex5) (-3 SERP0389-Glyc_Ethanol_NAD+-oxidoreductase) (-3 TCA_citrate-hydro-lyase) (3 TCA_citrate_synthase)
160	1,00	1	false	1	(1 AS_Aspartate_to_Alanine)
161	0,66	2	false	2	(1 AS_Serine_to_Cysteine) (1 Glyc_Actetate-CoA-ligase)
162	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductase_dATP)
163	1,00	1	false	1	(1 SERP2186-PurM_ATP_sulfate-adenylyltransferase)
164	1,00	3	false	3	(-1 AMP-energy_to_AMP-metabolism) (1 PurM_ADP-ribose-ribophosphohydrolase) (1 PurM_PRPP-synthetase)
165	1,00	2	false	2	(1 IQ-143-extern_to_IQ-) (1 SERP1403-MultiDrug-transport_efflux)
166	0,25	13	false	3	(1 FA_Syn_Acetyl-CoA_to_C16) (-6 TCA_citrate-hydro-lyase) (6 TCA_citrate_synthase)
167	0,51	1	false	1	(1 PyrM_UTP_L-glutamine-amido-ligase)
168	0,25	1	false	1	(1 AS_Phenylalanin_to_Tyrosine)
169	1,00	1	false	1	(1 PurM_5-nucleotidase_IMP)
170	1,00	2	false	2	(1 PurM_GDP-reductase) (1 PurM_IMP-dehydrogenase)
171	0,00	3	false	3	(1 IQ-143-extern_to_IQ-) (1 PurM_IMP-dehydrogenase) (1 SERP1944-MultiDrug-transport_efflux)
172	0,25	2	false	2	(1 PurM_IMP-dehydrogenase) (1 SERP1997-formate/nitrite-transport_efflux/import)
173	0,48	1	false	1	(1 PurM_5-nucleotidase_GMP)
174	0,25	1	false	1	(1 PyrM_cytidine-kinase_ITP)

175	1,00	1	false	1	(1 AS_Histidine_to_Glutamate)
176	1,00	1	false	1	(1 PyrM_cytidine-kinase_GTP)
177	1,00	13	false	3	(1 FA_Deg_C16_to_Acetyl-CoA) (6 TCA_citrate-hydro-lyase) (-6 TCA_citrate_synthase)
178	1,00	16	false	9	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (2 PurM_pyruvate-phosphotransferase_ATP) (-2 TCA_PEP-carboxylase)
179	0,48	1	false	1	(1 PyrM_cytidine-kinase_dUTP)
180	1,00	6	false	6	(-1 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-1 Glyc_ATP-alpha-D-glucokinase) (1 Glyc_ATP-beta-D-glucokinase) (1 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (1 Glyc_D-Glucose-1-epimerase) (1 PurM_DNA-directed-RNA-polymerase_ATP)
181	1,00	13	false	8	(-1 AMP-energy_to_AMP-metabolism) (-2 Glyc_alpha-D-Glucose-6-phosphate-ketol-isomerase2) (-2 Glyc_ATP-alpha-D-glucokinase) (2 Glyc_ATP-beta-D-glucokinase) (2 Glyc_beta-D-Glucose-6-phosphate-ketol-isomerase) (2 Glyc_D-Glucose-1-epimerase) (-1 PurM_adenylate-kinase_AMP) (1 SERP0687-spermidine/putrescine-transport_import)
182	0,41	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dUDP)
183	0,48	1	false	1	(1 PurM_dGTP-diphosphohydrolase)
184	1,00	1	false	1	(1 PurM_DNA-directed-RNA-polyermase_CTP)
185	1,00	1	false	1	(1 SERP0831-PurM_DNA-directed-DNA-polymerase_dGTP)
186	1,00	4	false	3	(1 AMP-energy_to_AMP-metabolism) (1 PurM_adenylate-kinase_AMP) (2 PurM_thioredoxin-oxidoreductased_dADP)
187	1,00	1	false	1	(1 PurM_thioredoxin-oxidoreductase_dCTP)
188	1,00	1	false	1	(1 AS_Tryptophan_to_Tryptamine)
189	1,00	3	false	3	(1 AS_Acetyl-CoA_to_L-Leucine) (-1 TCA_citrate-hydro-lyase) (1 TCA_citrate_synthase)
190	1,00	1	false	1	(1 AS_Homoserine_to_Threonine)
191	1,00	1	false	1	(1 PurM_5-nucleotidase_CMP)
192	1,00	1	false	1	(1 PyrM_cytidine-kinase_UTP)
193	1,00	1	false	1	(1 PyrM_uridine-kinase_dUTP)
194	1,00	1	false	1	(1 PyrM_uridine-kinase_ITP)
195	0,56	1	false	1	(1 PyrM_cytidine-kinase_dATP)
196	1,00	1	false	1	(1 SERP2060-glyerol-transport_import)
197	1,00	1	false	1	(1 PyrM_uridine-kinase_GTP)

[1] This data shows the elementary mode Analysis for *S. epidermidis RP62A* without GB-AP-238 .

