

Table 1: Reduced phagosome network - metabolites

Name	internal?	Connectivity
AA	false	1
Ac-sph	true	2
Actin	false	2
Actinpoly	false	2
ADP	true	7
ATP	true	7
CDP-cholin	false	2
CDP-DAG	true	2
cholin	true	3
cholinP	true	4
CMP	false	2
CTP	false	2
DAG	true	7
DAG-3P	false	1
ERM	true	2
ERM-PIP2	false	1
Ezrin	false	1
fatac	false	3
IcP	false	1
inositol	false	1
inositolTP	false	1
monoAGcholinP	true	2
P	false	2
PA	false	3
PC	false	4
PI	false	3
PIP	true	2
PIP2	true	3
PPi	false	2
S-1-P	false	1
sph	false	2
Sphmy	false	1
TAG	false	1
TM	false	1

Table 2: Reduced phagosome network - reactions

Enzyme name	reversible?	Reaction equation
Actindepoly	false	Actinpoly = 2 Actin
Actinnucl	false	ATP + 2 Actin = ADP + Actinpoly + P
CDPinoitra	true	CDP-DAG + inositol = CMP + PI
CDPsynth	false	CTP + PA = CDP-DAG + PPi
ceramidse	true	Ac-sph = fatac + sph
Cholinkin	true	ATP + cholin = ADP + cholinP
CholinPtf	true	CTP + cholinP = CDP-cholin + PPi
DAGchoIT	true	CMP + PC = CDP-cholin + DAG
DAGkin	true	ATP + DAG = ADP + DAG-3P
ERMfform	true	ERM + PIP2 = ERM-PIP2
ERMform	true	Ezrin + TM = ERM
Lipase	true	TAG = DAG + fatac
monoAGcholinPCtf	true	ADP + monoAGcholinP = ATP + cholin + fatac
PAP	true	PA = DAG + P
PI45diase	false	PIP2 = DAG + inositolP
PI4kin	true	ATP + PI = ADP + PIP
PI4P5kin	true	ATP + PIP = ADP + PIP2
PIdiase	false	PI = DAG + IcP
PLA2	true	PC = AA + monoAGcholinP
PLC	true	PC = DAG + cholinP
PLD	true	PC = PA + cholin
Sphmydias	true	Sphmy = Ac-sph + cholinP
SPK	true	ATP + sph = ADP + S-1-P

Table 3: Reduced phagosome network - Elementary Modes¹

#	Flux sum	Rev.?	Pathlength	Reactions	Net reaction
1	4	true	4	(-1 monoAGcholinPctf) (-1 PLA2) (1 PLD) (-1 SPK)	AA + S-1-P + fatac = PA + sph
2	2	true	2	(1 Lipase) (-1 PAP)	P + TAG = PA + fatac
3	6	true	5	(-1 ERMfform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (2 SPK)	ERM-PIP2 + 2 sph = Ezrin + PI + 2 S-1-P + TM
4	10	true	7	(-1 ERMfform) (-1 ERMform) (-2 monoAGcholinPctf) (-1 PI4kin) (-1 PI4P5kin) (-2 PLA2) (2 PLD)	2 AA + ERM-PIP2 + 2 fatac = Ezrin + 2 PA + PI + TM
5	3	true	3	(-1 DAGkin) (-1 PAP) (1 SPK)	DAG-3P + P + sph = PA + S-1-P
6	5	true	5	(1 DAGkin) (1 monoAGcholinPctf) (1 PAP) (1 PLA2) (-1 PLD)	2 PA = AA + DAG-3P + P + fatac
7	3	true	3	(-1 DAGkin) (-1 Lipase) (1 SPK)	DAG-3P + fatac + sph = S-1-P + TAG
8	5	true	5	(1 DAGkin) (1 Lipase) (1 monoAGcholinPctf) (1 PLA2) (-1 PLD)	PA + TAG = AA + DAG-3P + 2 fatac
9	8	true	6	(-2 DAGkin) (1 ERMfform) (1 ERMform) (-2 PAP) (1 PI4kin) (1 PI4P5kin)	2 DAG-3P + Ezrin + 2 P + PI + TM = ERM-PIP2 + 2 PA
10	8	true	6	(-2 DAGkin) (1 ERMfform) (1 ERMform) (-2 Lipase) (1 PI4kin) (1 PI4P5kin)	2 DAG-3P + Ezrin + PI + TM + 2 fatac = ERM-PIP2 + 2 TAG
11	2	true	2	(1 DAGcholT) (-1 PAP)	CMP + P + PC = CDP-cholin + PA
12	2	true	2	(1 DAGcholT) (-1 Lipase)	CMP + PC + fatac = CDP-cholin + TAG
13	3	true	3	(-1 DAGcholT) (-1 DAGkin) (1 SPK)	CDP-cholin + DAG-3P + sph = CMP + PC + S-1-P
14	5	true	5	(1 DAGcholT) (1 DAGkin) (1 monoAGcholinPctf) (1 PLA2) (-1 PLD)	CMP + PA + PC = AA + CDP-cholin + DAG-3P + fatac
15	8	true	6	(-2 DAGcholT) (-2 DAGkin) (1 ERMfform) (1 ERMform) (1 PI4kin) (1 PI4P5kin)	2 CDP-cholin + 2 DAG-3P + Ezrin + PI + TM = 2 CMP + ERM-PIP2 + 2 PC
16	3	true	3	(-1 CholinPtf) (1 PAP) (-1 PLC)	CDP-cholin + PA + PPi = CTP + P + PC
17	3	true	3	(-1 CholinPtf) (1 Lipase) (-1 PLC)	CDP-cholin + PPi + TAG = CTP + PC + fatac
18	4	true	4	(-1 CholinPtf) (-1 DAGkin) (-1 PLC) (1 SPK)	CDP-cholin + DAG-3P + PPi + sph = CTP + PC + S-1-P
19	6	true	6	(-1 CholinPtf) (-1 DAGkin) (-1 monoAGcholinPctf) (-1 PLA2) (-1 PLC) (1 PLD)	AA + CDP-cholin + DAG-3P + PPi + fatac = CTP + PA + PC
20	10	true	7	(2 CholinPtf) (2 DAGkin) (-1 ERMfform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (2 PLC)	2 CTP + ERM-PIP2 + 2 PC = 2 CDP-cholin + 2 DAG-3P + Ezrin + PI + 2 PPi + TM
21	3	true	3	(-1 CholinPtf) (1 DAGcholT) (-1 PLC)	CMP + PPi = CTP
22	5	true	5	(-1 Cholinkin) (-1 PAP) (1 PLC) (-1 PLD) (1 SPK)	P + sph = S-1-P
23	5	true	5	(-1 Cholinkin) (-1 monoAGcholinPctf) (-1 PAP) (-1 PLA2) (1 PLC)	AA + P + fatac = PA
24	5	true	5	(-1 Cholinkin) (-1 Lipase) (1 PLC) (-1 PLD) (1 SPK)	PA + fatac + sph = S-1-P + TAG

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25	5	true	5	(-1 Cholin) (-1 Lipase) (-1 monoAGcholinPctf) (-1 PLA2) (1 PLC)	AA + 2 fatic = TAG
26	12	true	8	(2 Cholin) (-1 ERMform) (-1 ERMform) (2 PAP) (-1 PI4kin) (-1 PI4P5kin) (-2 PLC) (2 PLD)	ERM-PIP2 = Ezrin + 2 P + PI + TM
27	12	true	8	(2 Cholin) (-1 ERMform) (-1 ERMform) (2 Lipase) (-1 PI4kin) (-1 PI4P5kin) (-2 PLC) (2 PLD)	ERM-PIP2 + 2 TAG = Ezrin + 2 PA + PI + TM + 2 fatic
28	4	true	4	(-1 Cholin) (1 DAGkin) (1 PLC) (-1 PLD)	PA = DAG-3P
29	6	true	6	(-1 Cholin) (1 DAGkin) (-1 monoAGcholinPctf) (-1 PLA2) (1 PLC) (-1 SPK)	AA + S-1-P + fatic = DAG-3P + sph
30	14	true	9	(-2 Cholin) (2 DAGkin) (-1 ERMform) (-1 ERMform) (-2 monoAGcholinPctf) (-1 PI4kin) (-1 PI4P5kin) (-2 PLA2) (2 PLC)	2 AA + ERM-PIP2 + 2 fatic = 2 DAG-3P + Ezrin + PI + TM
31	5	true	5	(-1 Cholin) (-1 DAGcholT) (1 PLC) (-1 PLD) (1 SPK)	CDP-cholin + PA + sph = CMP + PC + S-1-P
32	5	true	5	(-1 Cholin) (-1 DAGcholT) (-1 monoAGcholinPctf) (-1 PLA2) (1 PLC)	AA + CDP-cholin + fatic = CMP + PC
33	12	true	8	(2 Cholin) (2 DAGcholT) (-1 ERMform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (-2 PLC) (2 PLD)	2 CMP + ERM-PIP2 + 2 PC = 2 CDP-cholin + Ezrin + 2 PA + PI + TM
34	4	true	4	(-1 Cholin) (-1 CholinPtf) (-1 PLD) (1 SPK)	CDP-cholin + PA + PPI + sph = CTP + PC + S-1-P
35	4	true	4	(-1 Cholin) (-1 CholinPtf) (-1 monoAGcholinPctf) (-1 PLA2)	AA + CDP-cholin + PPI + fatic = CTP + PC
36	10	true	7	(2 Cholin) (2 CholinPtf) (-1 ERMform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (2 PLD)	2 CTP + ERM-PIP2 + 2 PC = 2 CDP-cholin + Ezrin + 2 PA + PI + 2 PPI + TM
37	5	true	5	(1 Cholin) (1 CholinPtf) (-1 DAGkin) (-1 PAP) (1 PLD)	CTP + DAG-3P + P + PC = CDP-cholin + 2 PA + PPI
38	5	true	5	(1 Cholin) (1 CholinPtf) (-1 DAGkin) (-1 Lipase) (1 PLD)	CTP + DAG-3P + PC + fatic = CDP-cholin + PA + PPI + TAG
39	5	true	5	(1 Cholin) (1 CholinPtf) (-1 DAGcholT) (-1 DAGkin) (1 PLD)	CTP + DAG-3P = CMP + PA + PPI
40	4	true	4	(-1 ceramide) (-1 PAP) (1 PLC) (-1 Sphmydias)	P + PC + fatic + sph = PA + Sphmy
41	4	true	4	(-1 ceramide) (-1 Lipase) (1 PLC) (-1 Sphmydias)	PC + 2 fatic + sph = Sphmy + TAG
42	5	true	5	(-1 ceramide) (1 DAGkin) (1 PLC) (-1 Sphmydias) (-1 SPK)	PC + S-1-P + fatic = DAG-3P + Sphmy
43	7	true	7	(-1 ceramide) (1 DAGkin) (1 monoAGcholinPctf) (1 PLA2) (1 PLC) (-1 PLD) (-1 Sphmydias)	PA + PC + sph = AA + DAG-3P + Sphmy
44	12	true	8	(2 ceramide) (-2 DAGkin) (1 ERMform) (1 ERMform) (1 PI4kin) (1 PI4P5kin) (-2 PLC) (2 Sphmydias)	2 DAG-3P + Ezrin + PI + 2 Sphmy + TM = ERM-PIP2 + 2 PC + 2 fatic + 2 sph
45	4	true	4	(-1 ceramide) (-1 DAGcholT) (1 PLC) (-1 Sphmydias)	CDP-cholin + fatic + sph = CMP + Sphmy
46	3	true	3	(1 ceramide) (1 CholinPtf) (1 Sphmydias)	CTP + Sphmy = CDP-cholin + PPI + fatic + sph
47	5	true	5	(-1 ceramide) (1 Cholin) (1 PLD) (-1 Sphmydias) (-1 SPK)	PC + S-1-P + fatic = PA + Sphmy

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48	5	true	5	(-1 ceramidse) (1 Cholinkin) (1 monoAGcholinPctf) (1 PLA2) (-1 Sphmydias)	PC + sph = AA + Sphmy
49	12	true	8	(2 ceramidse) (-2 Cholinkin) (1 ERMfform) (1 ERMform) (1 PI4kin) (1 PI4P5kin) (-2 PLD) (2 Sphmydias)	Ezrin + 2 PA + PI + 2 Sphmy + TM = ERM-PIP2 + 2 PC + 2 fatac + 2 sph
50	6	true	6	(1 ceramidse) (-1 Cholinkin) (1 DAGkin) (1 PAP) (-1 PLD) (1 Sphmydias)	2 PA + Sphmy = DAG-3P + P + PC + fatac + sph
51	6	true	6	(1 ceramidse) (-1 Cholinkin) (1 DAGkin) (1 Lipase) (-1 PLD) (1 Sphmydias)	PA + Sphmy + TAG = DAG-3P + PC + 2 fatac + sph
52	6	true	6	(1 ceramidse) (-1 Cholinkin) (1 DAGcholT) (1 DAGkin) (-1 PLD) (1 Sphmydias)	CMP + PA + Sphmy = CDP-cholin + DAG-3P + fatac + sph
53	2	false	2	(-1 PAP) (1 Pldiase)	P + PI = IcP + PA
54	2	false	2	(-1 Lipase) (1 Pldiase)	PI + fatac = IcP + TAG
55	3	false	3	(1 DAGkin) (1 Pldiase) (-1 SPK)	PI + S-1-P = DAG-3P + IcP + sph
56	5	false	5	(1 DAGkin) (1 monoAGcholinPctf) (1 Pldiase) (1 PLA2) (-1 PLD)	PA + PI = AA + DAG-3P + IcP + fatac
57	8	false	6	(2 DAGkin) (-1 ERMfform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (2 Pldiase)	ERM-PIP2 + PI = 2 DAG-3P + Ezrin + 2 IcP + TM
58	2	false	2	(-1 DAGcholT) (1 Pldiase)	CDP-cholin + PI = CMP + IcP + PC
59	3	false	3	(-1 CholinPtf) (1 Pldiase) (-1 PLC)	CDP-cholin + PI + PPI = CTP + IcP + PC
60	5	false	5	(1 Cholinkin) (1 Pldiase) (-1 PLC) (1 PLD) (-1 SPK)	PI + S-1-P = IcP + PA + sph
61	5	false	5	(1 Cholinkin) (1 monoAGcholinPctf) (1 Pldiase) (1 PLA2) (-1 PLC)	PI = AA + IcP + fatac
62	12	false	8	(2 Cholinkin) (-1 ERMfform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin) (2 Pldiase) (-2 PLC) (2 PLD)	ERM-PIP2 + PI = Ezrin + 2 IcP + 2 PA + TM
63	5	false	5	(-1 Cholinkin) (-1 CholinPtf) (1 DAGkin) (1 Pldiase) (-1 PLD)	CDP-cholin + PA + PI + PPI = CTP + DAG-3P + IcP + PC
64	4	false	4	(1 ceramidse) (1 Pldiase) (-1 PLC) (1 Sphmydias)	PI + Sphmy = IcP + PC + fatac + sph
65	6	false	6	(1 ceramidse) (-1 Cholinkin) (1 DAGkin) (1 Pldiase) (-1 PLD) (1 Sphmydias)	PA + PI + Sphmy = DAG-3P + IcP + PC + fatac + sph
66	6	false	5	(-1 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 SPK)	P + PI + 2 S-1-P = PA + inositolTP + 2 sph
67	10	false	7	(2 monoAGcholinPctf) (-1 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLA2) (-2 PLD)	P + PA + PI = 2 AA + 2 fatac + inositolTP
68	6	false	5	(-1 Lipase) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 SPK)	PI + 2 S-1-P + fatac = TAG + inositolTP + 2 sph
69	10	false	7	(-1 Lipase) (2 monoAGcholinPctf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLA2) (-2 PLD)	2 PA + PI = 2 AA + TAG + fatac + inositolTP
70	4	false	4	(-1 ERMfform) (-1 ERMform) (-1 PAP) (1 PI45diase)	ERM-PIP2 + P = Ezrin + PA + TM + inositolTP
71	4	false	4	(-1 ERMfform) (-1 ERMform) (-1 Lipase) (1 PI45diase)	ERM-PIP2 + fatac = Ezrin + TAG + TM + inositolTP