3. Daten der Simulationen von P. falciparum

1) Full list of enzymes of YANAsquare modes:
    1. Table S VI.3.1: List of enzmyes used to build metabolic web for *P. falciparum 3D7*.
2) Extreme modes calculated by YANAsquare models:
    1. Table S VI.3.2: Extreme modes of *P. falciparum 3D7* for a wildtype strain (no resistances, no compounds added).
    2. Table S VI.3.3: Extreme modes of *P. falciparum 3D7* for less active DHF and DHPS (Chloroquine resistant, Sulfodoxin added).
    3. Table S VI.3.4: Extreme modes of *P. falciparum 3D7* for less active ferrochelatase (Sulfadoxin resistant, Chloroquine added).
    4. Table S VI.3.5: Extreme modes of *P. falciparum 3D7* for mutlresistant strains (resistant to Sulfadoxin and Chloroquine, Chloroquine and Sulfadoxin added).
3) Extreme modes with added Methylene blue calculated by YANAsquare models:
    1. Table S VI.3.6: Extreme modes of *P. falciparum 3D7* for a wildtype strain (no resistances, methylene blue added).
    2. Table S VI.3.7: Extreme modes of *P. falciparum 3D7* for less active DHF and DHPS and added Methylene blue (Chloroquine resistant, Sulfadoxin and Methylene blue added).
    3. Table S VI.3.8: Extreme modes of *P. falciparum 3D7* for less active ferrochelatase and added Methylene blue (Sulfadoxin resistant, Chloroquine and Methylene blue added).
    4. Table S VI.3.9: Extreme modes of *P. falciparum 3D7* for mutlresistant strains and added Methylene blue (resistant to Sulfadoxin and Chloroquine, Chloroquine, Sulfadoxin and Methylene blue added).
4) Changes of pathway activities in Chloroquine/Sulfadoxine resistant strains:
    1. Table S VI.3.10: Comparison of pathway activities in Chloroquine/Sulfadoxin resistant strains.
    2. Table S VI.3.11: Comparison of pathway activities in Chloroquine/Sulfadoxin resistant strains with Methylene blue added.
    3. Table S VI.3.12: Comparison of the Wildtype strains with and without added Methylene blue.

1: Full list of enzymes of YANAsquare modes:

Table S VI.3.1: List of enzmyes used to build metabolic web for *P. falciparum 3D7.*

Enzyme name	reversible?	Reaction equation
1-cysPeroxiredoxin	true	2 GSH + ROOH = GSSG + H2O + ROH
1-cysteine-Glutaredoxin	true	GSH + Protein-SSG = GSSG + Protein-SH
1cys-glutaredoxin-like-protein1_EC:1.11.1.15	true	2 GSH + ROOH = GSSG + H2O + ROH
2-cys-Peroxiredoxin_EC:1.11.1.15_r2	true	ROOH + Trx(SH)2 = H2O + ROH + TrxS2
6-P-delta-Lactonase_EC:3.1.1.31	true	D-Glucono-15-lactone6-phosphate + H2O = 6-Phospho-D-gluconate
6-Phosphogluconatedehydrogenase_rn:R01528	false	6-Phospho-D-gluconate + NADP+ = CO2 + D-Ribulose5-phosphate + H+ + NADPH
Aldehyde_reductase_EC:1.1.1.21	false	Lactaldehyde + NAD+ = H+ + Methylglyoxal + NADH
Aldolase_EC:4.1.2.13_rn:R01070	true	beta-D-Fructose16-bisphosphate = D-Glyceraldehyde3-phosphate + Glyceronephosphate
Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066	true	2-Deoxy-D-ribose5-phosphate = Acetaldehyde + D-Glyceraldehyde3-phosphate
DHF_reducatse_EC:1.5.1.3_01x_rn:R00936	false	NAD+ + Tetrahydrofolate = Dihydrofolate + H+ + NADH
DHF_reducatse_EC:1.5.1.3_01x_rn:R00937	false	Folate + H+ + NADH = NAD+ + Tetrahydrofolate
DHF_reducatse_EC:1.5.1.3_01x_rn:R00939	false	Dihydrofolate + H+ + NADPH = NADP+ + Tetrahydrofolate
DHF_reducatse_EC:1.5.1.3_01x_rn:R00940	false	Folate + H+ + NADPH = NADP+ + Tetrahydrofolate
DHF_reducatse_EC:1.5.1.3_01x_rn:R02235	false	Folate + H+ + NADH = Dihydrofolate + NAD+
DHF_reducatse_EC:1.5.1.3_01x_rn:R02236	false	Folate + H+ + NADPH = Dihydrofolate + NADP+
DHPS_EC:2.5.1.15-rn:R03066	false	2-Amino-4-hydroxy-6-hydroxymethyl-78-dihydropteridine + ATP = AMP + Dihydropteroate
DHPS_EC:2.5.1.15-rn:R03067	false	2-Amino-78-dihydro-4-hydroxy-6-(diphosphooxymethyl)pteridine + 4-Aminobenzoate = Dihydropteroate + Diphosphate
Dihydrofolate_syntethase_EC:6.3.2.12-rn:R02237	false	ATP + Dihydropteroate + L-Glutamate = ADP + Dihydrofolate + Orthophosphate
Dihydroneopterin_aldolase_EC:4.1.2.25-rn:n/a	false	Dihydroneopterine + H2O = 2-Amino-4-hydroxy-6-hydroxymethyl-78-dihydropteridine + Orthophosphate
Enolase_EC:4.2.1.11_rn:R00658	true	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate
Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736	false	NADP+ + beta-D-Glucose6-phosphate = D-Glucono-15-lactone6-phosphate + H+ + NADPH
Glucose-Transporter	true	alpha-D-Glucose_ex = alpha-D-Glucose
Glutaredoxin2	true	2 GSH + ProteinS2 = GSSG + Protein(SH)2
Glutaredoxin3	true	2 GSH + ROOH = GSSG + H2O + ROH
Glutaredoxin4	true	2 GSH + Ribonucleotide-reductase-ox = GSSG + Ribunocleotide-reductase-red
Glutaredoxin5	true	GSH + ProteinSOH = H2O + Protein-SSG
Glutaredoxin6	true	ProteinS2 + Trx(SH)2 = Protein(SH)2 + TrxS2
Glutathion-peroxidase-like-Tpx_EC:1.11.1.9	true	2 ROOH + Trx(SH)2 = 2 H2O + ROH + TrxS2
Glutathion-S-Transferase2_EC:2.5.1.18	true	GSH + RX = HX + R-S-Glutathione
Glutathion-Synthase_EC:6.3.2.3	false	ATP + Glycine + gamma-L-Glutamyl-L-Cysteine = ADP + GSH + P

Glutathionereductase_EC:1.8.1.7_rn:00115	true	GSSG + H+ + NADPH = 2 GSH + NADP+
Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061	true	D-Glyceraldehyde3-phosphate + NAD+ + Orthophosphate = 3-Phospho-D-glyceroylphosphate + H+ + NADH
Glycinhydroymethyltransferase	true	L-Serine + Tetrahydrofolate = 510-Methylenetetrahydrofolate + Glycine + H2O
GlyoxalaseI_EC:4.4.1.5	false	GSH + Methylglyoxal = (R)-S-Lactoylglutathione + H2O
GlyoxalaseII_EC:3.1.2.6	false	(R)-S-Lactoylglutathione + H2O = GSH + R-Lactate
GTP_hydroalse_EC:3.5.4.16_01x-rn:R00428	false	GTP + H2O = Formamidopyrimidinenucleosidetriphosphate
GTP_hydroalse_EC:3.5.4.16_01x-rn:R04639	false	25-Diamino-6-(5-triphosphoryl-34-trihydroxy-2-oxopentyl)-amino-4-oxopyrimidine + H2O = 2-Amino-4-hydroxy-6-(erythro-123-trihydroxypropyl)dihydropteridinetriphosphate
GTP_hydroalse_EC:3.5.4.16_01x-rn:R05046	false	Formamidopyrimidinenucleosidetriphosphate + H2O = 25-Diaminopyrimidinenucleosidetriphosphate + Formate
GTP_hydroalse_EC:3.5.4.16_01x-rn:R05048	false	25-Diaminopyrimidinenucleosidetriphosphate = 25-Diamino-6-(5-triphosphoryl-34-trihydroxy-2-oxopentyl)-amino-4-oxopyrimidine
Hexokinase_2.7.1.1_rn:R01600	false	ATP + beta-D-Glucose = ADP + beta-D-Glucose6-phosphate
Hexokinase_2.7.1.1_rn:R01786	false	ATP + alpha-D-Glucose = ADP + alpha-D-Glucose6-phosphate
L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2	false	ATP + L-Cysteine + L-Glutamat = ADP + P + gamma-L-Glutamyl-L-Cysteine
Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703	true	H+ + NADH + Pyruvate = (S)-Lactate + NAD+
Monocarboxylate-Transporter	true	(S)-Lactate = (S)-Lactate_ex
MRP	false	ATP + GSH = ADP + GSHex + P
MRP-and/or_GSSG-Pumps	false	ATP + GSSG = ADP + GSSG_ex + P
One-carbon-pool_rn:R00945	true	L-Serine + Tetrahydrofolate = 510-Methylenetetrahydrofolate + Glycine + H2O
One-carbon-pool_rn:R02101	false	510-Methylenetetrahydrofolate + dUMP = Dihydrofolate + dTMP
One-carbon-pool_rn:R03940	false	10-Formyltetrahydrofolate + L-Methionyl-tRNA = N-Formylmethionyl-tRNA + Tetrahydrofolate
One-carbon-pool_rn:R04125	false	S-Aminomethyldihydrolipoylprotein + Tetrahydrofolate = 510-Methylenetetrahydrofolate + Dihydrolipoylprotein + NH3
Phosphofructokinase_EC:2.7.1.11_rn:R04779	false	ATP + beta-D-Fructose6-phosphate = ADP + beta-D-Fructose16-bisphosphate
Phosphoglucomustase_EC:5.4.2.2_rn:R01057	true	alpha-D-Ribose1-phosphate = D-Ribose5-phosphate
Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512	true	3-Phospho-D-glyceroylphosphate + ADP = 3-Phospho-D-glycerate + ATP
Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518	true	3-Phospho-D-glycerate = 2-Phospho-D-glycerate
Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739	true	alpha-D-Glucose6-phosphate = beta-D-Glucose6-phosphate
Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740	true	alpha-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321	true	beta-D-Glucose6-phosphate = beta-D-Fructose6-phosphate
Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015	true	D-Glyceraldehyde3-phosphate = Glyceronephosphate
Porphyrine_EC:1.3.3.3	false	CoproporphyrinogenIII + O2 = 2 CO2 + 2 H2O + Protoporpyhrinogen
Porphyrine_EC:1.3.3.4	false	3 O2 + 2 Protoporpyhrinogen = 6 H2O + 2 Protoporphyrin
Porphyrine_EC:2.3.1.37	false	Glycine + Succinyl-CoA = 5-Aminolevulinate + CO2 + CoA
Porphyrine_EC:2.5.1.-	false	Heme = HemeO