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72	7	false	5	(1 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-3 SPK)	PI + 3 S-1-P = DAG-3P + inositolTP + 3 sph
73	8	false	5	(-2 DAGkin) (-3 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin)	2 DAG-3P + 3 P + PI = 3 PA + inositolTP
74	13	false	7	(1 DAGkin) (3 monoAGcholinPCtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (3 PLA2) (-3 PLD)	3 PA + PI = 3 AA + DAG-3P + 3 fatac + inositolTP
75	8	false	5	(-2 DAGkin) (-3 Lipase) (1 PI45diase) (1 PI4kin) (1 PI4P5kin)	2 DAG-3P + PI + 3 fatac = 3 TAG + inositolTP
76	5	false	5	(1 DAGkin) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (-1 SPK)	ERM-PIP2 + S-1-P = DAG-3P + Ezrin + TM + inositolTP + sph
77	12	false	6	(2 DAGkin) (-3 ERMfform) (-3 ERMform) (2 PI45diase) (-1 PI4kin) (-1 PI4P5kin)	3 ERM-PIP2 = 2 DAG-3P + 3 Ezrin + PI + 3 TM + 2 inositolTP
78	7	false	7	(1 DAGkin) (-1 ERMfform) (-1 ERMform) (1 monoAGcholinPCtf) (1 PI45diase) (1 PLA2) (-1 PLD)	ERM-PIP2 + PA = AA + DAG-3P + Ezrin + TM + fatac + inositolTP
79	6	false	5	(-1 DAGcholT) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 SPK)	CDP-cholin + PI + 2 S-1-P = CMP + PC + inositolTP + 2 sph
80	10	false	7	(-1 DAGcholT) (2 monoAGcholinPCtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLA2) (-2 PLD)	CDP-cholin + 2 PA + PI = 2 AA + CMP + PC + 2 fatac + inositolTP
81	4	false	4	(-1 DAGcholT) (-1 ERMfform) (-1 ERMform) (1 PI45diase)	CDP-cholin + ERM-PIP2 = CMP + Ezrin + PC + TM + inositolTP
82	8	false	5	(-3 DAGcholT) (-2 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin)	3 CDP-cholin + 2 DAG-3P + PI = 3 CMP + 3 PC + inositolTP
83	7	false	6	(-1 CholinPtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-1 PLC) (-2 SPK)	CDP-cholin + PI + PPI + 2 S-1-P = CTP + PC + inositolTP + 2 sph
84	11	false	8	(-1 CholinPtf) (2 monoAGcholinPCtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLA2) (-1 PLC) (-2 PLD)	CDP-cholin + 2 PA + PI + PPI = 2 AA + CTP + PC + 2 fatac + inositolTP
85	5	false	5	(-1 CholinPtf) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (-1 PLC)	CDP-cholin + ERM-PIP2 + PPI = CTP + Ezrin + PC + TM + inositolTP
86	11	false	6	(-3 CholinPtf) (-2 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-3 PLC)	3 CDP-cholin + 2 DAG-3P + PI + 3 PPI = 3 CTP + 3 PC + inositolTP
87	9	false	7	(1 Cholinkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-1 PLC) (1 PLD) (-3 SPK)	PI + 3 S-1-P = PA + inositolTP + 3 sph
88	12	false	7	(-2 Cholinkin) (-3 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLC) (-2 PLD)	3 P + PI = PA + inositolTP
89	9	false	8	(1 Cholinkin) (1 monoAGcholinPCtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (1 PLA2) (-1 PLC) (-2 SPK)	PI + 2 S-1-P = AA + fatac + inositolTP + 2 sph
90	13	false	8	(1 Cholinkin) (3 monoAGcholinPCtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (3 PLA2) (-1 PLC) (-2 PLD)	2 PA + PI = 3 AA + 3 fatac + inositolTP
91	12	false	7	(-2 Cholinkin) (-3 Lipase) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLC) (-2 PLD)	2 PA + PI + 3 fatac = 3 TAG + inositolTP

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92	7	false	7	(1 Cholinkin) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (-1 PLC) (1 PLD) (-1 SPK)	ERM-PIP2 + S-1-P = Ezrin + PA + TM + inositolTP + sph
93	16	false	8	(2 Cholinkin) (-3 ERMfform) (-3 ERMform) (2 PI45diase) (-1 PI4kin) (-1 PI4P5kin) (-2 PLC) (2 PLD)	3 ERM-PIP2 = 3 Ezrin + 2 PA + PI + 3 TM + 2 inositolTP
94	7	false	7	(1 Cholinkin) (-1 ERMfform) (-1 ERMform) (1 monoAGcholinPctf) (1 PI45diase) (1 PLA2) (-1 PLC)	ERM-PIP2 = AA + Ezrin + TM + fatak + inositolTP
95	17	false	8	(3 Cholinkin) (-2 DAGkin) (3 monoAGcholinPctf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (3 PLA2) (-3 PLC)	2 DAG-3P + PI = 3 AA + 3 fatak + inositolTP
96	12	false	7	(-2 Cholinkin) (-3 DAGchoIT) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLC) (-2 PLD)	3 CDP-cholin + 2 PA + PI = 3 CMP + 3 PC + inositolTP
97	11	false	7	(-2 Cholinkin) (-3 CholinPtf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-1 PLC) (-2 PLD)	3 CDP-cholin + 2 PA + PI + 3 PPI = 3 CTP + 3 PC + inositolTP
98	10	false	7	(-2 Cholinkin) (-2 CholinPtf) (-1 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD)	2 CDP-cholin + P + PA + PI + 2 PPI = 2 CTP + 2 PC + inositolTP
99	10	false	7	(-2 Cholinkin) (-2 CholinPtf) (-1 Lipase) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD)	2 CDP-cholin + 2 PA + PI + 2 PPI + fatak = 2 CTP + 2 PC + TAG + inositolTP
100	13	false	7	(-3 Cholinkin) (-3 CholinPtf) (1 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-3 PLD)	3 CDP-cholin + 3 PA + PI + 3 PPI = 3 CTP + DAG-3P + 3 PC + inositolTP
101	7	false	7	(-1 Cholinkin) (-1 CholinPtf) (1 DAGkin) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (-1 PLD)	CDP-cholin + ERM-PIP2 + PA + PPI = CTP + DAG-3P + Ezrin + PC + TM + inositolTP
102	10	false	7	(-2 Cholinkin) (-2 CholinPtf) (-1 DAGchoIT) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD)	3 CDP-cholin + 2 PA + PI + 2 PPI = CMP + 2 CTP + 3 PC + inositolTP
103	8	false	7	(1 ceramidse) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-1 PLC) (1 Sphmydias) (-2 SPK)	PI + 2 S-1-P + Sphmy = PC + fatak + inositolTP + 3 sph
104	12	false	9	(1 ceramidse) (2 monoAGcholinPctf) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (2 PLA2) (-1 PLC) (-2 PLD) (1 Sphmydias)	2 PA + PI + Sphmy = 2 AA + PC + 3 fatak + inositolTP + sph
105	6	false	6	(1 ceramidse) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (-1 PLC) (1 Sphmydias)	ERM-PIP2 + Sphmy = Ezrin + PC + TM + fatak + inositolTP + sph
106	14	false	7	(3 ceramidse) (-2 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-3 PLC) (3 Sphmydias)	2 DAG-3P + PI + 3 Sphmy = 3 PC + 3 fatak + inositolTP + 3 sph
107	14	false	8	(3 ceramidse) (-2 Cholinkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-1 PLC) (-2 PLD) (3 Sphmydias)	2 PA + PI + 3 Sphmy = 3 PC + 3 fatak + inositolTP + 3 sph
108	12	false	8	(2 ceramidse) (-2 Cholinkin) (-1 PAP) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD) (2 Sphmydias)	P + PA + PI + 2 Sphmy = 2 PC + 2 fatak + inositolTP + 2 sph
109	12	false	8	(2 ceramidse) (-2 Cholinkin) (-1 Lipase) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD) (2 Sphmydias)	2 PA + PI + 2 Sphmy = 2 PC + TAG + fatak + inositolTP + 2 sph
110	16	false	8	(3 ceramidse) (-3 Cholinkin) (1 DAGkin) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-3 PLD) (3 Sphmydias)	3 PA + PI + 3 Sphmy = DAG-3P + 3 PC + 3 fatak + inositolTP + 3 sph

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111	8	false	8	(1 ceramidse) (-1 Cholinkin) (1 DAGkin) (-1 ERMfform) (-1 ERMform) (1 PI45diase) (1 PLD) (1 Sphmydias)	ERM-PIP2 + PA + Sphmy = DAG-3P + Ezrin + PC + TM + fatac + inositolTP + sph
112	12	false	8	(2 ceramidse) (-2 Cholinkin) (-1 DAGcholT) (1 PI45diase) (1 PI4kin) (1 PI4P5kin) (-2 PLD) (2 Sphmydias)	CDP-cholin + 2 PA + PI + 2 Sphmy = CMP + 3 PC + 2 fatac + inositolTP + 2 sph
113	2	false	2	(1 CDPinotra) (1 CDPsynth)	CTP + PA + inositol = CMP + PI + PPi
114	2	false	2	(1 Actinnucl) (-1 SPK)	2 Actin + S-1-P = Actinpoly + P + sph
115	4	false	4	(1 Actinnucl) (1 monoAGcholinPCtf) (1 PLA2) (-1 PLD)	2 Actin + PA = AA + Actinpoly + P + fatac
116	6	false	5	(2 Actinnucl) (-1 ERMfform) (-1 ERMform) (-1 PI4kin) (-1 PI4P5kin)	4 Actin + ERM-PIP2 = 2 Actinpoly + Ezrin + 2 P + PI + TM
117	3	false	3	(1 Actinnucl) (-1 DAGkin) (-1 PAP)	2 Actin + DAG-3P = Actinpoly + PA
118	3	false	3	(1 Actinnucl) (-1 DAGkin) (-1 Lipase)	2 Actin + DAG-3P + fatac = Actinpoly + P + TAG
119	3	false	3	(1 Actinnucl) (-1 DAGcholT) (-1 DAGkin)	2 Actin + CDP-cholin + DAG-3P = Actinpoly + CMP + P + PC
120	4	false	4	(1 Actinnucl) (-1 CholinPtf) (-1 DAGkin) (-1 PLC)	2 Actin + CDP-cholin + DAG-3P + PPi = Actinpoly + CTP + P + PC
121	5	false	5	(1 Actinnucl) (-1 Cholinkin) (-1 PAP) (1 PLC) (-1 PLD)	2 Actin = Actinpoly
122	5	false	5	(1 Actinnucl) (-1 Cholinkin) (-1 Lipase) (1 PLC) (-1 PLD)	2 Actin + PA + fatac = Actinpoly + P + TAG
123	6	false	6	(1 Actinnucl) (1 Cholinkin) (-1 DAGkin) (1 monoAGcholinPCtf) (1 PLA2) (-1 PLC)	2 Actin + DAG-3P = AA + Actinpoly + P + fatac
124	5	false	5	(1 Actinnucl) (-1 Cholinkin) (-1 DAGcholT) (1 PLC) (-1 PLD)	2 Actin + CDP-cholin + PA = Actinpoly + CMP + P + PC
125	4	false	4	(1 Actinnucl) (-1 Cholinkin) (-1 CholinPtf) (-1 PLD)	2 Actin + CDP-cholin + PA + PPi = Actinpoly + CTP + P + PC
126	5	false	5	(1 Actinnucl) (1 ceramidse) (-1 DAGkin) (-1 PLC) (1 Sphmydias)	2 Actin + DAG-3P + Sphmy = Actinpoly + P + PC + fatac + sph
127	5	false	5	(1 Actinnucl) (1 ceramidse) (-1 Cholinkin) (-1 PLD) (1 Sphmydias)	2 Actin + PA + Sphmy = Actinpoly + P + PC + fatac + sph
128	1	false	1	(1 Actindepoly)	Actinpoly = 2 Actin

¹ The actin nucleation modes are listed from mode 114 onwards. Only these phospholipids did also stimulate actin nucleation in experiments with phagosomes.

Table 4: Extended phagosome network - metabolites

Name	internal?	Connectivity	Description
1-Acyl-sn-glycero-3-Pcholine	true	3	1-Acyl-sn-glycero-3-phosphocholine
1-Acyl-sn-glycero-3-PEtOHamine	true	2	1-Acyl-sn-glycero-3-phosphoethanolamine
1-Acyl-sn-glycerol3-P	false	2	1-Acyl-sn-glycerol 3-phosphate
1,2-Diacyl-sn-glycerol	true	4	1,2-Diacyl-sn-glycerol
2-Acyl-sn-glycero-3-Pcholine	false	1	2-Acyl-sn-glycero-3-phosphocholine
2-Acyl-sn-glycero-3-PEtOHamine	false	1	2-Acyl-sn-glycero-3-phosphoethanolamine
2-Acyl-sn-glycerol3-P	false	1	2-Acyl-sn-glycerol 3-phosphate
Ac	false	1	Acetate
Ac-CoA	false	1	Acetyl-CoA
Accholine	true	2	Acetylcholine
Acyl-CoA	false	4	Acyl-CoA
AcylDHAP	false	1	Acylglycerone phosphate
Adenosyl-L-homoCys	false	1	S-Adenosyl-L-homocysteine
Adenosyl-L-Met	false	1	S-Adenosyl-L-methionine
Cardiolipin	false	2	Cardiolipin
CDP-choline	false	2	CDP-choline
CDP-diacylglycerol	true	3	CDP-diacylglycerol
CDP-EtOHamine	false	1	CDP-ethanolamine
Choline	true	6	Choline
CholineP	true	3	Choline phosphate
CMP	false	3	CMP
CoA	false	5	CoA
CTP	false	3	CTP
D-Glucuronate	false	1	D-Glucuronate
DHAP	true	3	Glycerone phosphate
EtOHamine	true	4	Ethanolamine
EtOHamineP	true	3	Ethanolamine phosphate
FAD	false	1	FAD
FADH2	false	1	FADH2
Fattyacid	false	6	Fatty acid
G6P	false	1	D-Glucose 6-phosphate
Glycerol	false	1	Glycerol
inositol	true	5	myo-Inositol
inositol_TEP_1345	true	3	D-myo-Inositol 1,3,4,5-tetrakisphosphate
inositolBP_14	true	2	D-myo-Inositol 1,4-bisphosphate
inositolBP_34	true	2	D-myo-Inositol 3,4-bisphosphate
inositolHP	false	1	myo-Inositol hexakisphosphate

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inositolP_1	true	2	Inositol 1-phosphate
inositolP_3	true	2	D-myo-Inositol 3-phosphate
inositolP_4	true	2	myo-Inositol 4-phosphate
inositolPP_13456	true	2	D-myo-Inositol 1,3,4,5,6-pentakisphosphate
inositolTEP_1456	true	2	D-myo-Inositol 1,4,5,6-tetrakisphosphate
inositolTP_134	true	2	D-myo-Inositol 1,3,4-trisphosphate
inositolTP_145	true	5	D-myo-Inositol 1,4,5-trisphosphate
L-Ser	false	2	L-Serine
NAD+	false	1	NAD+
NADH	false	1	NADH
Oxygen	false	1	Oxygen
PA	true	6	Phosphatidate
PC	true	5	Phosphatidylcholine
Phosphatidyl-N-methylEtOHamine	false	1	Phosphatidyl-N-methylethanolamine
PhosphatidylEtOHamine	true	5	Phosphatidylethanolamine
Phosphatidylglycerol	false	2	Phosphatidylglycerol
PI	false	3	1-Phosphatidyl-D-myo-inositol
PIP2_45	true	5	1-Phosphatidyl-D-myo-inositol 4,5-bisphosphate
PIP3_345	true	2	Phosphatidylinositol-3,4,5-trisphosphate
PIP_3	false	1	1-Phosphatidyl-1D-myo-inositol 3-phosphate
PIP_4	true	3	1-Phosphatidyl-1D-myo-inositol 4-phosphate
PSer	true	3	Phosphatidylserine
sn-glycero-3-Pcholine	false	2	sn-glycero-3-Phosphocholine
sn-glycero-3-PEtOHamine	false	2	sn-glycero-3-Phosphoethanolamine
sn-Glycerol3-P	true	4	sn-Glycerol 3-phosphate
Sterol	false	1	Sterol
Sterylester	false	1	Steryl ester

Table 5: Extended phagosome network - reactions

Enzyme name	rev.?	Reaction equation	Annotation
rn:R00840	true	inositolP_1 = G6P	1L-myo-Inositol-1-phosphate lyase (isomerizing) [5.5.1.4]
rn:R00842	false	NAD+ + sn-Glycerol3-P = DHAP + NADH	sn-Glycerol-3-phosphate:NAD+ 2-oxidoreductase [1.1.1.8 , 1.1.1.94]
rn:R00848	false	FAD + sn-Glycerol3-P = DHAP + FADH2	sn-Glycerol-3-phosphate:(acceptor) 2-oxidoreductase [1.1.99.5]
rn:R00851	false	Acyl-CoA + sn-Glycerol3-P = 1-Acyl-sn-glycerol3-P + CoA	acyl-CoA:sn-glycerol-3-phosphate 1-O-acyltransferase [2.3.1.15]
rn:R01013	true	Acyl-CoA + DHAP = AcylDHAP + CoA	Acyl-CoA:glycerone-phosphate O-acyltransferase [2.3.1.42]
rn:R01021	false	Choline = CholineP	ATP:choline phosphotransferase [2.7.1.32]
rn:R01023	false	Ac-CoA + Choline = Accholine + CoA	Acetyl-CoA:choline O-acetyltransferase [2.3.1.6]
rn:R01026	false	Accholine = Ac + Choline	Acetylcholine aetylhydrolase [3.1.1.7]
rn:R01184	false	Oxygen + inositol = D-Glucuronate	myo-Inositol:oxygen oxidoreductase [1.13.99.1]
rn:R01185	false	inositolP_1 = inositol	myo-Inositol 1-phosphate phosphahydrolase [3.1.3.25]
rn:R01186	false	inositolP_4 = inositol	myo-Inositol 4-phosphate phosphahydrolase [3.1.3.25]
rn:R01187	false	inositolP_3 = inositol	1D-myo-Inositol 3-phosphate phosphahydrolase [3.1.3.25]
rn:R01310	false	PC = Choline + PA	Phosphatidylcholine phosphatidohydrolase [3.1.4.4]
rn:R01315	false	PC = 1-Acyl-sn-glycero-3-Pcholine + Fattyacid	Phosphatidylcholine 2-acylhylolase [3.1.1.4]
rn:R01321	false	12-Diacyl-sn-glycerol + CDP-choline = CMP + PC	CDPcholine:1,2-diacylglycerol cholinephosphotransferase [2.7.8.2]
rn:R01468	false	EtOHamine = EtOHamineP	ATP:ethanolamine O-phosphotransferase [2.7.1.82]
rn:R01799	false	CTP + PA = CDP-diacylglycerol	CTP:phosphatidate cytidyltransferase [2.7.7.41]
rn:R01802	false	CDP-diacylglycerol + inositol = CMP + PI	CDPdiacylglycerol:myo-inositol 3-phosphatidyltransferase [2.7.8.11]
rn:R01890	false	CTP + CholineP = CDP-choline	CTP:choline-phosphate cytidyltransferase [2.7.7.15]
rn:R02030	false	CDP-diacylglycerol + Phosphatidylglycerol = CMP + Cardiolipin	[2.7.8.-]
rn:R02038	false	CTP + EtOHamineP = CDP-EtOHamine	CTP:ethanolamine-phosphate cytidyltransferase [2.7.7.14]
rn:R02051	false	PhosphatidylEtOHamine = EtOHamine + PA	Phosphatidylethanolamine phosphatidohydrolase [3.1.4.4]
rn:R02053	false	PhosphatidylEtOHamine = 1-Acyl-sn-glycero-3-PEtOHamine + Fattyacid	Phosphatidylethanolamine 2-acylhylolase [3.1.1.4]
rn:R02055	false	PSer = PhosphatidylEtOHamine	Phosphatidyl-L-serine carboxy-lyase [4.1.1.65]
rn:R02056	false	Adenosyl-L-Met + PhosphatidylEtOHamine = Adenosyl-L-homoCys + Phosphatidyl-N-methylEtOHamine	S-Adenosyl-L-methionine:phosphatidylethanolamine N-methyltransferase [2.1.1.17]
rn:R02114	false	PC + Sterol = 1-Acyl-sn-glycero-3-Pcholine + Sterylester	Phosphatidylcholine:sterol O-acyltransferase [2.3.1.43]
rn:R02239	false	PA = 12-Diacyl-sn-glycerol	1,2-Diacyl-sn-glycerol 3-phosphate phosphohydrolase [3.1.3.4]
rn:R02240	false	12-Diacyl-sn-glycerol = PA	ATP:1,2-diacylglycerol 3-phosphotransferase [2.7.1.107]
rn:R02241	false	CoA + PA = 1-Acyl-sn-glycerol3-P + Acyl-CoA	[2.3.1.51]