Porphyrine_EC:2.5.1.61	false	H2O + 4 Porphobilinogen = Hydroxymethylbilane + 4 NH3
Porphyrine_EC:4.1.1.37	false	UroporphyrinogenI = 4 CO2 + CoproporphyrinogenI
Porphyrine_EC:4.1.1.37_2	false	UroporphyrinogenIII = 4 CO2 + CoproporphyrinogenIII
Porphyrine_EC:4.2.1.24	false	5-Aminolevulinate = 2 H2O + Porphobilinogen
Porphyrine_EC:4.2.1.75	false	Hydroxymethylbilane = H2O + UroporphyrinogenIII
Porphyrine_EC:4.4.1.17	false	Apocytochromec + Heme = Cytochromec
Porphyrine_EC:4.99.1.1	false	Fe2+ + Protoporphyrin = 2 H+ + Heme
Porphyrine_EC:COX15	false	HemeO = HemeA
Porphyrine_EC:spontan	false	Hydroxymethylbilane = UroporphyrinogenI
Pyruvate_kinase_EC:2.7.1.40_rn:R00200	false	ADP + Phosphoenolpyruvate = ATP + Pyruvate
Ribonucleotide-Reductase_EC:1.17.4.1_R04294	true	2-desoxyribonucleoside-diphosphat + H2O + Ribonucleotide-reductase-ox + Thioredoxindisulfide = Ribunocleotide-reductase-red + Thioredoxin + ribonucleoside-disphosphat
Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017	true	H2O + Ribonucleotide-reductase-ox + Thioredoxindisulfide + dADP = ADP + Ribunocleotide-reductase-red + Thioredoxin
Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018	true	H2O + Ribonucleotide-reductase-ox + Thioredoxindisulfide + dUDP = Ribunocleotide-reductase-red + Thioredoxin + UDP
Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019	true	H2O + Ribonucleotide-reductase-ox + Thioredoxindisulfide + dGDP = GDP + Ribunocleotide-reductase-red + Thioredoxin
Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024	true	H2O + Ribonucleotide-reductase-ox + Thioredoxindisulfide + dCDP = CDP + Ribunocleotide-reductase-red + Thioredoxin
Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049	false	ATP + D-Ribose5-phosphate = 5-Phospho-alpha-D-ribose1-diphosphate + AMP
Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056	true	D-Ribose5-phosphate = D-Ribulose5-phosphate
Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529	true	D-Ribulose5-phosphate = D-Xylulose5-phosphate
spontan	false	D-Glyceraldehyde3-phosphate = Methylglyoxal + P
spontan2	false	Glyceronephosphate = Methylglyoxal + P
Superoxide-dismutase_EC:1.15.1.1	false	2 H+ + 2 O2- = H2O2 + O2
Thioredoxin	true	FADH2 + ProteinS2 = FAD + Protein(SH)2
Thioredoxin-depPeroxidase	true	Protein-O- + Thioredoxin = H2O + Protein + Thioredoxindisulfide
Thioredoxin2	true	GSSG + Trx(SH)2 = 2 GSH + TrxS2
Thioredoxinreductase_EC:1.6.4.5.	false	H+ + NADPH + TrxS2 = NADP+ + Trx(SH)2
Transketolase_EC:2.2.1.1_rn:R01641	true	D-Ribose5-phosphate + D-Xylulose5-phosphate = D-Glyceraldehyde3-phosphate + D-Sedoheptulose7-phosphate
Transketolase_EC:2.2.1.1_rn:R01830	true	D-Glyceraldehyde3-phosphate + beta-D-Fructose6-phosphate = D-Erythrose4-phosphate + D-Xylulose5-phosphate
triphosphate_lyase_EC:4.2.3.12-rn:R04286	false	2-Amino-4-hydroxy-6-(erythro-123-trihydroxypropyl)dihydropteridinetriphosphate + 2 H2O = 6-Pyruvoyltetrahydropterin + Triphosphate
triphosphate_phosphohydrolase_EC:3.1.3.1_rn:R04620	false	2-Amino-4-hydroxy-6-(erythro-123-trihydroxypropyl)dihydropteridinetriphosphate + 3 H2O = Dihydroneopterine + 3 Orthophosphate