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rn:R02746	false	1-Acyl-sn-glycero-3-Pcholine = Fattyacid + sn-glycero-3-Pcholine	1-Acyl-sn-glycero-3-phosphocholine acylhydrolase [3.1.1.5]
rn:R02747	false	2-Acyl-sn-glycero-3-Pcholine = Fattyacid + sn-glycero-3-Pcholine	2-Acyl-sn-glycero-3-phosphocholine acylhydrolase [3.1.1.5]
rn:R03361	false	PI = PIP ₄	ATP:1-Phosphatidyl-1D-myo-inositol 4-phosphotransferase [2.7.1.67]
rn:R03362	false	PI = PIP ₃	ATP:1-phosphatidyl-1D-myo-inositol 3-phosphotransferase [2.7.1.137]
rn:R03393	false	inositolBP ₁₄ = inositolP ₄	D-myo-Inositol-1,4-bisphosphate 1-phosphohydrolase [3.1.3.57]
rn:R03394	false	inositolTP ₁₄₅ = inositolBP ₁₄	D-myo-Inositol-1,4,5-trisphosphate 5-phosphohydrolase [3.1.3.56]
rn:R03416	false	1-Acyl-sn-glycero-3-PEtOHamine = Fattyacid + sn-glycero-3-PEtOHamine	1-Acyl-sn-glycero-3-phosphoethanolamine aldehydohydrolase [3.1.1.5]
rn:R03417	false	2-Acyl-sn-glycero-3-PEtOHamine = Fattyacid + sn-glycero-3-PEtOHamine	L-2-Lysophosphatidylethanolamine aldehydohydrolase [3.1.1.5]
rn:R03427	false	inositolTP ₁₃₄ = inositolBP ₃₄	D-myo-Inositol 1,3,4-trisphosphate 1-phosphohydrolase [3.1.3.57]
rn:R03430	false	inositol_TEP ₁₃₄₅ = inositolTP ₁₃₄	D-myo-Inositol 1,3,4,5-tetrakisphosphate 5-phosphohydrolase [3.1.3.56]
rn:R03433	false	inositolTP ₁₄₅ = inositol_TEP ₁₃₄₅	ATP:1D-myo-inositol-1,4,5-trisphosphate 3-phosphotransferase [2.7.1.127]
rn:R03434	false	inositol_TEP ₁₃₄₅ = inositolTP ₁₄₅	D-myo-Inositol 1,3,4,5-tetrakisphosphate 3-phosphohydrolase [3.1.3.62]
rn:R03435	false	PIP _{2_45} = 12-Diacyl-sn-glycerol + inositolTP ₁₄₅	1-Phosphatidyl-1D-myo-inositol-4,5-bisphosphate inositoltrisphosphohydrolase [3.1.4.11]
rn:R03469	false	PIP ₄ = PIP _{2_45}	ATP:1-phosphatidyl-1D-myo-inositol-4-phosphate 5-phosphotransferase [2.7.1.68]
rn:R04372	false	inositolBP ₃₄ = inositolP ₃	D-myo-Inositol-3,4-bisphosphate 4-phosphohydrolase [3.1.3.66]
rn:R04404	false	PIP _{2_45} = PIP ₄	Phosphatidyl-myo-inositol-4,5-bisphosphate 4-phosphohydrolase [3.1.3.36]
rn:R04513	false	PIP _{3_345} = PIP _{2_45}	Phosphatidylinositol-3,4,5-trisphosphate 3-phosphohydrolase [3.1.3.67]
rn:R04545	false	PIP _{2_45} = PIP _{3_345}	ATP:1-phosphatidyl-1D-myo-inositol-4,5-bisphosphate 3-phosphotransferase [2.7.1.153]
rn:R05202	true	inositolHP = inositolPP ₁₃₄₅₆	unknown [2.7.1.-]
rn:R05800	false	inositolTP ₁₄₅ = inositolTEP ₁₄₅₆	ATP:1D-myo-inositol-1,4,5-trisphosphate 6-phosphotransferase [2.7.1.151]
rn:R05801	false	inositolTEP ₁₄₅₆ = inositolPP ₁₃₄₅₆	ATP:1D-myo-inositol-1,4,5-trisphosphate 6-phosphotransferase [2.7.1.151]
rn:R06870	false	EtOHamineP = EtOHamine	Phosphoethanolamine phosphohydrolase [3.1.3.75]
rn:R06871	false	CholineP = Choline	Phosphocholine phosphohydrolase [3.1.3.75]

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rn:R06872	true	Acyl-CoA + sn-Glycerol3-P = 2-Acyl-sn-glycerol3-P + CoA	Acyl-CoA:sn-glycerol-3-phosphate 2-O-acyltransferase []
rn:R07376	false	L-Ser + PhosphatidylEtOHamine = EtOHamine + PSer	[]
rn:R07377	false	L-Ser + PC = Choline + PSer	[]
rn:R07390	false	2 Phosphatidylglycerol = Cardiolipin + Glycerol	[2.7.8.-]

Table 6: Extended phagosome network - Elementary Modes

#	Flux sum	Rev.?	Pathlength	Reactions	Net reaction
1	1	false	1	(1 m:R03417)	2-Acyl-sn-glycero-3-PEtOHamine = Fattyacid + sn-glycero-3-PEtOHamine
2	1	false	1	(1 m:R07390)	2 Phosphatidylglycerol = Cardiolipin + Glycerol
3	3	false	3	(-1 m:R00840) (1 m:R01184) (1 m:R01185)	G6P + Oxygen = D-Glucuronate
4	2	false	2	(1 m:R00851) (-1 m:R06872)	2-Acyl-sn-glycerol3-P = 1-Acyl-sn-glycerol3-P
5	2	false	2	(1 m:R04513) (1 m:R04545)	no net reaction
6	3	false	3	(1 m:R00848) (1 m:R01013) (-1 m:R06872)	2-Acyl-sn-glycerol3-P + FAD = AcylDHAP + FADH2
7	3	false	3	(1 m:R00842) (1 m:R01013) (-1 m:R06872)	2-Acyl-sn-glycerol3-P + NAD+ = AcylDHAP + NADH
8	2	false	2	(1 m:R01468) (1 m:R06870)	no net reaction
9	1	false	1	(1 m:R03362)	PI = PIP_3
10	1	false	1	(1 m:R02747)	2-Acyl-sn-glycero-3-Pcholine = Fattyacid + sn-glycero-3-Pcholine
11	2	false	2	(1 m:R01021) (1 m:R06871)	no net reaction
12	4	false	4	(1 m:R01468) (1 m:R02038) (1 m:R02055) (1 m:R07376)	CTP + L-Ser = CDP-EtOHamine
13	5	false	5	(1 m:R01021) (1 m:R01310) (1 m:R01321) (1 m:R01890) (1 m:R02239)	CTP = CMP
14	2	false	2	(1 m:R01023) (1 m:R01026)	Ac-CoA = Ac + CoA
15	9	false	9	(1 m:R01021) (1 m:R01321) (1 m:R01468) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R02239) (1 m:R07377)	2 CTP + L-Ser = CDP-EtOHamine + CMP
16	2	false	2	(1 m:R03433) (1 m:R03434)	no net reaction
17	2	false	2	(1 m:R02239) (1 m:R02240)	no net reaction
18	11	false	11	(1 m:R01021) (1 m:R01310) (1 m:R01321) (1 m:R01890) (1 m:R02241) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CTP + CoA + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CMP + inositolHP
19	12	false	12	(1 m:R01021) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	2 CTP + PI + Phosphatidylglycerol = 2 CMP + Cardiolipin + inositolHP
20	14	false	14	(-1 m:R00840) (1 m:R01021) (1 m:R01185) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	2 CTP + G6P = 2 CMP + inositolHP
21	14	false	14	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01310) (1 m:R01321) (1 m:R01890) (1 m:R02241) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CTP + CoA + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CMP + D-Glucuronate

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22	15	false	15	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	2 CTP + Oxygen + PI + Phosphatidylglycerol = 2 CMP + Cardiolipin + D-Glucuronate
23	14	false	14	(1 m:R01021) (1 m:R01187) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	2 CTP = 2 CMP
24	12	false	12	(1 m:R01021) (1 m:R01321) (1 m:R01890) (1 m:R02055) (1 m:R02056) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801) (1 m:R07377)	Adenosyl-L-Met + CTP + L-Ser + PI = Adenosyl-L-homoCys + CMP + Phosphatidyl-N-methylEtOHamine + inositolHP
25	15	false	15	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01321) (1 m:R01890) (1 m:R02055) (1 m:R02056) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372) (1 m:R07377)	Adenosyl-L-Met + CTP + L-Ser + Oxygen + PI = Adenosyl-L-homoCys + CMP + D-Glucuronate + Phosphatidyl-N-methylEtOHamine
26	2	false	2	(1 m:R03469) (1 m:R04404)	no net reaction
27	15	false	15	(1 m:R01021) (1 m:R01321) (1 m:R01468) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R02241) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801) (1 m:R07377)	2 CTP + CoA + L-Ser + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CDP-EtOHamine + CMP + inositolHP
28	16	false	16	(1 m:R01021) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801) (1 m:R07377)	3 CTP + L-Ser + PI + Phosphatidylglycerol = CDP-EtOHamine + 2 CMP + Cardiolipin + inositolHP
29	18	false	18	(-1 m:R00840) (1 m:R01021) (1 m:R01185) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801) (1 m:R07377)	3 CTP + G6P + L-Ser = CDP-EtOHamine + 2 CMP + inositolHP
30	18	false	18	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01321) (1 m:R01468) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R02241) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372) (1 m:R07377)	2 CTP + CoA + L-Ser + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CDP-EtOHamine + CMP + D-Glucuronate
31	19	false	19	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372) (1 m:R07377)	3 CTP + L-Ser + Oxygen + PI + Phosphatidylglycerol = CDP-EtOHamine + 2 CMP + Cardiolipin + D-Glucuronate

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32	18	false	18	(1 m:R01021) (1 m:R01187) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372) (1 m:R07377)	3 CTP + L-Ser = CDP-EtOHamine + 2 CMP
33	13	false	13	(1 m:R01021) (1 m:R01321) (1 m:R01890) (1 m:R02053) (1 m:R02055) (1 m:R03361) (1 m:R03416) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801) (1 m:R07377)	CTP + L-Ser + PI = CMP + 2 Fattyacid + inositolHP + sn-glycero-3-PEtOHamine
34	16	false	16	(1 m:R01021) (1 m:R01184) (1 m:R01187) (1 m:R01321) (1 m:R01890) (1 m:R02053) (1 m:R02055) (1 m:R03361) (1 m:R03416) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372) (1 m:R07377)	CTP + L-Ser + Oxygen + PI = CMP + D-Glucuronate + 2 Fattyacid + sn-glycero-3-PEtOHamine
35	9	false	9	(1 m:R01315) (1 m:R01321) (1 m:R02746) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CDP-choline + PI = CMP + 2 Fattyacid + inositolHP + sn-glycero-3-Pcholine
36	12	false	12	(1 m:R01184) (1 m:R01187) (1 m:R01315) (1 m:R01321) (1 m:R02746) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CDP-choline + Oxygen + PI = CMP + D-Glucuronate + 2 Fattyacid + sn-glycero-3-Pcholine
37	12	false	12	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01310) (1 m:R01321) (1 m:R01890) (1 m:R02241) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CTP + CoA + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CMP + D-Glucuronate
38	13	false	13	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	2 CTP + Oxygen + PI + Phosphatidylglycerol = 2 CMP + Cardiolipin + D-Glucuronate
39	12	false	12	(1 m:R01021) (1 m:R01186) (1 m:R01310) (1 m:R01321) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	2 CTP = 2 CMP
40	13	false	13	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01321) (1 m:R01890) (1 m:R02055) (1 m:R02056) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469) (1 m:R07377)	Adenosyl-L-Met + CTP + L-Ser + Oxygen + PI = Adenosyl-L-homoCys + CMP + D-Glucuronate + Phosphatidyl-N-methylEtOHamine
41	16	false	16	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01321) (1 m:R01468) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R02241) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469) (1 m:R07377)	2 CTP + CoA + L-Ser + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + CDP-EtOHamine + CMP + D-Glucuronate
42	17	false	17	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01890) (1 m:R02030) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469) (1 m:R07377)	3 CTP + L-Ser + Oxygen + PI + Phosphatidylglycerol = CDP-EtOHamine + 2 CMP + Cardiolipin + D-Glucuronate

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43	16	false	16	(1 m:R01021) (1 m:R01186) (1 m:R01321) (1 m:R01468) (1 m:R01799) (1 m:R01802) (1 m:R01890) (1 m:R02038) (1 m:R02051) (1 m:R02055) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469) (1 m:R07377)	3 CTP + L-Ser = CDP-EtOHamine + 2 CMP
44	14	false	14	(1 m:R01021) (1 m:R01184) (1 m:R01186) (1 m:R01321) (1 m:R01890) (1 m:R02053) (1 m:R02055) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03416) (1 m:R03435) (1 m:R03469) (1 m:R07377)	CTP + L-Ser + Oxygen + PI = CMP + D-Glucuronate + 2 Fattyacid + sn-glycero-3-PEtOHamine
45	10	false	10	(1 m:R01184) (1 m:R01186) (1 m:R01315) (1 m:R01321) (1 m:R02746) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CDP-choline + Oxygen + PI = CMP + D-Glucuronate + 2 Fattyacid + sn-glycero-3-Pcholine
46	8	false	8	(1 m:R02240) (1 m:R02241) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CoA + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + inositolHP
47	9	false	9	(1 m:R01799) (1 m:R02030) (1 m:R02240) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CTP + PI + Phosphatidylglycerol = CMP + Cardiolipin + inositolHP
48	11	false	11	(-1 m:R00840) (1 m:R01185) (1 m:R01799) (1 m:R01802) (1 m:R02240) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CTP + G6P = CMP + inositolHP
49	11	false	11	(1 m:R01184) (1 m:R01187) (1 m:R02240) (1 m:R02241) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CoA + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + D-Glucuronate
50	12	false	12	(1 m:R01184) (1 m:R01187) (1 m:R01799) (1 m:R02030) (1 m:R02240) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CTP + Oxygen + PI + Phosphatidylglycerol = CMP + Cardiolipin + D-Glucuronate
51	11	false	11	(1 m:R01187) (1 m:R01799) (1 m:R01802) (1 m:R02240) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CTP = CMP
52	9	false	9	(1 m:R01184) (1 m:R01186) (1 m:R02240) (1 m:R02241) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CoA + Oxygen + PI = 1-Acyl-sn-glycerol3-P + Acyl-CoA + D-Glucuronate
53	10	false	10	(1 m:R01184) (1 m:R01186) (1 m:R01799) (1 m:R02030) (1 m:R02240) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CTP + Oxygen + PI + Phosphatidylglycerol = CMP + Cardiolipin + D-Glucuronate
54	9	false	9	(1 m:R01186) (1 m:R01799) (1 m:R01802) (1 m:R02240) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CTP = CMP
55	9	false	9	(1 m:R01321) (1 m:R02114) (1 m:R02746) (1 m:R03361) (1 m:R03435) (1 m:R03469) (-1 m:R05202) (1 m:R05800) (1 m:R05801)	CDP-choline + PI + Sterol = CMP + Fattyacid + Sterylester + inositolHP + sn-glycero-3-Pcholine

large phagosome EMs

56	12	false	12	(1 m:R01184) (1 m:R01187) (1 m:R01321) (1 m:R02114) (1 m:R02746) (1 m:R03361) (1 m:R03427) (1 m:R03430) (1 m:R03433) (1 m:R03435) (1 m:R03469) (1 m:R04372)	CDP-choline + Oxygen + PI + Sterol = CMP + D-Glucuronate + Fattyacid + Sterylester + sn-glycero-3-Pcholine
57	10	false	10	(1 m:R01184) (1 m:R01186) (1 m:R01321) (1 m:R02114) (1 m:R02746) (1 m:R03361) (1 m:R03393) (1 m:R03394) (1 m:R03435) (1 m:R03469)	CDP-choline + Oxygen + PI + Sterol = CMP + D-Glucuronate + Fattyacid + Sterylester + sn-glycero-3-Pcholine

Table 7: *S. saprophyticus* network - metabolites

Name	internal?	Connectivity	Description
(5-P-D-R)anthranilate	true	2	N-(5-Phospho-D-ribosyl)anthranilate
1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	true	2	1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose_5-phosphate
2-(A-Hydroxyethyl)thiamine_diP	true	3	2-(alpha-Hydroxyethyl)thiamine_diphosphate
2-Oxobutanoate	true	2	2-Oxobutanoate
2-P-D-GA	true	2	2-Phospho-D-glycerate
23-Dihydrodipicolinate	true	2	2,3-Dihydrodipicolinate
2345-Tetrahydrodipicolinate	true	2	2,3,4,5-Tetrahydrodipicolinate
3-(4-Hydroxyphenyl)PYR	true	2	3-(4-Hydroxyphenyl)pyruvate
3-(Imidazol-4-yl)-2-oxopropyl_P	true	2	3-(Imidazol-4-yl)-2-oxopropyl_phosphate
3-DehydroShi	true	2	3-Dehydroshikimate
3-Methyl-2-oxobutanoate	true	3	3-Methyl-2-oxobutanoate
3-P-D-GA	true	2	3-Phospho-D-glycerate
3-P-D-glyceroyl_P	true	2	3-Phospho-D-glyceroyl_phosphate
4-Imidazolone-5-propanoate	true	3	4-Imidazolone-5-propanoate
4-P-L-Asp	true	2	4-Phospho-L-aspartate
5-O-(1-Carboxyvinyl)-3-PShi	true	2	5-O-(1-Carboxyvinyl)-3-phosphoshikimate
510-MethyleneTHF	true	2	5,10-Methylenetetrahydrofolate
6PGlucon	true	2	6-Phospho-D-gluconate
Ac	true	4	Acetate
Ac-CoA	true	6	Acetyl-CoA
Acetaldehyde	true	1	Acetaldehyde
AICAR	true	2	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide
AKG	true	14	2-Oxoglutarate
Ala-tRNA(ex)	false	1	Ala-tRNA(ex)
Anthranilate	true	2	Anthranilate
Arg-tRNA(ex)	false	1	Arg-tRNA(ex)
Asn-tRNA(ex)	false	1	Asn-tRNA(ex)
Asp-tRNA(ex)	false	1	Asp-tRNA(ex)
Carbamoyl_P	true	2	Carbamoyl_phosphate
Chor	true	3	Chorismate
cis-Acon	true	2	cis-Aconitate
Cit	true	2	Citrate
CoA	true	9	CoA
Cys-tRNA(ex)	false	1	Cys-tRNA(ex)
D-Ala	true	2	D-Alanine
D-E4P	true	3	D-Erythrose_4-phosphate
D-erythro-1-(Imidazol-4-yl)glycerol_3-P	true	2	D-erythro-1-(Imidazol-4-yl)glycerol_3-phosphate

SAP metabolites

D-F	true	2	D-Fructose
D-F_16-BP	true	3	D-Fructose_1,6-bisphosphate
D-F_6-P	true	6	D-Fructose_6-phosphate
D-G(ex)	false	1	D-Glucose(ex)
D-G_6-P	true	4	D-Glucose_6-phosphate
D-Glu	true	2	D-Glutamate
D-Glucono-15-lactone_6-P	true	2	D-Glucono-1,5-lactone_6-phosphate
D-Ri_5-P	true	3	D-Ribose_5-phosphate
D-Ru_5-P	true	3	D-Ribulose_5-phosphate
D-S7P	true	2	D-Sedoheptulose_7-phosphate
D-Xu_5-P	true	3	D-Xylulose_5-phosphate
DAHP	true	2	2-Dehydro-3-deoxy-D-arabino-heptonate_7-phosphate
DHQ	true	2	3-Dehydroquinate
FAD	false	1	FAD
FADH2	false	1	FADH2
Formamide	true	1	Formamide
Formimino-L-Glu	true	2	N-Formimino-L-glutamate
Fum	true	3	Fumarate
GA_P	true	7	(2R)-2-Hydroxy-3-(phosphonoxy)-propanal
Gln-tRNA(ex)	false	1	Gln-tRNA(ex)
Glu-tRNA(ex)	false	1	Glu-tRNA(ex)
Gly	true	3	Glycine
Gly-tRNA(ex)	false	1	Gly-tRNA(ex)
Glycerone_P	true	2	Glycerone_phosphate
His-tRNA(ex)	false	1	His-tRNA(ex)
Ile-tRNA(ex)	false	1	Ile-tRNA(ex)
Indoleglycerol_P	true	2	Indoleglycerol_phosphate
IsoCit	true	2	Isocitrate
L-Ala	true	2	L-Alanine
L-Arg	true	4	L-Arginine
L-Asn	true	2	L-Asparagine
L-Asp	true	5	L-Aspartate
L-Asp_4-semialdehyde	true	3	L-Aspartate_4-semialdehyde
L-Citrulline	true	3	L-Citrulline
L-Cys	true	3	L-Cysteine
L-Gln	true	5	L-Glutamine
L-Glu	true	17	L-Glutamate
L-His	true	3	L-Histidine
L-Histidinol	true	2	L-Histidinol
L-Histidinol_P	true	2	L-Histidinol_phosphate

SAP metabolites

L-HomoCys	true	2	L-Homocysteine
L-HomoSer	true	3	L-Homoserine
L-Ile	true	2	L-Isoleucine
L-Leu	true	2	L-Leucine
L-Lys	true	2	L-Lysine
L-Met	true	2	L-Methionine
L-Orn	true	5	L-Ornithine
L-PhenylAla	true	2	L-Phenylalanine
L-Pro	true	3	L-Proline
L-Ser	true	5	L-Serine
L-Thr	true	3	L-Threonine
L-Try	true	2	L-Tryptophane
L-Tyr	true	2	L-Tyrosine
L-Val	true	2	L-Valine
Leu-tRNA(ex)	false	1	Leu-tRNA(ex)
Lys-tRNA(ex)	false	1	Lys-tRNA(ex)
Mal	true	3	(S)-Malate
Met-tRNA(ex)	false	1	Met-tRNA(ex)
NAD+	false	12	NAD+
NADH	false	12	NADH
NADP+	true	11	NADP+
NADPH	true	11	NADPH
NH3	true	11	NH3
NH3(ex)	false	1	NH3(ex)
O-Ac-L-Ser	true	2	O-Acetyl-L-serine
O-P-L-homoSer	true	2	O-Phospho-L-homoserine
OAA	true	5	Oxaloacetate
OASucc	true	2	Oxalosuccinate
PEP	true	7	Phosphoenolpyruvate
Phe-tRNA(ex)	false	1	Phe-tRNA(ex)
PhenylPYR	true	2	Phenylpyruvate
PR-AMP	true	2	Phosphoribosyl-AMP
PR-ATP	true	2	Phosphoribosyl-ATP
PR-formimino-AICAR-P	true	2	5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4-carboxamide
Prephenate	true	3	Prephenate
Pribulosyl-formimino-AICAR-P	true	2	N-(5-Phospho-D-1-ribulosylformimino)-5-amino-1-(5-phospho-D-ribosyl)-4-imidazolecarboxamide
Pro-tRNA(ex)	false	1	Pro-tRNA(ex)
PRPP	true	4	5-Phospho-D-ribose_1-diphosphate
Purine(ex)	false	1	Purine(ex)

SAP metabolites

PYR	true	13	Pyruvate
Pyrimidine(ex)	false	1	Pyrimidine(ex)
Ser-tRNA(ex)	false	1	Ser-tRNA(ex)
Shi	true	2	Shikimate
Shi_3-P	true	2	Shikimate_3-phosphate
Succ	true	3	Succinate
SuccCoA	true	3	Succinyl-CoA
Sucrose_6-P	true	1	Sucrose_6-phosphate
THF	true	2	Tetrahydrofolate
Thiamin_diP	true	3	Thiamin_diphosphate
Thr-tRNA(ex)	false	1	Thr-tRNA(ex)
Try-tRNA(ex)	false	1	Try-tRNA(ex)
Tyr-tRNA(ex)	false	1	Tyr-tRNA(ex)
Urea	true	2	Urea
Urocanate	true	2	Urocanate
Val-tRNA(ex)	false	1	Val-tRNA(ex)

Table 8: *S. saprophyticus* network - reactions

Enzyme name	rev.?	Reaction equation	Annotation
rn:E0001	false	L-PhenylAla = Phe-tRNA(ex)	PheX [6.1.1.20]
rn:E0002	false	L-Tyr = Tyr-tRNA(ex)	TyrX [6.1.1.1]
rn:E0003	false	L-Try = Try-tRNA(ex)	TryX [6.1.1.-]
rn:E0004	false	L-His = His-tRNA(ex)	HisX [6.1.1.21]
rn:E0005	false	L-Met = Met-tRNA(ex)	MetX [6.1.1.10]
rn:E0006	false	L-Thr = Thr-tRNA(ex)	ThrX [6.1.1.3]
rn:E0007	false	Gly = Gly-tRNA(ex)	GlyX [6.1.1.14]
rn:E0008	false	L-Ser = Ser-tRNA(ex)	SerX [6.1.1.11]
rn:E0009	false	L-Cys = Cys-tRNA(ex)	CysX [6.1.1.16]
rn:E0010	false	L-Lys = Lys-tRNA(ex)	LysX [6.1.1.6]
rn:E0011	false	L-Asn = Asn-tRNA(ex)	AsnX [6.1.1.22]
rn:E0012	false	L-Asp = Asp-tRNA(ex)	AspX [6.1.1.12]
rn:E0013	false	L-Ala = Ala-tRNA(ex)	AlaX [6.1.1.7]
rn:E0014	false	L-Pro = Pro-tRNA(ex)	ProX [6.1.1.15]
rn:E0015	false	L-Arg = Arg-tRNA(ex)	ArgX [6.1.1.19]
rn:E0016	false	L-Glu = Glu-tRNA(ex)	GluX [6.1.1.17]
rn:E0017	false	L-Gln = Gln-tRNA(ex)	GlnX [6.1.1.17]
rn:E0018	false	L-Ile = Ile-tRNA(ex)	IleX [6.1.1.5]
rn:E0019	false	L-Val = Val-tRNA(ex)	ValX [6.1.1.9]
rn:E0020	false	L-Leu = Leu-tRNA(ex)	LeuX [6.1.1.4]
rn:N001	false	AICAR = Purine(ex)	PurineMeta []
rn:N002	false	PRPP = Pyrimidine(ex)	PyrimidineMeta []
rn:R001	false	PYR = PEP	PPDK [2.7.9.1]
rn:R002	false	4-Imidazolone-5-propanoate = 2 L-Glu	HisMetaEnzOxReDase [1.14.13.-]
rn:U0015	false	1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P = Indoleglycerol_P	indole-3-glycerolphosphatesynthase [4.1.1.48]
rn:U0018	false	L-Gln = Carbamoyl_P + L-Glu	carbamoyl-phosphatesynthase [6.3.5.5]
rn:U0020	false	23-Dihydrodipicolinate + NADPH = 2345-Tetrahydrodipicolinate + NADP+	dihydrodipicolinate reductase [1.3.1.26]
rn:U0021	false	DAHP = DHQ	3-dehydroquinate synthase [4.2.3.4]
rn:U0038	false	3-Methyl-2-oxobutanoate + L-Glu = AKG + L-Val	branched-chain amino acid aminotransferase [2.6.1.42]
rn:U0045	false	4-Imidazolone-5-propanoate = Formimino-L-Glu	imidazolone propionase [3.5.2.7]
rn:U0047	false	4-P-L-Asp + NADPH = L-Asp_4-semialdehyde + NADP+	aspartate semialdehyde dehydrogenase [1.2.1.11]
rn:U0048	false	PR-formimino-AICAR-P = Pribulosyl-formimino-AICAR-P	putative phosphoribosylformimino-5-aminoimidazolecarboxamide ribotide isomerase [5.3.1.16]
rn:U0049	false	510-MethyleneTHF + Gly = L-Ser + THF	serine hydroxymethyltransferase [2.1.2.1]

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rn:U0050	false	L-HomoCys = L-Met	5-methyltetrahydropteroyltriglutamate-homocysteinemethyltransferase [2.1.1.14]
rn:U0052	false	5-O-(1-Carboxyvinyl)-3-PShi = Chor	chorismatesynthase [4.2.3.5]
rn:U0057	false	Anthranilate + PRPP = (5-P-D-R)anthranilate	anthranilatephosphoribosyltransferase [2.4.2.18]
rn:U0058	false	L-Asp + L-Gln = L-Asn + L-Glu	asparagine synthase [6.3.5.4]
rn:U0059	false	L-Asp = 4-P-L-Asp	asparto kinase II [2.7.2.4]
rn:U0061	false	L-Glu + NH ₃ = L-Gln	glutamine-ammonialigase [6.3.1.2]
rn:U0062	false	L-HomoSer = O-P-L-homoSer	homoserinekinase [2.7.1.39]
rn:U0065	false	Shi = Shi_3-P	shikimatekinase(SK) [2.7.1.71]
rn:U0068	false	Carbamoyl_P + L-Orn = L-Citrulline	ornithinecarbamoyltransferase [2.1.3.3]
rn:U0072	false	Chor + NH ₃ = Anthranilate + PYR	anthranilatesynthase [4.1.3.27]
rn:U0073	false	Chor = Prephenate	chorismatemutase [5.4.99.5]
		D-erythro-1-(Imidazol-4-yl)glycerol_3-P = 3-(Imidazol-4-yl)-2-oxopropyl_P	imidazoleglycerol-phosphatedehydratase [4.2.1.19]
rn:U0075	false		
rn:U0089	false	L-Arg = L-Citrulline + NH ₃	argininedeiminase [3.5.3.6]
rn:U0090	false	L-Arg = L-Orn + Urea	arginase [3.5.3.1]
rn:U0093	false	L-Glu + OAA = AKG + L-Asp	aspartate transaminase [2.6.1.1]
rn:U0095	false	L-Asp_4-semialdehyde + PYR = 23-Dihydrodipicolinate	dihydrodipicolinate synthase [4.2.1.52]
rn:U0100	true	L-Glu = D-Glu	glutamateracemase [5.1.1.3]
rn:U0104	false	L-Histidinol + 2 NAD ⁺ = L-His + 2 NADH	putative histidinoldehydrogenase [1.1.1.23]
rn:U0105	false	L-Histidinol_P = L-Histidinol	putative histidinol phosphatase [3.1.3.15]
rn:U0106	true	L-HomoSer + NADP ⁺ = L-Asp_4-semialdehyde + NADPH	homoserine dehydrogenase [1.1.1.3]
rn:U0112	false	L-Orn = L-Pro + NH ₃	putative ornithinecyclodeaminase [4.3.1.12]
rn:U0114	false	Ac-CoA + L-Ser = CoA + O-Ac-L-Ser	serineO-acetyltransferase [2.3.1.30]
rn:U0116	false	Indoleglycerol_P + L-Ser = GA_P + L-Try	tryptophan synthase [4.2.1.20]
rn:U0117	false	NH ₃ + PYR = L-Ser	thereoninedehydratase [4.3.1.19, 4.3.1.17]
rn:U0121	false	L-Thr = 2-Oxobutanoate + NH ₃	thereoninedehydratase [4.3.1.19]
		Pribulosyl-formimino-AICAR-P = AICAR + D-erythro-1-(Imidazol-4-yl)glycerol_3-P	amidotransferasehisH [2.4.2.-]
rn:U0125	false		
rn:U0126	false	(5-P-D-R)anthranilate = 1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	phosphoriborylanthranilateisomerase [5.3.1.24]
rn:U0134	false	Formimino-L-Glu = Formamide + L-Glu	hypothetical protein,similartoformiminoglutamase [3.5.3.8]
rn:U0138	false	O-P-L-homoSer = L-Thr	threoninesynthase [4.2.3.1]
rn:U0141	false	D-E4P + PEP = DAHP	phospho-2-dehydro-3-deoxyheptonate aldo [2.5.1.54]
rn:U0142	false	PEP + Shi_3-P = 5-O-(1-Carboxyvinyl)-3-PShi	3-phosphoshikimate1-carboxyvinyltransferase [2.5.1.19]
rn:U0143	false	PR-AMP = PR-formimino-AICAR-P	histidinebiosynthesisbifunctionalproteinHisIE [3.5.4.19]
rn:U0144	false	PR-ATP = PR-AMP	histidinebiosynthesisbifunctionalproteinHisIE [3.6.1.31]
rn:U0145	false	PRPP = PR-ATP	ATPphosphoribosyltransferase [2.4.2.17]
rn:U0146	false	NAD ⁺ + Prephenate = 3-(4-Hydroxyphenyl)PYR + NADH	prephenatedehydrogenase [1.3.1.12]