2: Extreme modes calculated by YANAsquare models

Table S VI.3.2: Extreme modes of *P. falciparum 3D7* for a wildtype strain (no resistances, no compounds added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0,03550214	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0,18927750	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0,24827750	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0,12242836	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0,05332433	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0,21577177	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0,35187177	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0,13847177	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0,05332433	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0,13847177	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0,57607120	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0,05332433	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0,05332433	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	0,02767480	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0,13847177	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0,14189903	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0,14112955	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0,17966192	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0,11928531	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0,10219637	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)

21	0,14100070	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0,09630498	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0,15464255	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0,10150761	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0,00000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0,19287431	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0,14112955	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0,00000000	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0,07247485	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0,00000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0,00000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0,00000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0,02733251	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0,02895586	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1

					Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0,28335771	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.3: Extreme modes of *P. falciparum 3D7* for less active DHF and DHPS (Chloroquine resistant, Sulfadoxin added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.004165815	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0.180262233	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0.239262169	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0.103040009	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0.054126352	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0.224549750	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.360649601	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0.147249834	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0.054126352	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0.147249834	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0.509545893	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0.054126352	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0.054126352	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	-0.115070754	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0.147249834	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0.078911521	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.132262225	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0.170683240	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0.096690900	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.122356648	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.141054461	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)

22	0.135861652	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0.100397666	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.144504901	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.000000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.192916676	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.132262225	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.000000000	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.067293057	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.000000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.000000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.000000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.023118816	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.000000000	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-

35	0.158425136	7	false	7	Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.4: Extreme modes of *P. falciparum 3D7* for less active ferrochelatase (Sulfadoxin resistant, Chloroquine added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.01107674	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0.17461941	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0.23361941	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0.07739945	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0.05463234	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0.23049611	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.36659613	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0.15319611	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0.05463234	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0.15319611	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0.60540687	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0.05463234	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0.05463234	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	0.04239609	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0.15319611	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0.14807101	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.12632956	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0.18053624	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0.09472815	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1

					Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.11093138	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.14099469	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0.02300644	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0.20981061	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.09053873	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.00000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.19306453	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.12632956	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.38889148	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.12087227	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.00000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.00000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.02399060	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.00000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2

					Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.00681835	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0.20008914	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.5: Extreme modes of *P. falciparum 3D7* for mutlresistant strains (resistant to Sulfadoxin and Chloroquine, Chloroquine, Sulfadoxin and methyleine blue added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.013981991	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0.161130841	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0.220130969	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	-0.108441632	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0.055877240	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0.243857043	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.379957338	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0.166556876	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0.055877240	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0.166556876	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0.566519587	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0.055877240	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0.055877240	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	-0.095919650	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0.166556876	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0.148983275	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.113048484	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

18	0.180699041	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0.142813939	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.109719497	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.140891848	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0.021482206	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0.204131870	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.093981883	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.000000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.192968332	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.113048484	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.381630913	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.078878107	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.000000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.000000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.000000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8

					Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.024497192	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.008718887	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0.193498730	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

3: Extreme modes with added Methylene blue calculated by YANAsquare models:

Table S VI.3.6: Extreme modes of *P. falciparum 3D7* for a wildtype strain (no resistances, methylene blue added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0,03415607	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0,16843896	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0,11743894	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0,15070773	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0,05314473	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0,10707029	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0,22619036	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0,13669031	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0,05314473	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0,13669031	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0,45818687	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0,05314473	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0,05314473	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	0,04829026	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0,13669031	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	0,03022726	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0,12055349	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0,17932449	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0,08158773	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0,08830794	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)

21	0,14097235	1 false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0,01934514	7 false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0,14896761	18 false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0,08502037	16 false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0,04974439	8 false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0,15315625	3 false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0,12055349	6 false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0,00000000	6 false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0,05172020	6 false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0,00000000	9 false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0,00000000	39 false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0,00000000	83 false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0,02822463	83 false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0,01911563	7 false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1

					Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0,28090636	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.7: Extreme modes of *P. falciparum 3D7* for less active DHF and DHPS and added Methylene blue (Chloroquine resistant, Sulfadoxin and Methylene blue added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.003705426	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0.149361218	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0.098361138	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0.104657833	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	-0.056415281	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0.126174031	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.245294218	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0.155794078	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	-0.056415281	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0.155794078	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0.352528658	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	-0.056415281	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	-0.056415281	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	0.067393939	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0.155794078	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0.082763049	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.101381174	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0.162657571	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)

19	0.098216298	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.123514449	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.140921560	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0.067778062	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0.104497504	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.142020949	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.000000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.186286383	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.101381174	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.000000000	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.067597773	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.000000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.000000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.000000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.023006859	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8

					Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.000000000	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0.155981439	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.8: Extreme modes of *P. falciparum 3D7* for less active ferrochelatase and added Methylene blue (Sulfadoxin resistant, Chloroquine and Methylene blue added.

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.007981358	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	0.171036125	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	0.120036123	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	0.160669895	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0.052926801	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	0.104625852	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.223745857	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	0.134245853	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0.052926801	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	0.134245853	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	0.156853481	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0.052926801	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0.052926801	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	-0.105908604	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	0.134245853	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	-0.140226218	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.123108687	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0.170898526	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0.117972578	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.086218620	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.140997978	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)

22	0.000000000	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.)
23	0.206731012	18	false	13	(1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.115753221	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.000000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.186355577	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.123108687	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.379371542	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.064238597	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.000000000	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.000000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.024073026	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.000000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.000000000	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-

					Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)
35	0.198307345	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

Table S VI.3.9: Extreme modes of *P. falciparum 3D7* for mutlresistant strains and added Methylene blue (Chloroquine and Sulfadoxin resistant, Chloroqune, Sulfadoxin and Methylene blue added).

#	Activity	Flux sum	Reversible?	Pathlength	Reactions
1	0.01441165	2	true	2	(-1 Glycinhydroymethyltransferase) (1 One-carbon-pool_rn:R00945)
2	-0.17549682	3	true	3	(1 2-cys-Peroxiredoxin_EC:1.11.1.15_r2) (-1 Glutaredoxin6) (1 Thioredoxin)
3	-0.12454966	3	true	3	(-1 Glutaredoxin6) (1 Glutathion-peroxidase-like-Tpx_EC:1.11.1.9) (1 Thioredoxin)
4	-0.06292834	3	true	3	(-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R03321)
5	0.05879846	2	true	2	(1 Ribonucleotide-Reductase_EC:1.17.4.1_R04294) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017)
6	-0.10010707	4	true	4	(-1 1cys-glutaredoxin-like-protein1_EC:1.11.1.15) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
7	0.28805035	4	true	4	(-1 1-cysPeroxiredoxin) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
8	-0.12969505	4	true	4	(-1 Glutaredoxin3) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
9	0.05879846	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02024)
10	-0.12969505	5	true	5	(-1 Glutaredoxin2) (1 Glutaredoxin4) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin) (-1 Thioredoxin-depPeroxidase)
11	-0.49878081	6	true	6	(-1 Glutaredoxin4) (1 Glutaredoxin6) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (-1 Thioredoxin2)
12	0.05879846	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02018)
13	0.05879846	2	true	2	(-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02019)
14	-0.04138897	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutathion-S-Transferase2_EC:2.5.1.18) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
15	-0.12969505	5	true	5	(-1 1-cysteine-Glutaredoxin) (1 Glutaredoxin4) (-1 Glutaredoxin5) (-1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin-depPeroxidase)
16	0.09069177	6	true	5	(1 Desoxyribosephosphataldolase_EC:4.1.2.4_rn:R01066) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-1 Transketolase_EC:2.2.1.1_rn:R01641)
17	0.05863309	5	false	5	(1 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
18	0.17072246	12	false	11	(1 Enolase_EC:4.2.1.11_rn:R00658) (1 Glyceraldehyde-3P-dehydroase_EC:1.2.1.12_rn:R01061) (1 Lactate_dehydrogenase_EC:1.1.1.27_rn:R00703) (1 Monocarboxylate-Transporter) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphoglycerate-kinase_EC:2.7.2.3_rn:R01512) (1 Phosphoglycerate_mutase_EC:5.4.2.1_rn:R01518) (1 Pyruvate_kinase_EC:2.7.1.40_rn:R00200) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 Transketolase_EC:2.2.1.1_rn:R01641)
19	0.10431479	6	false	6	(1 Hexokinase_2.7.1.1_rn:R01600) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
20	0.08565630	2	false	2	(1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-P-pyrophosphokinase_EC:2.7.6.1_rn:R01049)
21	0.14102903	1	false	1	(1 Superoxide-dismutase_EC:1.15.1.1)
22	0.00000000	7	false	7	(-1 Glutaredoxin4) (1 Glutaredoxin6) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-