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rn:U0147	false	Prephenate = PhenylPYR	prephenate dehydratase [4.2.1.51]
rn:U0155	false	3-DehydroShi + NADPH = NADP+ + Shi	shikimate dehydrogenase [1.1.1.25]
rn:U0160	false	Urea = 2 NH ₃	urease [3.5.1.5]
rn:U0161	false	Urocanate = 4-Imidazolone-5-propanoate	urocanate hydratase [4.2.1.49]
rn:U0166	false	3-(Imidazol-4-yl)-2-oxopropyl_P + L-Glu = AKG + L-Histidinol_P	putative histidinol-phosphate aminotransferase [2.6.1.9]
rn:U0167	false	L-Glu + PhenylPYR = AKG + L-PhenylAla	putative histidinol-phosphate aminotransferase [2.6.1.9]
rn:U0168	false	3-(4-Hydroxyphenyl)PYR + L-Glu = AKG + L-Tyr	putative histidinol-phosphate transaminase [2.6.1.9]
rn:U0179	false	Acetaldehyde + NAD+ = Ac + NADH	aldehyde dehydrogenase [1.2.1.3]
rn:U0188	false	DHQ = 3-DehydroShi	enolase [4.2.1.11, 4.2.1.10]
rn:U0195	false	PYR + Thiamin_diP = 2-(A-Hydroxyethyl)thiamine_diP	pyruvate dehydrogenase_ acetolactate synthase [1.2.4.1, 2.2.1.6]
rn:U0198	false	O-Ac-L-Ser = Ac + L-Cys	cysteine synthase [2.5.1.47]
rn:U0209	false	D-Ala = L-Ala	alanine racemase [5.1.1.1]
rn:U0238	false	GA_P + NAD+ = 3-P-D-glyceroyl_P + NADH	glyceraldehyde-3-phosphate dehydrogenase [1.2.1.12]
rn:U0239	false	Glycerone_P = GA_P	triose phosphate isomerase [5.3.1.1]
rn:U0244	false	Mal + NAD+ = NADH + OAA	MDH [1.1.1.37]
rn:U0245	true	Mal + NAD+ = NADH + PYR	malate dehydrogenase homolog [1.1.1.38]
rn:U0246	false	Fum = Mal	fumarate hydratase, class-II [4.2.1.2]
rn:U0255	false	3-P-D-GA = 2-P-D-GA	phosphoglycerate mutase [5.4.2.1]
rn:U0256	false	2-P-D-GA = PEP	enolase [4.2.1.11]
rn:U0260	false	6PGlucon + NADP+ = D-Ru_5-P + NADPH	phosphogluconate dehydrogenase [1.1.1.44]
rn:U0267	false	Ac-CoA + OAA = Cit + CoA	citrate synthase [2.3.3.1]
rn:U0269	false	PEP = PYR	pyruvate kinase [2.7.1.40]
rn:U0270	false	3-P-D-glyceroyl_P = 3-P-D-GA	phosphoglycerate kinase [2.7.2.3]
rn:U0271	false	Ac + CoA = Ac-CoA	acetyl-CoA synthetase AND ligase [6.2.1.1]
rn:U0274	false	D-F = D-F_6-P	fructokinase, putative [2.7.1.4]
rn:U0276	false	D-F_6-P = D-F_16-BP	6-phosphofructokinase [2.7.1.11]
rn:U0280	false	D-Ri_5-P = PRPP	ribose-phosphate pyrophosphokinase [2.7.6.1]
rn:U0284	false	OAA = PEP	phosphoenolpyruvate carboxykinase [4.1.1.49]
rn:U0287	false	PYR = OAA	pyruvate carboxylase [6.4.1.1]
rn:U0288	true	CoA + Succ = SuccCoA	succinyl-CoA synthetase [6.2.1.5]
rn:U0294	false	D-F_16-BP = D-F_6-P	fructose-bisphosphatase [3.1.3.11]
rn:U0295	true	D-F_6-P + GA_P = D-E4P + D-Xu_5-P	transketolase [2.2.1.1]
rn:U0297	false	D-Glucono-15-lactone_6-P = 6PGlucon	Spon_PGLactonohydrolase [3.1.1.31]
rn:U0301	false	D-G_6-P + NADP+ = D-Glucono-15-lactone_6-P + NADPH	glucose-6-phosphate 1-dehydrogenase [1.1.1.49]
rn:U0302	false	D-G_6-P = D-F_6-P	glucose-6-phosphate isomerase A [5.3.1.9]
rn:U0311	false	D-Ru_5-P = D-Ri_5-P	ribose 5-phosphate isomerase A [5.3.1.6]
rn:U0314	false	D-Ru_5-P = D-Xu_5-P	ribulose-phosphate 3-epimerase [5.1.3.1]
rn:U0315	true	D-S7P + GA_P = D-E4P + D-F_6-P	Transaldolase superfamily [2.2.1.2]

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rn:U0316	true	D-S7P + GA_P = D-Ri_5-P + D-Xu_5-P	transketolase [2.2.1.1]
rn:U0324	false	IsoCit + NADP+ = NADPH + OASucc	isocitrate dehydrogenase [1.1.1.42]
rn:U0335	false	OASucc = AKG	isocitrate dehydrogenase [1.1.1.42]
rn:U0345	false	FAD + Succ = FADH2 + Fum	succinate dehydrogenase [1.3.99.1]
rn:U0348	false	Sucrose_6-P = D-F + D-G_6-P	sucrose-6-phosphatehydrolase [3.2.1.26]
rn:U0358	false	cis-Acon = IsoCit	aconitate hydratase [4.2.1.3]
rn:U0359	false	Cit = cis-Acon	aconitate hydratase [4.2.1.3]
rn:U0360	false	D-F_16-BP = GA_P + Glycerone_P	fructose-bisphosphate aldolase [4.1.2.13]
rn:U0372	false	AKG + L-Gln + NADPH = 2 L-Glu + NADP+	glutamatesynthase [1.4.1.13]
rn:U0384	false	L-His = NH3 + Urocanate	histidineammonia-lyase [4.3.1.3]
rn:U0522	true	NH3(ex) = NH3	probabile ammonium transporter [2.A.49]
rn:U0534	false	D-G(ex) + PEP = D-G_6-P + PYR	glucose-specific PTS [2.7.1.69, 2.7.3.9]
rn:U0673	true	AKG + D-Ala = D-Glu + PYR	D-alanineaminotransferase [2.6.1.21]
rn:U0986	false	2 L-Glu + NADH = AKG + L-Orn + NAD+	EZComp_UreaOrnSyn [1.5.1.12, 2.6.1.13]
rn:U0987	false	2345-Tetrahydrodipicolinate + L-Glu + SuccCoA = AKG + CoA + L-Lys + Succ	EZComp_LysSyn [2.3.1.117, 2.6.1.17, 3.5.1.18, 5.1.1.7, 4.1.1.20]
rn:U0988	false	AKG + CoA + NAD+ = NADH + SuccCoA	EZComp_TCASuccinyl [1.2.4.2, 2.3.1.61, 1.8.1.4]
rn:U0989	false	2-(A-Hydroxyethyl)thiamine_diP + 2-Oxobutanoate + L-Glu + NADPH = AKG + L-Ile + NADP+ + Thiamin_diP	EZComp_Ile_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9, 2.6.1.42]
rn:U0990	false	2-(A-Hydroxyethyl)thiamine_diP + NADPH + PYR = 3-Methyl-2-oxobutanoate + NADP+ + Thiamin_diP	EZComp_Val_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9]
rn:U0991	false	3-Methyl-2-oxobutanoate + Ac-CoA + L-Glu + NAD+ = AKG + CoA + L-Leu + NADH	EZComp_Leu_Meta [2.3.3.13, 4.2.1.33, 1.1.1.85, 2.6.1.42]
rn:U0993	false	L-Asp + L-Citrulline = Fum + L-Arg	EZComp_Fum_Asp [4.3.2.1, 6.3.4.5]
rn:U0994	false	CoA + NAD+ + PYR = Ac-CoA + NADH	EZComp_PyrAcetylCoA [1.2.4.1, 2.3.1.12, 1.8.1.4]
rn:U0995	false	Gly + NAD+ + THF = 510-MethyleneTHF + NADH + NH3	EZComp_GlySerThrMeta [2.1.2.10, 1.8.1.4, 1.4.4.2]
rn:U0996	false	Ac-CoA + L-Cys + L-HomoSer = Ac + CoA + L-HomoCys + NH3 + PYR	EZComp_MetMeta [2.3.1.31, 2.5.1.48, 4.4.1.8]
rn:U0997	false	AKG + L-Orn + NADH + 2 NADPH = 2 L-Pro + NAD+ + 2 NADP+	EZComp_UreaMeta [1.5.1.2, 1.5.1.12, 2.6.1.13]

Table 9: *S. saprophyticus* network - Elementary Modes discussed in the results section¹

#	Flux sum	Rev. ²	Length	Reactions ³	Net reaction
4	190	false	25	(12 m:E0012) (12 m:U0061) (12 m:U0093) (12 m:U0238) (12 m:U0239) (12 m:U0244) (-12 m:U0245) (12 m:U0255) (12 m:U0256) (6 m:U0260) (5 m:U0269) (12 m:U0270) (5 m:U0276) (-2 m:U0295) (6 m:U0297) (6 m:U0301) (1 m:U0302) (2 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (5 m:U0360) (12 m:U0372) (12 m:U0522) (7 m:U0534)	5 7 D-G(ex) + 12 NAD ⁺ + 12 NH ₃ (ex) = 12 Asp-tRNA(ex) + 12 NADH
5	226	false	26	(12 m:E0011) (12 m:U0058) (24 m:U0061) (12 m:U0093) (12 m:U0238) (5 m:U0239) (12 m:U0244) (-12 m:U0245) (12 m:U0255) (12 m:U0256) (6 m:U0260) (5 m:U0269) (12 m:U0270) (5 m:U0276) (-2 m:U0295) (6 m:U0297) (6 m:U0301) (1 m:U0302) (2 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (5 m:U0360) (12 m:U0372) (24 m:U0522) (7 m:U0534)	7 D-G(ex) + 12 NAD ⁺ + 24 NH ₃ (ex) = 12 Asn-tRNA(ex) + 12 NADH
6	103	false	27	(5 m:E0008) (6 m:U0061) (6 m:U0089) (6 m:U0093) (5 m:U0117) (5 m:U0238) (2 m:U0239) (6 m:U0244) (6 m:U0246) (5 m:U0255) (5 m:U0256) (3 m:U0260) (2 m:U0269) (5 m:U0270) (2 m:U0276) (-1 m:U0295) (3 m:U0297) (3 m:U0301) (1 m:U0311) (2 m:U0314) (1 m:U0315) (-1 m:U0316) (2 m:U0360) (6 m:U0372) (5 m:U0522) (3 m:U0534) (6 m:U0993)	3 D-G(ex) + 11 NAD ⁺ + 5 NH ₃ (ex) = 11 NADH + 5 Ser-tRNA(ex)
7	88	false	27	(5 m:E0012) (6 m:U0061) (1 m:U0089) (6 m:U0093) (5 m:U0238) (2 m:U0239) (6 m:U0244) (-5 m:U0245) (1 m:U0246) (5 m:U0255) (5 m:U0256) (3 m:U0260) (2 m:U0269) (5 m:U0270) (2 m:U0276) (-1 m:U0295) (3 m:U0297) (3 m:U0301) (1 m:U0311) (2 m:U0314) (1 m:U0315) (-1 m:U0316) (2 m:U0360) (6 m:U0372) (5 m:U0522) (3 m:U0534) (1 m:U0993)	3 D-G(ex) + 6 NAD ⁺ + 5 NH ₃ (ex) = 5 Asp-tRNA(ex) + 6 NADH
8	103	false	28	(5 m:E0011) (5 m:U0058) (11 m:U0061) (1 m:U0089) (6 m:U0093) (5 m:U0238) (2 m:U0239) (6 m:U0244) (-5 m:U0245) (1 m:U0246) (5 m:U0255) (5 m:U0256) (3 m:U0260) (2 m:U0269) (5 m:U0270) (2 m:U0276) (-1 m:U0295) (3 m:U0297) (3 m:U0301) (1 m:U0311) (2 m:U0314) (1 m:U0315) (-1 m:U0316) (2 m:U0360) (6 m:U0372) (10 m:U0522) (3 m:U0534) (1 m:U0993)	3 D-G(ex) + 6 NAD ⁺ + 10 NH ₃ (ex) = 5 Asn-tRNA(ex) + 6 NADH

SAP EMs

21	188	false	32	(1 m:E0010) (8 m:E0011) (1 m:U0020) (1 m:U0047) (8 m:U0058) (1 m:U0059) (18 m:U0061) (9 m:U0093) (1 m:U0095) (10 m:U0238) (4 m:U0239) (9 m:U0244) (-9 m:U0245) (10 m:U0255) (10 m:U0256) (6 m:U0260) (4 m:U0269) (10 m:U0270) (4 m:U0276) (1 m:U0288) (-2 m:U0295) (6 m:U0297) (6 m:U0301) (2 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (4 m:U0360) (10 m:U0372) (18 m:U0522) (6 m:U0534) (1 m:U0987)	6 D-G(ex) + 10 NAD ⁺ + 18 NH ₃ (ex) = 8 Asn-tRNA(ex) + Lys-tRNA(ex) + 10 NADH
22	136	false	34	(1 m:E0010) (4 m:E0019) (1 m:U0020) (4 m:U0038) (1 m:U0047) (1 m:U0059) (6 m:U0061) (1 m:U0093) (1 m:U0095) (4 m:U0195) (10 m:U0238) (4 m:U0239) (1 m:U0244) (-1 m:U0245) (10 m:U0255) (10 m:U0256) (6 m:U0260) (4 m:U0269) (10 m:U0270) (4 m:U0276) (1 m:U0288) (-2 m:U0295) (6 m:U0297) (6 m:U0301) (2 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (4 m:U0360) (6 m:U0372) (6 m:U0522) (6 m:U0534) (1 m:U0987) (4 m:U0990)	6 D-G(ex) + 10 NAD ⁺ + 6 NH ₃ (ex) = Lys-tRNA(ex) + 10 NADH + 4 Val-tRNA(ex)
24	88	false	29	(5 m:E0013) (6 m:U0061) (1 m:U0089) (1 m:U0093) (5 m:U0100) (5 m:U0209) (5 m:U0238) (2 m:U0239) (1 m:U0244) (1 m:U0246) (5 m:U0255) (5 m:U0256) (3 m:U0260) (2 m:U0269) (5 m:U0270) (2 m:U0276) (-1 m:U0295) (3 m:U0297) (3 m:U0301) (1 m:U0311) (2 m:U0314) (1 m:U0315) (-1 m:U0316) (2 m:U0360) (6 m:U0372) (5 m:U0522) (3 m:U0534) (-5 m:U0673) (1 m:U0993)	3 D-G(ex) + 6 NAD ⁺ + 5 NH ₃ (ex) = 5 Ala-tRNA(ex) + 6 NADH

¹ complete list available from the authors on request

² reversible

³ reaction identifiers are taken from KEGG, for annotations see the reaction table

Table 10: *S. aureus* network - metabolites

Name	internal?	Connectivity	Description
(5-P-D-R)anthranilate	true	2	N-(5-Phospho-D-ribosyl)anthranilate
1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	true	2	1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose_5-phosphate
2-(A-Hydroxyethyl)thiamine_diP	true	3	2-(alpha-Hydroxyethyl)thiamine_diphosphate
2-Oxobutanoate	true	2	2-Oxobutanoate
2-P-D-GA	true	2	2-Phospho-D-glycerate
23-Dihydrodipicolinate	true	2	2,3-Dihydrodipicolinate
2345-Tetrahydrodipicolinate	true	2	2,3,4,5-Tetrahydrodipicolinate
3-(4-Hydroxyphenyl)PYR	true	2	3-(4-Hydroxyphenyl)pyruvate
3-(Imidazol-4-yl)-2-oxopropyl_P	true	2	3-(Imidazol-4-yl)-2-oxopropyl_phosphate
3-DehydroShi	true	2	3-Dehydroshikimate
3-Methyl-2-oxobutanoate	true	3	3-Methyl-2-oxobutanoate
3-P-D-GA	true	2	3-Phospho-D-glycerate
3-P-D-glyceroyl_P	true	2	3-Phospho-D-glyceroyl_phosphate
4-Imidazolone-5-propanoate	true	2	4-Imidazolone-5-propanoate
4-P-L-Asp	true	2	4-Phospho-L-aspartate
5-O-(1-Carboxyvinyl)-3-PShi	true	2	5-O-(1-Carboxyvinyl)-3-phosphoshikimate
510-MethyleneTHF	true	2	5,10-Methylenetetrahydrofolate
6PGlucon	true	2	6-Phospho-D-gluconate
Ac	true	4	Acetate
Ac-CoA	true	6	Acetyl-CoA
Acetaldehyde	true	2	Acetaldehyde
AICAR	true	2	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide
AKG	true	14	2-Oxoglutarate
Ala-tRNA(ex)	false	1	Ala-tRNA(ex)
Anthranilate	true	2	Anthranilate
Arg-tRNA(ex)	false	1	Arg-tRNA(ex)
Asn-tRNA(ex)	false	1	Asn-tRNA(ex)
Asp-tRNA(ex)	false	1	Asp-tRNA(ex)
Carbamoyl_P	true	3	Carbamoyl_phosphate
Chor	true	3	Chorismate
cis-Acon	true	2	cis-Aconitate
Cit	true	2	Citrate
CoA	true	9	CoA
Cys-tRNA(ex)	false	1	Cys-tRNA(ex)
D-Ala	true	2	D-Alanine
D-E4P	true	3	D-Erythrose_4-phosphate
D-erythro-1-(Imidazol-4-yl)glycerol_3-P	true	2	D-erythro-1-(Imidazol-4-yl)glycerol_3-phosphate

SA metabolites

D-F	true	2	D-Fructose
D-F_16-BP	true	3	D-Fructose_1,6-bisphosphate
D-F_6-P	true	6	D-Fructose_6-phosphate
D-G(ex)	false	1	D-Glucose(ex)
D-G_6-P	true	4	D-Glucose_6-phosphate
D-Glu	true	2	D-Glutamate
D-Glucono-15-lactone_6-P	true	2	D-Glucono-1,5-lactone_6-phosphate
D-Ri_5-P	true	3	D-Ribose_5-phosphate
D-Ru_5-P	true	3	D-Ribulose_5-phosphate
D-S7P	true	2	D-Sedoheptulose_7-phosphate
D-Xu_5-P	true	3	D-Xylulose_5-phosphate
DAHP	true	2	2-Dehydro-3-deoxy-D-arabino-heptonate_7-phosphate
DHQ	true	2	3-Dehydroquinate
FAD	false	1	FAD
FADH2	false	1	FADH2
Formamide	true	1	Formamide
Formimino-L-Glu	true	2	N-Formimino-L-glutamate
Fum	true	3	Fumarate
GA_P	true	7	(2R)-2-Hydroxy-3-(phosphonoxy)-propanal
Gln-tRNA(ex)	false	1	Gln-tRNA(ex)
Glu-tRNA(ex)	false	1	Glu-tRNA(ex)
Gly	true	4	Glycine
Gly-tRNA(ex)	false	1	Gly-tRNA(ex)
Glycerone_P	true	2	Glycerone_phosphate
His-tRNA(ex)	false	1	His-tRNA(ex)
Ile-tRNA(ex)	false	1	Ile-tRNA(ex)
Indoleglycerol_P	true	2	Indoleglycerol_phosphate
IsoCit	true	2	Isocitrate
L-Ala	true	2	L-Alanine
L-Arg	true	4	L-Arginine
L-Asn	true	2	L-Asparagine
L-Asp	true	5	L-Aspartate
L-Asp_4-semialdehyde	true	3	L-Aspartate_4-semialdehyde
L-Citrulline	true	3	L-Citrulline
L-Cys	true	3	L-Cysteine
L-Gln	true	5	L-Glutamine
L-Glu	true	16	L-Glutamate
L-His	true	3	L-Histidine
L-Histidinol	true	2	L-Histidinol
L-Histidinol_P	true	2	L-Histidinol_phosphate

SA metabolites

L-HomoCys	true	2	L-Homocysteine
L-HomoSer	true	3	L-Homoserine
L-Ile	true	2	L-Isoleucine
L-Leu	true	2	L-Leucine
L-Lys	true	2	L-Lysine
L-Met	true	2	L-Methionine
L-Orn	true	5	L-Ornithine
L-PhenylAla	true	2	L-Phenylalanine
L-Pro	true	3	L-Proline
L-Ser	true	5	L-Serine
L-Thr	true	4	L-Threonine
L-Try	true	2	L-Tryptophane
L-Tyr	true	2	L-Tyrosine
L-Val	true	2	L-Valine
Leu-tRNA(ex)	false	1	Leu-tRNA(ex)
Lys-tRNA(ex)	false	1	Lys-tRNA(ex)
Mal	true	3	(S)-Malate
Menaquinol	true	1	Menaquinol
Menaquinone	true	1	Menaquinone
Met-tRNA(ex)	false	1	Met-tRNA(ex)
NAD+	false	11	NAD+
NADH	false	11	NADH
NADP+	true	11	NADP+
NADPH	true	11	NADPH
NH3	true	12	NH3
NH3(ex)	false	1	NH3(ex)
O-Ac-L-Ser	true	2	O-Acetyl-L-serine
O-P-L-homoSer	true	2	O-Phospho-L-homoserine
OAA	true	5	Oxaloacetate
OASucc	true	2	Oxalosuccinate
PEP	true	6	Phosphoenolpyruvate
Phe-tRNA(ex)	false	1	Phe-tRNA(ex)
PhenylPYR	true	2	Phenylpyruvate
PR-AMP	true	2	Phosphoribosyl-AMP
PR-ATP	true	2	Phosphoribosyl-ATP
PR-formimino-AICAR-P	true	2	5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4-carboxamide
Prephenate	true	3	Prephenate
Pribulosyl-formimino-AICAR-P	true	2	N-(5-Phospho-D-1-ribulosylformimino)-5-amino-1-(5-phospho-D-ribosyl)-4-imidazolecarboxamide
Pro-tRNA(ex)	false	1	Pro-tRNA(ex)
PRPP	true	4	5-Phospho-D-ribose_1-diphosphate

SA metabolites

Purine(ex)	false	1	Purine(ex)
PYR	true	12	Pyruvate
Pyrimidine(ex)	false	1	Pyrimidine(ex)
Ser-tRNA(ex)	false	1	Ser-tRNA(ex)
Shi	true	2	Shikimate
Shi_3-P	true	2	Shikimate_3-phosphate
Succ	true	3	Succinate
SuccCoA	true	3	Succinyl-CoA
Sucrose_6-P	true	1	Sucrose_6-phosphate
THF	true	2	Tetrahydrofolate
Thiamin_diP	true	3	Thiamin_diphosphate
Thr-tRNA(ex)	false	1	Thr-tRNA(ex)
Try-tRNA(ex)	false	1	Try-tRNA(ex)
Tyr-tRNA(ex)	false	1	Tyr-tRNA(ex)
Urea	true	2	Urea
Urocanate	true	2	Urocanate
Val-tRNA(ex)	false	1	Val-tRNA(ex)

Table 11: *S. aureus* network - reactions

Enzyme name	rev.?	Reaction equation	Annotation
RN:E0001	false	L-PhenylAla = Phe-tRNA(ex)	PheX [6.1.1.20]
RN:E0002	false	L-Tyr = Tyr-tRNA(ex)	TyrX [6.1.1.1]
RN:E0003	false	L-Try = Try-tRNA(ex)	TryX [6.1.1.-]
RN:E0004	false	L-His = His-tRNA(ex)	HisX [6.1.1.21]
RN:E0005	false	L-Met = Met-tRNA(ex)	MetX [6.1.1.10]
RN:E0006	false	L-Thr = Thr-tRNA(ex)	ThrX [6.1.1.3]
RN:E0007	false	Gly = Gly-tRNA(ex)	GlyX [6.1.1.14]
RN:E0008	false	L-Ser = Ser-tRNA(ex)	SerX [6.1.1.11]
RN:E0009	false	L-Cys = Cys-tRNA(ex)	CysX [6.1.1.16]
RN:E0010	false	L-Lys = Lys-tRNA(ex)	LysX [6.1.1.6]
RN:E0011	false	L-Asn = Asn-tRNA(ex)	AsnX [6.1.1.22]
RN:E0012	false	L-Asp = Asp-tRNA(ex)	AspX [6.1.1.12]
RN:E0013	false	L-Ala = Ala-tRNA(ex)	AlaX [6.1.1.7]
RN:E0014	false	L-Pro = Pro-tRNA(ex)	ProX [6.1.1.15]
RN:E0015	false	L-Arg = Arg-tRNA(ex)	ArgX [6.1.1.19]
RN:E0016	false	L-Glu = Glu-tRNA(ex)	GluX [6.1.1.17]
RN:E0017	false	L-Gln = Gln-tRNA(ex)	GlnX [6.1.1.17]
RN:E0018	false	L-Ile = Ile-tRNA(ex)	IleX [6.1.1.5]
RN:E0019	false	L-Val = Val-tRNA(ex)	ValX [6.1.1.9]
RN:E0020	false	L-Leu = Leu-tRNA(ex)	LeuX [6.1.1.4]
RN:Nucl01	false	AICAR = Purine(ex)	PurineMeta []
RN:Nucl02	false	PRPP = Pyrimidine(ex)	PyrimidineMeta []
RN:R0015	false	1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P = Indoleglycerol_P	indole-3-glycerolphosphatesynthase [4.1.1.48]
RN:R0018	false	L-Gln = Carbamoyl_P + L-Glu	carbamoyl-phosphatesynthase [6.3.5.5]
RN:R0020	false	23-Dihydrodipicolinate + NADPH = 2345-Tetrahydrodipicolinate + NADP+	dihydrodipicolinate reductase [1.3.1.26]
RN:R0021	false	DAHPh = DHQ	3-dehydroquinatesynthase [4.2.3.4]
RN:R0038	false	3-Methyl-2-oxobutanoate + L-Glu = AKG + L-Val	branched-chainaminoacidaminotransferase [2.6.1.42]
RN:R0045	false	4-Imidazolone-5-propanoate = Formimino-L-Glu	imidazolonepropionase [3.5.2.7]
RN:R0047	false	4-P-L-Asp + NADPH = L-Asp_4-semialdehyde + NADP+	aspartate semialdehyde dehydrogenase [1.2.1.11]
RN:R0048	false	PR-formimino-AICAR-P = Pribulosyl-formimino-AICAR-P	putative phosphoribosylformimino-5-aminoimidazolecarboxamideriboti-deisomerase [5.3.1.16]
RN:R0049	false	510-MethyleneTHF + Gly = L-Ser + THF	serinehydroxymethyltransferase [2.1.2.1]
RN:R0050	false	L-HomoCys = L-Met	5-methyltetrahydropteroyltriglutamate-homocysteinemethyltransferase [2.1.1.14]

SA reactions

RN:R0052	false	5-O-(1-Carboxyvinyl)-3-PShi = Chor	chorismatesynthase [4.2.3.5]
RN:R0057	false	Anthranilate + PRPP = (5-P-D-R)anthranilate	anthranilatephosphoribosyltransferase [2.4.2.18]
RN:R0058	false	L-Asp + L-Gln = L-Asn + L-Glu	asparagine synthase [6.3.5.4]
RN:R0059	false	L-Asp = 4-P-L-Asp	asparto kinase II [2.7.2.4]
RN:R0061	false	L-Glu + NH ₃ = L-Gln	glutamine-ammonialigase [6.3.1.2]
RN:R0062	false	L-HomoSer = O-P-L-homoSer	homoserinekinase [2.7.1.39]
RN:R0065	false	Shi = Shi_3-P	shikimatekinase(SK) [2.7.1.71]
RN:R0068	false	Carbamoyl_P + L-Orn = L-Citrulline	ornithinecarbamoyltransferase [2.1.3.3]
RN:R0072	false	Chor + NH ₃ = Anthranilate + PYR	anthranilatesynthase [4.1.3.27]
RN:R0073	false	Chor = Prephenate	chorismatemutase [5.4.99.5]
		D-erythro-1-(Imidazol-4-yl)glycerol_3-P = 3-(Imidazol-4-yl)-2-oxopropyl_P	imidazoleglycerol-phosphatedehydratase [4.2.1.19]
RN:R0075	false		
RN:R0089	false	L-Arg = L-Citrulline + NH ₃	argininedeiminase [3.5.3.6]
RN:R0090	false	L-Arg = L-Orn + Urea	arginase [3.5.3.1]
RN:R0093	false	L-Glu + OAA = AKG + L-Asp	aspartate transaminase [2.6.1.1]
RN:R0095	false	L-Asp_4-semialdehyde + PYR = 23-Dihydrodipicolinate	dihydrodipicolinate synthase [4.2.1.52]
RN:R0100	true	L-Glu = D-Glu	glutamateracemase [5.1.1.3]
RN:R0104	false	L-Histidinol + 2 NAD ⁺ = L-His + 2 NADH	putative histidinoldehydrogenase [1.1.1.23]
RN:R0105	false	L-Histidinol_P = L-Histidinol	putative histidinol phosphatase [3.1.3.15]
RN:R0106	true	L-HomoSer + NADP ⁺ = L-Asp_4-semialdehyde + NADPH	homoserine dehydrogenase [1.1.1.3]
RN:R0112	false	L-Orn = L-Pro + NH ₃	putative ornithinecyclodeaminase [4.3.1.12]
RN:R0114	false	Ac-CoA + L-Ser = CoA + O-Ac-L-Ser	serineO-acetyltransferase [2.3.1.30]
RN:R0116	false	Indoleglycerol_P + L-Ser = GA_P + L-Try	tryptophan synthase [4.2.1.20]
RN:R0117	false	NH ₃ + PYR = L-Ser	thereoninedehydratase [4.3.1.19, 4.3.1.17]
RN:R0120	true	L-Thr = Acetaldehyde + Gly	putative threoninealdolase [4.1.2.5]
RN:R0121	false	L-Thr = 2-Oxobutanoate + NH ₃	thereoninedehydratase [4.3.1.19]
		Pribulosyl-formimino-AICAR-P = AICAR + D-erythro-1-(Imidazol-4-yl)glycerol_3-P	amidotransferasehisH [2.4.2.-]
RN:R0125	false		
RN:R0126	false	(5-P-D-R)anthranilate = 1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	phosphoriborylanthranilateisomerase [5.3.1.24]
RN:R0134	false	Formimino-L-Glu = Formamide + L-Glu	hypothetical protein,similartoformiminoglutamase [3.5.3.8]
RN:R0138	false	O-P-L-homoSer = L-Thr	threoninesynthase [4.2.3.1]
RN:R0141	false	D-E4P + PEP = DAHP	phospho-2-dehydro-3-deoxyheptonate aldo [2.5.1.54]
RN:R0142	false	PEP + Shi_3-P = 5-O-(1-Carboxyvinyl)-3-PShi	3-phosphoshikimate1-carboxyvinyltransferase [2.5.1.19]
RN:R0143	false	PR-AMP = PR-formimino-AICAR-P	histidinebiosynthesisbifunctionalproteinHisIE [3.5.4.19]
RN:R0144	false	PR-ATP = PR-AMP	histidinebiosynthesisbifunctionalproteinHisIE [3.6.1.31]
RN:R0145	false	PRPP = PR-ATP	ATPphosphoribosyltransferase [2.4.2.17]
RN:R0146	false	NAD ⁺ + Prephenate = 3-(4-Hydroxyphenyl)PYR + NADH	prephenatedehydrogenase [1.3.1.12]
RN:R0147	false	Prephenate = PhenylPYR	prephenate dehydratase [4.2.1.51]

SA reactions

RN:R0155	false	3-DehydroShi + NADPH = NADP+ + Shi	shikimatedehydrogenease [1.1.1.25]
RN:R0160	false	Urea = 2 NH3	urease [3.5.1.5]
RN:R0161	false	Urocanate = 4-Imidazolone-5-propanoate	urocanatehydratase [4.2.1.49]
RN:R0166	false	3-(Imidazol-4-yl)-2-oxopropyl_P + L-Glu = AKG + L-Histidinol_P	putative histidinol-phosphateaminotransferase [2.6.1.9]
RN:R0167	false	L-Glu + PhenylPYR = AKG + L-PhenylAla	putative histidinol-phosphateaminotransferase [2.6.1.9]
RN:R0168	false	3-(4-Hydroxyphenyl)PYR + L-Glu = AKG + L-Tyr	putative histidinol-phosphatetransaminase [2.6.1.9]
RN:R0179	false	Acetaldehyde + NAD+ = Ac + NADH	aldehyde dehydrogenase [1.2.1.3]
RN:R0188	false	DHQ = 3-DehydroShi	enolase [4.2.1.11, 4.2.1.10]
RN:R0195	false	PYR + Thiamin_diP = 2-(A-Hydroxyethyl)thiamine_diP	pyruvate dehydrogenase_acetolactatesynthase [1.2.4.1, 2.2.1.6]
RN:R0198	false	O-Ac-L-Ser = Ac + L-Cys	cysteinesynthase [2.5.1.47]
RN:R0208	false	NH3 = Carbamoyl_P	carbamatekinase [2.7.2.2]
RN:R0209	false	D-Ala = L-Ala	alanineracemase [5.1.1.1]
RN:R0238	false	GA_P + NAD+ = 3-P-D-glyceroyl_P + NADH	glyceraldehyde-3-phosphate dehydrogenase [1.2.1.12]
RN:R0239	false	Glycerone_P = GA_P	triosephosphate isomerase [5.3.1.1]
RN:R0243	false	Mal + Menaquinone = Menaquinol + OAA	malate:quinoneoxidoreductase [1.1.99.16]
RN:R0245	true	Mal + NAD+ = NADH + PYR	malatedehydrogenase homolog [1.1.1.38]
RN:R0246	false	Fum = Mal	fumarate hydratase, class-II [4.2.1.2]
RN:R0255	false	3-P-D-GA = 2-P-D-GA	phosphoglycerate mutase [5.4.2.1]
RN:R0256	false	2-P-D-GA = PEP	enolase [4.2.1.11]
RN:R0260	false	6PGlucon + NADP+ = D-Ru_5-P + NADPH	phosphogluconate dehydrogenase [1.1.1.44]
RN:R0267	false	Ac-CoA + OAA = Cit + CoA	citrate synthase [2.3.3.1]
RN:R0269	false	PEP = PYR	pyruvate kinase [2.7.1.40]
RN:R0270	false	3-P-D-glyceroyl_P = 3-P-D-GA	phosphoglycerate kinase [2.7.2.3]
RN:R0271	false	Ac + CoA = Ac-CoA	acetyl-CoA synthetase AND ligase [6.2.1.1]
RN:R0274	false	D-F = D-F_6-P	fructokinase, putative [2.7.1.4]
RN:R0276	false	D-F_6-P = D-F_16-BP	6-phosphofructokinase [2.7.1.11]
RN:R0280	false	D-Ri_5-P = PRPP	ribose-phosphate pyrophosphokinase [2.7.6.1]
RN:R0284	false	OAA = PEP	phosphoenolpyruvate carboxykinase [4.1.1.49]
RN:R0287	false	PYR = OAA	pyruvate carboxylase [6.4.1.1]
RN:R0288	true	CoA + Succ = SuccCoA	succinyl-CoA synthetase [6.2.1.5]
RN:R0294	false	D-F_16-BP = D-F_6-P	fructose-bisphosphatase [3.1.3.11]
RN:R0295	true	D-F_6-P + GA_P = D-E4P + D-Xu_5-P	transketolase [2.2.1.1]
RN:R0297	false	D-Glucono-15-lactone_6-P = 6PGlucon	Spon_PGLactonohydrolase [3.1.1.31]
RN:R0301	false	D-G_6-P + NADP+ = D-Glucono-15-lactone_6-P + NADPH	glucose-6-phosphate 1-dehydrogenase [1.1.1.49]
RN:R0302	false	D-G_6-P = D-F_6-P	glucose-6-phosphate isomerase A [5.3.1.9]
RN:R0311	false	D-Ru_5-P = D-Ri_5-P	ribose 5-phosphate isomerase A [5.3.1.6]
RN:R0314	false	D-Ru_5-P = D-Xu_5-P	ribulose-phosphate 3-epimerase [5.1.3.1]
RN:R0315	true	D-S7P + GA_P = D-E4P + D-F_6-P	Transaldolase superfamily [2.2.1.2]