23	0.22160177	18	false	13	Reductase_EC:1.17.4.1_rn:R02017) (-1 Thioredoxin) (1 Thioredoxin-depPeroxidase) (1 Thioredoxinreductase_EC:1.6.4.5.) (1 6-P-delta-Lactonase_EC:3.1.1.31) (1 6-Phosphogluconatedehydrogenase_rn:R01528) (1 Glucose-6-phosphate1-dehydrg.EC:1.1.1.49_rn:R02736) (2 Glutaredoxin4) (2 Glutathionereductase_EC:1.8.1.7_rn:00115) (-2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02739) (-1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (-2 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (-1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Thioredoxin-depPeroxidase) (-1 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
24	0.05909384	16	false	8	(1 Aldolase_EC:4.1.2.13_rn:R01070) (1 Phosphofructokinase_EC:2.7.1.11_rn:R04779) (-5 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (-1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (-2 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (-2 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (-3 Transketolase_EC:2.2.1.1_rn:R01641) (-1 Transketolase_EC:2.2.1.1_rn:R01830)
25	0.00000000	8	false	7	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan) (1 Transketolase_EC:2.2.1.1_rn:R01641)
26	0.10850367	3	false	3	(1 Aldehyde_reductase_EC:1.1.1.21) (1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6)
27	0.05863309	6	false	5	(2 1-cysteine-Glutaredoxin) (-1 Glutaredoxin4) (1 MRP-and/or_GSSG-Pumps) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
28	0.36747103	6	false	6	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00936) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)
29	0.05430869	6	false	6	(1 Glucose-Transporter) (1 Hexokinase_2.7.1.1_rn:R01786) (1 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphohexoseisomerase_EC:5.3.1.9_rn:R02740) (1 Transketolase_EC:2.2.1.1_rn:R01641) (1 Transketolase_EC:2.2.1.1_rn:R01830)
30	0.11664678	9	false	8	(1 GlyoxalaseI_EC:4.4.1.5) (1 GlyoxalaseII_EC:3.1.2.6) (2 Phosphoglucomustase_EC:5.4.2.2_rn:R01057) (1 Phosphotrioseisomerase_EC:5.3.1.1_rn:R01015) (1 Ribose-Phosphat-Isomerase_EC:5.3.1.6_rn:R01056) (1 Ribulose-P-3-Epimerase_EC:5.1.3.1_rn:R01529) (1 spontan2) (1 Transketolase_EC:2.2.1.1_rn:R01641)
31	0.00000000	39	false	12	(4 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-4 Glutaredoxin4) (-4 Glutathionereductase_EC:1.8.1.7_rn:00115) (4 Glycinhydroymethyltransferase) (4 One-carbon-pool_rn:R02101) (4 Porphyrine_EC:2.3.1.37) (1 Porphyrine_EC:2.5.1.61) (1 Porphyrine_EC:4.1.1.37) (4 Porphyrine_EC:4.2.1.24) (1 Porphyrine_EC:spontan) (4 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (4 Thioredoxin-depPeroxidase)
32	0.00000000	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1-Fe2+accumulation) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
33	0.02408068	83	false	15	(8 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-8 Glutaredoxin4) (-8 Glutathionereductase_EC:1.8.1.7_rn:00115) (8 Glycinhydroymethyltransferase) (8 One-carbon-pool_rn:R02101) (2 Porphyrine_EC:1.3.3.3) (1 Porphyrine_EC:1.3.3.4) (8 Porphyrine_EC:2.3.1.37) (2 Porphyrine_EC:2.5.1.61) (2 Porphyrine_EC:4.1.1.37_2) (8 Porphyrine_EC:4.2.1.24) (2 Porphyrine_EC:4.2.1.75) (2 Porphyrine_EC:4.99.1.1) (8 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (8 Thioredoxin-depPeroxidase)
34	0.01260773	7	false	7	(-1 1-cysteine-Glutaredoxin) (1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (1 Glutathion-Synthase_EC:6.3.2.3) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 Glycinhydroymethyltransferase) (1 L-Gluthamat-L-cysteine-Synthase_EC:6.3.2.2) (1 One-carbon-pool_rn:R02101)

35	0.18607812	7	false	7	(1 DHF_reducatse_EC:1.5.1.3_01x_rn:R00939) (-1 Glutaredoxin4) (-1 Glutathionereductase_EC:1.8.1.7_rn:00115) (1 One-carbon-pool_rn:R02101) (1 One-carbon-pool_rn:R04125) (1 Ribonucleotide-Reductase_EC:1.17.4.1_rn:R02017) (1 Thioredoxin-depPeroxidase)

4: Changes of pathway activities in Chloroquine and Sulfadoxin resistant strains:

Table S VI.3.10: Comparison of pathway activities in Chloroquine/Sulfadoxin resistant strains.

Extreme Mode #	WT no compounds added Activity	Chloroquine resistant Activity	Sulfadoxine resistant Activity
1	0,03550214	0,00416582	0,01107674
2	0,18927750	0,18026223	0,17461941
3	0,24827750	0,23926217	0,23361941
4	0,12242836	0,10304001	0,07739945
5	0,05332433	0,05412635	0,05463234
6	0,21577177	0,22454975	0,23049611
7	0,35187177	0,36064960	0,36659613
8	0,13847177	0,14724983	0,15319611
9	0,05332433	0,05412635	0,05463234
10	0,13847177	0,14724983	0,15319611
11	0,57607120	0,50954589	0,60540687
12	0,05332433	0,05412635	0,05463234
13	0,05332433	0,05412635	0,05463234
14	0,02767480	-0,11507075	0,04239609
15	0,13847177	0,14724983	0,15319611
16	-0,14189903	-0,07891152	-0,14807101
17	0,14112955	0,13226223	0,12632956
18	0,17966192	0,17068324	0,18053624
19	0,11928531	0,09669090	0,09472815
20	0,10219637	0,12235665	0,11093138
21	0,14100070	0,14105446	0,14099469
22	0,09630498	0,13586165	0,02300644
23	0,15464255	0,10039767	0,20981061
24	0,10150761	0,14450490	0,09053873
25	0,00000000	0,00000000	0,00000000
26	0,19287431	0,19291668	0,19306453
27	0,14112955	0,13226223	0,12632956
28	0,00000000	0,00000000	0,38889148
29	0,07247485	0,06729306	0,12087227
30	0,00000000	0,00000000	0,00000000
31	0,00000000	0,00000000	0,00000000
32	0,00000000	0,00000000	0,02399060
33	0,02733251	0,02311882	0,00000000
34	0,02895586	0,00000000	0,00681835
35	0,28335771	0,15842514	0,20008914

Table S VI.3.11: Comparison of pathway activities in Chloroquine/Sulfadoxin resistant strains with Methylene blue added.