SA reactions

RN:R0316	true	$D\text{-S7P} + GA_P = D\text{-Ri_5-P} + D\text{-Xu_5-P}$	transketolase [2.2.1.1]
RN:R0324	false	$IsoCit + NADP^+ = NADPH + OASucc$	isocitrate dehydrogenase [1.1.1.42]
RN:R0335	false	$OASucc = AKG$	isocitrate dehydrogenase [1.1.1.42]
RN:R0345	false	$FAD + Succ = FADH_2 + Fum$	succinate dehydrogenase [1.3.99.1]
RN:R0348	false	$Sucrose_6\text{-P} = D\text{-F} + D\text{-G_6-P}$	sucrose-6-phosphatehydrolase [3.2.1.26]
RN:R0358	false	$cis\text{-Acon} = IsoCit$	aconitate hydratase [4.2.1.3]
RN:R0359	false	$Cit = cis\text{-Acon}$	aconitate hydratase [4.2.1.3]
RN:R0360	false	$D\text{-F_16-BP} = GA_P + Glycerone_P$	fructose-bisphosphate aldolase [4.1.2.13]
RN:R0372	false	$AKG + L\text{-Gln} + NADPH = 2\ L\text{-Glu} + NADP^+$	glutamatesynthase [1.4.1.13]
RN:R0384	false	$L\text{-His} = NH_3 + Urocanate$	histidineammonia-lyase [4.3.1.3]
RN:R0522	true	$NH_3(ex) = NH_3$	probabale ammonium transporter [2.A.49]
RN:R0534	false	$D\text{-G}(ex) + PEP = D\text{-G_6-P} + PYR$	glucose-specific PTS [2.7.1.69, 2.7.3.9]
RN:R0673	true	$AKG + D\text{-Ala} = D\text{-Glu} + PYR$	D-alanineaminotransferase [2.6.1.21]
RN:R0986	false	$2\ L\text{-Glu} + NADH = AKG + L\text{-Orn} + NAD^+$	EZComp_UreaOrnSyn [1.5.1.12, 2.6.1.13]
RN:R0987	false	$2345\text{-Tetrahydrodipicolinate} + L\text{-Glu} + SuccCoA = AKG + CoA + L\text{-Lys} + Succ$	EZComp_LysSyn [2.3.1.117, 2.6.1.17, 3.5.1.18, 5.1.1.7, 4.1.1.20]
RN:R0988	false	$AKG + CoA + NAD^+ = NADH + SuccCoA$	EZComp_TCASuccinyl [1.2.4.2, 2.3.1.61, 1.8.1.4]
RN:R0989	false	$2\text{-}(A\text{-Hydroxyethyl})thiamine_diP + 2\text{-Oxobutanoate} + L\text{-Glu} + NADPH = AKG + L\text{-Ile} + NADP^+ + Thiamin_diP$	EZComp_Ile_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9, 2.6.1.42]
RN:R0990	false	$2\text{-}(A\text{-Hydroxyethyl})thiamine_diP + NADPH + PYR = 3\text{-Methyl-2-ox-obutanoate} + NADP^+ + Thiamin_diP$	EZComp_Val_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9]
RN:R0991	false	$3\text{-Methyl-2-oxobutanoate} + Ac\text{-CoA} + L\text{-Glu} + NAD^+ = AKG + CoA + L\text{-Leu} + NADH$	EZComp_Leu_Meta [2.3.3.13, 4.2.1.33, 1.1.1.85, 2.6.1.42]
RN:R0993	false	$L\text{-Asp} + L\text{-Citrulline} = Fum + L\text{-Arg}$	EZComp_Fum_Asp [4.3.2.1, 6.3.4.5]
RN:R0994	false	$CoA + NAD^+ + PYR = Ac\text{-CoA} + NADH$	EZComp_PyrAcetylCoA [1.2.4.1, 2.3.1.12, 1.8.1.4]
RN:R0995	false	$Gly + NAD^+ + THF = 510\text{-MethyleneTHF} + NADH + NH_3$	EZComp_GlySerThrMeta [2.1.2.10, 1.8.1.4, 1.4.4.2]
RN:R0996	false	$Ac\text{-CoA} + L\text{-Cys} + L\text{-HomoSer} = Ac + CoA + L\text{-HomoCys} + NH_3 + PYR$	EZComp_MetMeta [2.3.1.31, 2.5.1.48, 4.4.1.8]
RN:R0997	false	$AKG + L\text{-Orn} + NADH + 2\ NADPH = 2\ L\text{-Pro} + NAD^+ + 2\ NADP^+$	EZComp_UreaMeta [1.5.1.2, 1.5.1.12, 2.6.1.13]

Table 12: *S. aureus* network - Elementary Modes discussed in the results section¹

#	Flux	sum Rev. ²	Length	Reactions ³	Net reaction
3	25	false	16	(1 RN:Nucl02) (2 RN:R0061) (2 RN:R0089) (2 RN:R0093) (2 RN:R0245) (2 RN:R0246) (1 RN:R0260) (1 RN:R0280) (1 RN:R0284) (3 RN:R0287) (1 RN:R0297) (1 RN:R0301) (1 RN:R0311) (2 RN:R0372) (1 RN:R0534) (2 RN:R0993)	D-G(ex) + 2 NAD ⁺ = 2 NADH + Pyrimidine(ex)
19	428	false	35	(5 RN:E0001) (11 RN:E0019) (5 RN:R0021) (11 RN:R0038) (5 RN:R0052) (16 RN:R0061) (5 RN:R0065) (5 RN:R0073) (5 RN:R0141) (5 RN:R0142) (5 RN:R0147) (5 RN:R0155) (5 RN:R0167) (5 RN:R0188) (11 RN:R0195) (32 RN:R0238) (15 RN:R0239) (32 RN:R0255) (32 RN:R0256) (16 RN:R0260) (32 RN:R0270) (15 RN:R0276) (-2 RN:R0295) (16 RN:R0297) (16 RN:R0301) (6 RN:R0302) (7 RN:R0311) (9 RN:R0314) (7 RN:R0315) (-7 RN:R0316) (15 RN:R0360) (16 RN:R0372) (16 RN:R0522) (22 RN:R0534) (11 RN:R0990)	22 D-G(ex) + 32 NAD ⁺ + 16 NH ₃ (ex) = 32 NADH + 5 Phe-tRNA(ex) + 11 Val-tRNA(ex)
21	239	false	36	(3 RN:E0001) (11 RN:E0009) (3 RN:R0021) (3 RN:R0052) (3 RN:R0061) (3 RN:R0065) (3 RN:R0073) (11 RN:R0114) (11 RN:R0117) (3 RN:R0141) (3 RN:R0142) (3 RN:R0147) (3 RN:R0155) (3 RN:R0167) (3 RN:R0188) (11 RN:R0198) (17 RN:R0238) (9 RN:R0239) (17 RN:R0255) (17 RN:R0256) (3 RN:R0260) (17 RN:R0270) (11 RN:R0271) (9 RN:R0276) (1 RN:R0295) (3 RN:R0297) (3 RN:R0301) (8 RN:R0302) (2 RN:R0311) (1 RN:R0314) (2 RN:R0315) (-2 RN:R0316) (9 RN:R0360) (3 RN:R0372) (14 RN:R0522) (11 RN:R0534)	11 D-G(ex) + 17 NAD ⁺ + 14 NH ₃ (ex) = 11 Cys-tRNA(ex) + 17 NADH + 3 Phe-tRNA(ex)
81	289	false	36	(5 RN:E0013) (5 RN:E0018) (6 RN:Nucl02) (5 RN:R0047) (5 RN:R0059) (15 RN:R0061) (5 RN:R0062) (5 RN:R0093) (5 RN:R0100) (-5 RN:R0106) (5 RN:R0121) (5 RN:R0138) (5 RN:R0195) (5 RN:R0209) (15 RN:R0238) (6 RN:R0239) (15 RN:R0255) (15 RN:R0256) (15 RN:R0260) (15 RN:R0270) (6 RN:R0276) (6 RN:R0280) (5 RN:R0287) (-3 RN:R0295) (15 RN:R0297) (15 RN:R0301) (9 RN:R0311) (6 RN:R0314) (3 RN:R0315) (-3 RN:R0316) (6 RN:R0360) (15 RN:R0372) (10 RN:R0522) (15 RN:R0534) (-5 RN:R0673) (5 RN:R0989)	15 D-G(ex) + 15 NAD ⁺ + 10 NH ₃ (ex) = 5 Ala-tRNA(ex) + 5 Ile-tRNA(ex) + 15 NADH + 6 Pyrimidine(ex)

SA EMs

				(13 RN:E0001) (10 RN:E0018) (13 RN:R0021) (10 RN:R0047) (13 RN:R0052) (10 RN:R0059) (33 RN:R0061) (10 RN:R0062) (13 RN:R0065) (13 RN:R0073) (10 RN:R0093) (-10 RN:R0106) (10 RN:R0121) (10 RN:R0138) (13 RN:R0141) (13 RN:R0142) (13 RN:R0147) (13 RN:R0155) (13 RN:R0167) (13 RN:R0188) (10 RN:R0195) (46 RN:R0238) (21 RN:R0239) (46 RN:R0255) (46 RN:R0256) (38 RN:R0260) (46 RN:R0270) (21 RN:R0276) (18 RN:R0284) (28 RN:R0287) (-4 RN:R0295) (38 RN:R0297) (38 RN:R0301) (17 RN:R0311) (21 RN:R0314) (17 RN:R0315) (-17 RN:R0316) (21 RN:R0360) (33 RN:R0372) (23 RN:R0522) (38 RN:R0534) (10 RN:R0989)	38 D-G(ex) + 46 NAD ⁺ + 23 NH ₃ (ex) = 10 Ile-tRNA(ex) + 46 NADH + 13 Phe-tRNA(ex)
91	853	false	42	(3 RN:E0001) (2 RN:E0006) (10 RN:E0008) (3 RN:R0021) (2 RN:R0047) (3 RN:R0052) (2 RN:R0059) (5 RN:R0061) (2 RN:R0062) (3 RN:R0065) (3 RN:R0073) (2 RN:R0093) (-2 RN:R0106) (10 RN:R0117) (2 RN:R0138) (3 RN:R0141) (3 RN:R0142) (3 RN:R0147) (3 RN:R0155) (3 RN:R0167) (3 RN:R0188) (18 RN:R0238) (9 RN:R0239) (18 RN:R0255) (18 RN:R0256) (6 RN:R0260) (18 RN:R0270) (9 RN:R0276) (2 RN:R0287) (6 RN:R0297) (6 RN:R0301) (6 RN:R0302) (3 RN:R0311) (3 RN:R0314) (3 RN:R0315) (-3 RN:R0316) (9 RN:R0360) (5 RN:R0372) (15 RN:R0522) (12 RN:R0534)	12 D-G(ex) + 18 NAD ⁺ + 15 NH ₃ (ex) = 18 NADH + 3 Phe-tRNA(ex) + 10 Ser-tRNA(ex) + 2 Thr-tRNA(ex)
100	241	false	40		

¹ complete list available from the authors on request

² reversible

³ reaction identifiers are taken from KEGG, for annotations see the reaction table

Table 13: *S. epidermidis* network - metabolites

Name	internal?	Connectivity	Description
(5-P-D-R)anthranilate	true	2	N-(5-Phospho-D-ribosyl)anthranilate
1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	true	2	1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose_5-phosphate
2-(A-Hydroxyethyl)thiamine_diP	true	3	2-(alpha-Hydroxyethyl)thiamine_diphosphate
2-Oxobutanoate	true	2	2-Oxobutanoate
2-P-D-GA	true	2	2-Phospho-D-glycerate
23-Dihydrodipicolinate	true	2	2,3-Dihydrodipicolinate
2345-Tetrahydrodipicolinate	true	2	2,3,4,5-Tetrahydrodipicolinate
3-(4-Hydroxyphenyl)PYR	true	2	3-(4-Hydroxyphenyl)pyruvate
3-(Imidazol-4-yl)-2-oxopropyl_P	true	2	3-(Imidazol-4-yl)-2-oxopropyl_phosphate
3-DehydroShi	true	2	3-Dehydroshikimate
3-Methyl-2-oxobutanoate	true	3	3-Methyl-2-oxobutanoate
3-P-D-GA	true	2	3-Phospho-D-glycerate
3-P-D-glyceroyl_P	true	2	3-Phospho-D-glyceroyl_phosphate
4-Imidazolone-5-propanoate	true	1	4-Imidazolone-5-propanoate
4-P-L-Asp	true	2	4-Phospho-L-aspartate
5-O-(1-Carboxyvinyl)-3-PShi	true	2	5-O-(1-Carboxyvinyl)-3-phosphoshikimate
510-MethyleneTHF	true	2	5,10-Methylenetetrahydrofolate
6PGlucon	true	2	6-Phospho-D-gluconate
Ac	true	4	Acetate
Ac-CoA	true	6	Acetyl-CoA
Acetaldehyde	true	2	Acetaldehyde
AICAR	true	2	1-(5-Phosphoribosyl)-5-amino-4-imidazolecarboxamide
AKG	true	15	2-Oxoglutarate
Ala-tRNA(ex)	false	1	Ala-tRNA(ex)
Anthranilate	true	2	Anthranilate
Arg-tRNA(ex)	false	1	Arg-tRNA(ex)
Asn-tRNA(ex)	false	1	Asn-tRNA(ex)
Asp-tRNA(ex)	false	1	Asp-tRNA(ex)
Carbamoyl_P	true	3	Carbamoyl_phosphate
Chor	true	3	Chorismate
cis-Acon	true	2	cis-Aconitate
Cit	true	2	Citrate
CoA	true	9	CoA
Cys-tRNA(ex)	false	1	Cys-tRNA(ex)
D-Ala	true	2	D-Alanine
D-E4P	true	3	D-Erythrose_4-phosphate
D-erythro-1-(Imidazol-4-yl)glycerol_3-P	true	2	D-erythro-1-(Imidazol-4-yl)glycerol_3-phosphate

SEP metabolites

D-F	true	2	D-Fructose
D-F_16-BP	true	3	D-Fructose_1,6-bisphosphate
D-F_6-P	true	6	D-Fructose_6-phosphate
D-G(ex)	false	1	D-Glucose(ex)
D-G_6-P	true	4	D-Glucose_6-phosphate
D-Glu	true	2	D-Glutamate
D-Glucono-15-lactone_6-P	true	2	D-Glucono-1,5-lactone_6-phosphate
D-Ri_5-P	true	3	D-Ribose_5-phosphate
D-Ru_5-P	true	3	D-Ribulose_5-phosphate
D-S7P	true	2	D-Sedoheptulose_7-phosphate
D-Xu_5-P	true	3	D-Xylulose_5-phosphate
DAHP	true	2	2-Dehydro-3-deoxy-D-arabino-heptonate_7-phosphate
DHQ	true	2	3-Dehydroquinate
FAD(ex)	false	1	FAD
FADH2(ex)	false	1	FADH2
Formamide	true	1	Formamide
Formimino-L-Glu	true	2	N-Formimino-L-glutamate
Fum	true	3	Fumarate
GA_P	true	7	(2R)-2-Hydroxy-3-(phosphonoxy)-propanal
Gln-tRNA(ex)	false	1	Gln-tRNA(ex)
Glu-tRNA(ex)	false	1	Glu-tRNA(ex)
Gly	true	4	Glycine
Gly-tRNA(ex)	false	1	Gly-tRNA(ex)
Glycerone_P	true	2	Glycerone_phosphate
His-tRNA(ex)	false	1	His-tRNA(ex)
Ile-tRNA(ex)	false	1	Ile-tRNA(ex)
Indoleglycerol_P	true	2	Indoleglycerol_phosphate
IsoCit	true	2	Isocitrate
L-Ala	true	2	L-Alanine
L-Arg	true	3	L-Arginine
L-Asn	true	2	L-Asparagine
L-Asp	true	5	L-Aspartate
L-Asp_4-semialdehyde	true	3	L-Aspartate_4-semialdehyde
L-Citrulline	true	3	L-Citrulline
L-Cys	true	3	L-Cysteine
L-Gln	true	5	L-Glutamine
L-Glu	true	18	L-Glutamate
L-Glu_5-semialdehyde	true	2	L-Glutamate_5-semialdehyde
L-His	true	2	L-Histidine
L-Histidinol	true	2	L-Histidinol