Extreme Mode #	WT methylene blue added Activity	Chloroquine resistant, MB added Activity	Sulfadoxine resistant, MB added Activity
1	0,03415607	0,00370543	0,00798136
2	0,16843896	0,14936122	0,17103613
3	0,11743894	0,09836114	0,12003612
4	0,15070773	0,10465783	0,16066990
5	0,05314473	-0,05641528	0,05292680
6	0,10707029	0,12617403	0,10462585
7	0,22619036	0,24529422	0,22374586
8	0,13669031	0,15579408	0,13424585
9	0,05314473	-0,05641528	0,05292680
10	0,13669031	0,15579408	0,13424585
11	0,45818687	0,35252866	0,15685348
12	0,05314473	-0,05641528	0,05292680
13	0,05314473	-0,05641528	0,05292680
14	0,04829026	0,06739394	-0,10590860
15	0,13669031	0,15579408	0,13424585
16	0,03022726	-0,08276305	-0,14022622
17	0,12055349	0,10138117	0,12310869
18	0,17932449	0,16265757	0,17089853
19	0,08158773	0,09821630	0,11797258
20	0,08830794	0,12351445	0,08621862
21	0,14097235	0,14092156	0,14099798
22	0,01934514	0,06777806	0,00000000
23	0,14896761	0,10449750	0,20673101
24	0,08502037	0,14202095	0,11575322
25	0,04974439	0,00000000	0,00000000
26	0,15315625	0,18628638	0,18635558
27	0,12055349	0,10138117	0,12310869
28	0,00000000	0,00000000	0,37937154
29	0,05172020	0,06759777	0,06423860
30	0,00000000	0,00000000	0,00000000
31	0,00000000	0,00000000	0,00000000
32	0,00000000	0,00000000	0,02407303
33	0,02822463	0,02300686	0,00000000
34	0,01911563	0,00000000	0,00000000
35	0,28090636	0,15598144	0,19830735

Table S VI.3.12: Comparison of the Wildtype strains with and without added Methylene blue.

Extreme Mode #	WT methylene blue added Activity	WT no compounds added Activity	Change enzyme flux [%]: No compounds vs MB added	Abbreviations[1]
1	0,03415607	0,03550214	-0,13	FS
2	0,16843896	0,18927750	-2,08	PP
3	0,11743894	0,24827750	-13,08	PP
4	0,15070773	0,12242836	2,83	CK
5	0,05314473	0,05332433	-0,02	DP
6	0,10707029	0,21577177	-10,87	PP
7	0,22619036	0,35187177	-12,57	PP
8	0,13669031	0,13847177	-0,18	PP
9	0,05314473	0,05332433	-0,02	DP
10	0,13669031	0,13847177	-0,18	PP
11	0,45818687	0,57607120	-11,79	PP
12	0,05314473	0,05332433	-0,02	DP
13	0,05314473	0,05332433	-0,02	DP
14	0,04829026	0,02767480	2,06	PP
15	0,13669031	0,13847177	-0,18	PP
16	0,03022726	-0,14189903	-17,21	RNM
17	0,12055349	0,14112955	-2,06	PP
18	0,17932449	0,17966192	-0,03	GK
19	0,08158773	0,11928531	-3,77	RNM
20	0,08830794	0,10219637	-1,39	RNM
21	0,14097235	0,14100070	0,00	SoP
22	0,01934514	0,09630498	-7,70	PP
23	0,14896761	0,15464255	-0,57	GK
24	0,08502037	0,10150761	-1,65	GK
25	0,04974439	0,00000000	4,97	GK
26	0,15315625	0,19287431	-3,97	LP
27	0,12055349	0,14112955	-2,06	PP
28	0,00000000	0,00000000	0,00	PPuG
29	0,05172020	0,07247485	-2,08	GK
30	0,00000000	0,00000000	0,00	GK
31	0,00000000	0,00000000	0,00	HeP
32	0,00000000	0,00000000	0,00	HeP
33	0,02822463	0,02733251	0,09	HeP
34	0,01911563	0,02895586	-0,98	GP
35	0,28090636	0,28335771	-0,25	PP

[1] Abbreviations: Folate synthesis (FS); Protein Protection (PP); Conversion of ketosugars (CK); Desoxyribunucleotide production (DP); Ribosephosphate for nucleotide metabolism (RNM); Generation of ketosugars (GK); Superoxide protection (SoP); Lactacte production (LP); PP using glutathionreductase (PpuG); Heme protection (HeP); Glutathion production (GP).