SEP metabolites

L-Histidinol_P	true	2	L-Histidinol_phosphate
L-HomoCys	true	2	L-Homocysteine
L-HomoSer	true	3	L-Homoserine
L-Ile	true	2	L-Isoleucine
L-Leu	true	2	L-Leucine
L-Lys	true	2	L-Lysine
L-Met	true	2	L-Methionine
L-Orn	true	5	L-Ornithine
L-PhenylAla	true	2	L-Phenylalanine
L-Pro	true	3	L-Proline
L-Ser	true	5	L-Serine
L-Thr	true	4	L-Threonine
L-Try	true	2	L-Tryptophane
L-Tyr	true	2	L-Tyrosine
L-Val	true	2	L-Valine
Leu-tRNA(ex)	false	1	Leu-tRNA(ex)
Lys-tRNA(ex)	false	1	Lys-tRNA(ex)
Mal	true	4	(S)-Malate
Menaquinol	true	1	Menaquinol
Menaquinone	true	1	Menaquinone
Met-tRNA(ex)	false	1	Met-tRNA(ex)
NAD+	false	13	NAD+
NADH	false	13	NADH
NADP+	true	11	NADP+
NADPH	true	11	NADPH
NH3	true	11	NH3
NH3(ex)	false	1	NH3(ex)
O-Ac-L-Ser	true	2	O-Acetyl-L-serine
O-P-L-homoSer	true	2	O-Phospho-L-homoserine
OAA	true	6	Oxaloacetate
OASucc	true	2	Oxalosuccinate
PEP	true	6	Phosphoenolpyruvate
Phe-tRNA(ex)	false	1	Phe-tRNA(ex)
PhenylPYR	true	2	Phenylpyruvate
PR-AMP	true	2	Phosphoribosyl-AMP
PR-ATP	true	2	Phosphoribosyl-ATP
PR-formimino-AICAR-P	true	2	5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4-carboxamide
Prephenate	true	3	Prephenate
Pribulosyl-formimino-AICAR-P	true	2	N-(5-Phospho-D-1-ribulosylformimino)-5-amino-1-(5-phospho-D-ribosyl)-4-imidazolecarboxamide
Pro-tRNA(ex)	false	1	Pro-tRNA(ex)

SEP metabolites

PRPP	true	4	5-Phospho-D-ribose_1-diphosphate
Purine(ex)	false	1	Purine(ex)
PYR	true	12	Pyruvate
Pyrimidine(ex)	false	1	Pyrimidine(ex)
Ser-tRNA(ex)	false	1	Ser-tRNA(ex)
Shi	true	2	Shikimate
Shi_3-P	true	2	Shikimate_3-phosphate
Succ	true	3	Succinate
SuccCoA	true	3	Succinyl-CoA
Sucrose_6-P	true	1	Sucrose_6-phosphate
THF	true	2	Tetrahydrofolate
Thiamin_diP	true	3	Thiamin_diphosphate
Thr-tRNA(ex)	false	1	Thr-tRNA(ex)
Try-tRNA(ex)	false	1	Try-tRNA(ex)
Tyr-tRNA(ex)	false	1	Tyr-tRNA(ex)
Urea	true	1	Urea
Val-tRNA(ex)	false	1	Val-tRNA(ex)

Table 14: *S. epidermidis* network - reactions

Enzyme name	rev.?	Reaction equation	Annotation
rn:E0001	false	L-PhenylAla = Phe-tRNA(ex)	PheX [6.1.1.20]
rn:E0002	false	L-Tyr = Tyr-tRNA(ex)	TyrX [6.1.1.1]
rn:E0003	false	L-Try = Try-tRNA(ex)	TryX [6.1.1.-]
rn:E0004	false	L-His = His-tRNA(ex)	HisX [6.1.1.21]
rn:E0005	false	L-Met = Met-tRNA(ex)	MetX [6.1.1.10]
rn:E0006	false	L-Thr = Thr-tRNA(ex)	ThrX [6.1.1.3]
rn:E0007	false	Gly = Gly-tRNA(ex)	GlyX [6.1.1.14]
rn:E0008	false	L-Ser = Ser-tRNA(ex)	SerX [6.1.1.11]
rn:E0009	false	L-Cys = Cys-tRNA(ex)	CysX [6.1.1.16]
rn:E0010	false	L-Lys = Lys-tRNA(ex)	LysX [6.1.1.6]
rn:E0011	false	L-Asn = Asn-tRNA(ex)	AsnX [6.1.1.22]
rn:E0012	false	L-Asp = Asp-tRNA(ex)	AspX [6.1.1.12]
rn:E0013	false	L-Ala = Ala-tRNA(ex)	AlaX [6.1.1.7]
rn:E0014	false	L-Pro = Pro-tRNA(ex)	ProX [6.1.1.15]
rn:E0015	false	L-Arg = Arg-tRNA(ex)	ArgX [6.1.1.19]
rn:E0016	false	L-Glu = Glu-tRNA(ex)	GluX [6.1.1.17]
rn:E0017	false	L-Gln = Gln-tRNA(ex)	GlnX [6.1.1.17]
rn:E0018	false	L-Ile = Ile-tRNA(ex)	IleX [6.1.1.5]
rn:E0019	false	L-Val = Val-tRNA(ex)	ValX [6.1.1.9]
rn:E0020	false	L-Leu = Leu-tRNA(ex)	LeuX [6.1.1.4]
rn:N01	false	AICAR = Purine(ex)	PurineMeta []
rn:N02	false	PRPP = Pyrimidine(ex)	PyrimidineMeta []
rn:U0015	false	1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P = Indoleglycerol_P	indole-3-glycerolphosphatesynthase [4.1.1.48]
rn:U0018	false	L-Gln = Carbamoyl_P + L-Glu	carbamoyl-phosphatesynthase [6.3.5.5]
rn:U0020	false	23-Dihydrodipicolinate + NADPH = 2345-Tetrahydrodipicolinate + NADP+	dihydrodipicolinate reductase [1.3.1.26]
rn:U0021	false	DAHP = DHQ	3-dehydroquinate synthase [4.2.3.4]
rn:U0038	false	3-Methyl-2-oxobutanoate + L-Glu = AKG + L-Val	branched-chain amino acid aminotransferase [2.6.1.42]
rn:U0045	false	4-Imidazolone-5-propanoate = Formimino-L-Glu	imidazolone propionase [3.5.2.7]
rn:U0047	false	4-P-L-Asp + NADPH = L-Asp_4-semialdehyde + NADP+	aspartate semialdehyde dehydrogenase [1.2.1.11]
rn:U0048	false	PR-formimino-AICAR-P = Pribulosyl-formimino-AICAR-P	putative phosphoribosylformimino-5-aminoimidazolecarboxamide ribotidesomerase [5.3.1.16]
rn:U0049	false	510-MethyleneTHF + Gly = L-Ser + THF	serine hydroxymethyltransferase [2.1.2.1]
rn:U0050	false	L-HomoCys = L-Met	5-methyltetrahydropteroyltriglutamate-homocysteine methyltransferase [2.1.1.14]

SEP reactions

rn:U0052	false	5-O-(1-Carboxyvinyl)-3-PShi = Chor	chorismatesynthase [4.2.3.5]
rn:U0057	false	Anthranilate + PRPP = (5-P-D-R)anthranilate	anthranilatephosphoribosyltransferase [2.4.2.18]
rn:U0058	false	L-Asp + L-Gln = L-Asn + L-Glu	asparagine synthase [6.3.5.4]
rn:U0059	false	L-Asp = 4-P-L-Asp	asparto kinase II [2.7.2.4]
rn:U0061	false	L-Glu + NH ₃ = L-Gln	glutamine-ammonialigase [6.3.1.2]
rn:U0062	false	L-HomoSer = O-P-L-homoSer	homoserinekinase [2.7.1.39]
rn:U0065	false	Shi = Shi_3-P	shikimatekinase(SK) [2.7.1.71]
rn:U0068	false	Carbamoyl_P + L-Orn = L-Citrulline	ornithinecarbamoyltransferase [2.1.3.3]
rn:U0072	false	Chor + NH ₃ = Anthranilate + PYR	anthranilatesynthase [4.1.3.27]
rn:U0073	false	Chor = Prephenate	chorismatemutase [5.4.99.5]
		D-erythro-1-(Imidazol-4-yl)glycerol_3-P = 3-(Imidazol-4-yl)-2-oxopropyl_P	imidazoleglycerol-phosphatedehydratase [4.2.1.19]
rn:U0075	false		
rn:U0089	false	L-Arg = L-Citrulline + NH ₃	argininedeiminase [3.5.3.6]
rn:U0093	false	L-Glu + OAA = AKG + L-Asp	aspartate transaminase [2.6.1.1]
rn:U0095	false	L-Asp_4-semialdehyde + PYR = 2,3-Dihydrodipicolinate	dihydrodipicolinate synthase [4.2.1.52]
rn:U0100	true	L-Glu = D-Glu	glutamateracemase [5.1.1.3]
rn:U0101	true	L-Glu_5-semialdehyde + NAD ⁺ = L-Glu + NADH	1-pyrroline-5-carboxylatedehydrogenase [1.5.1.12]
rn:U0104	false	L-Histidinol + 2 NAD ⁺ = L-His + 2 NADH	putative histidinoldehydrogenase [1.1.1.23]
rn:U0105	false	L-Histidinol_P = L-Histidinol	putative histidinol phosphatase [3.1.3.15]
rn:U0106	true	L-HomoSer + NADP ⁺ = L-Asp_4-semialdehyde + NADPH	homoserine dehydrogenase [1.1.1.3]
rn:U0111	true	AKG + L-Orn = L-Glu + L-Glu_5-semialdehyde	ornithineaminotransferase [2.6.1.13]
rn:U0112	false	L-Orn = L-Pro + NH ₃	putative ornithinecyclodeaminase [4.3.1.12]
rn:U0114	false	Ac-CoA + L-Ser = CoA + O-Ac-L-Ser	serineO-acetyltransferase [2.3.1.30]
rn:U0116	false	Indoleglycerol_P + L-Ser = GA_P + L-Try	tryptophan synthase [4.2.1.20]
rn:U0117	false	NH ₃ + PYR = L-Ser	thereoninedehydratase [4.3.1.19, 4.3.1.17]
rn:U0120	true	L-Thr = Acetaldehyde + Gly	putative threoninealdolase [4.1.2.5]
rn:U0121	false	L-Thr = 2-Oxobutanoate + NH ₃	thereoninedehydratase [4.3.1.19]
		Pribulosyl-formimino-AICAR-P = AICAR + D-erythro-1-(Imidazol-4-yl)glycerol_3-P	amidotransferasehisH [2.4.2.-]
rn:U0125	false		
		(5-P-D-R)anthranilate = 1-(2-Carboxyphenylamino)-1-deoxy-D-Ru_5-P	phosphoriborylanthranilateisomerase [5.3.1.24]
rn:U0126	false		
rn:U0134	false	Formimino-L-Glu = Formamide + L-Glu	hypothetical protein,similartoformiminoglutamase [3.5.3.8]
rn:U0138	false	O-P-L-homoSer = L-Thr	threoninesynthase [4.2.3.1]
rn:U0141	false	D-E4P + PEP = DAHP	phospho-2-dehydro-3-deoxyheptonate aldo [2.5.1.54]
rn:U0142	false	PEP + Shi_3-P = 5-O-(1-Carboxyvinyl)-3-PShi	3-phosphoshikimate1-carboxyvinyltransferase [2.5.1.19]
rn:U0143	false	PR-AMP = PR-formimino-AICAR-P	histidinebiosynthesisbifunctionalproteinHisIE [3.5.4.19]
rn:U0144	false	PR-ATP = PR-AMP	histidinebiosynthesisbifunctionalproteinHisIE [3.6.1.31]
rn:U0145	false	PRPP = PR-ATP	ATPphosphoribosyltransferase [2.4.2.17]

SEP reactions

rn:U0146	false	NAD ⁺ + Prephenate = 3-(4-Hydroxyphenyl)PYR + NADH	prephenatedehydrogenase [1.3.1.12]
rn:U0147	false	Prephenate = PhenylPYR	prephenate dehydratase [4.2.1.51]
rn:U0155	false	3-DehydroShi + NADPH = NADP ⁺ + Shi	shikimatedehydrogenase [1.1.1.25]
rn:U0160	false	Urea = 2 NH ₃	urease [3.5.1.5]
rn:U0166	false	3-(Imidazol-4-yl)-2-oxopropyl_P + L-Glu = AKG + L-Histidinol_P	putative histidinol-phosphateaminotransferase [2.6.1.9]
rn:U0167	false	L-Glu + PhenylPYR = AKG + L-PhenylAla	putativehistidinol-phosphateaminotransferase [2.6.1.9]
rn:U0168	false	3-(4-Hydroxyphenyl)PYR + L-Glu = AKG + L-Tyr	putative histidinol-phosphatetransaminase [2.6.1.9]
rn:U0179	false	Acetaldehyde + NAD ⁺ = Ac + NADH	aldehyde dehydrogenase [1.2.1.3]
rn:U0188	false	DHQ = 3-DehydroShi	enolase [4.2.1.11, 4.2.1.10]
rn:U0195	false	PYR + Thiamin_diP = 2-(A-Hydroxyethyl)thiamine_diP	pyruvate dehydrogenase_ acetolactatesynthase [1.2.4.1, 2.2.1.6]
rn:U0198	false	O-Ac-L-Ser = Ac + L-Cys	cysteinesynthase [2.5.1.47]
rn:U0208	false	NH ₃ = Carbamoyl_P	carbamatekinase [2.7.2.2]
rn:U0209	false	D-Ala = L-Ala	alanineracemase [5.1.1.1]
rn:U0238	false	GA_P + NAD ⁺ = 3-P-D-glyceroyl_P + NADH	glyceraldehyde-3-phosphate dehydrogenase [1.2.1.12]
rn:U0239	false	Glycerone_P = GA_P	triosephosphate isomerase [5.3.1.1]
rn:U0243	false	Mal + Menaquinone = Menaquinol + OAA	malate:quinoneoxidoreductase [1.1.99.16]
rn:U0244	false	Mal + NAD ⁺ = NADH + OAA	MDH [1.1.1.37]
rn:U0245	true	Mal + NAD ⁺ = NADH + PYR	malatedehydrogenase homolog [1.1.1.38]
rn:U0246	false	Fum = Mal	fumarate hydratase, class-II [4.2.1.2]
rn:U0255	false	3-P-D-GA = 2-P-D-GA	phosphoglycerate mutase [5.4.2.1]
rn:U0256	false	2-P-D-GA = PEP	enolase [4.2.1.11]
rn:U0260	false	6PGlucon + NADP ⁺ = D-Ru_5-P + NADPH	phosphogluconate dehydrogenase [1.1.1.44]
rn:U0267	false	Ac-CoA + OAA = Cit + CoA	citrate synthase [2.3.3.1]
rn:U0269	false	PEP = PYR	pyruvate kinase [2.7.1.40]
rn:U0270	false	3-P-D-glyceroyl_P = 3-P-D-GA	phosphoglycerate kinase [2.7.2.3]
rn:U0271	false	Ac + CoA = Ac-CoA	acetyl-CoA synthetase AND ligase [6.2.1.1]
rn:U0274	false	D-F = D-F_6-P	fructokinase,putative [2.7.1.4]
rn:U0276	false	D-F_6-P = D-F_16-BP	6-phosphofructokinase [2.7.1.11]
rn:U0280	false	D-Ri_5-P = PRPP	ribose-phosphate pyrophosphokinase [2.7.6.1]
rn:U0284	false	OAA = PEP	phosphoenolpyruvate carboxykinase [4.1.1.49]
rn:U0287	false	PYR = OAA	pyruvate carboxylase [6.4.1.1]
rn:U0288	true	CoA + Succ = SuccCoA	succinyl-CoA synthetase [6.2.1.5]
rn:U0294	false	D-F_16-BP = D-F_6-P	fructose-bisphosphatase [3.1.3.11]
rn:U0295	true	D-F_6-P + GA_P = D-E4P + D-Xu_5-P	transketolase [2.2.1.1]
rn:U0297	false	D-Glucono-15-lactone_6-P = 6PGlucon	Spon_PGLactonohydrolase [3.1.1.31]
rn:U0301	false	D-G_6-P + NADP ⁺ = D-Glucono-15-lactone_6-P + NADPH	glucose-6-phosphate 1-dehydrogenase [1.1.1.49]
rn:U0302	false	D-G_6-P = D-F_6-P	glucose-6-phosphate isomerase A [5.3.1.9]
rn:U0311	false	D-Ru_5-P = D-Ri_5-P	ribose 5-phosphate isomerase A [5.3.1.6]

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rn:U0314	false	D-Ru_5-P = D-Xu_5-P	ribulose-phosphate 3-epimerase [5.1.3.1]
rn:U0315	true	D-S7P + GA_P = D-E4P + D-F_6-P	Transaldolase superfamily [2.2.1.2]
rn:U0316	true	D-S7P + GA_P = D-Ri_5-P + D-Xu_5-P	transketolase [2.2.1.1]
rn:U0324	false	IsoCit + NADP+ = NADPH + OASucc	isocitrate dehydrogenase [1.1.1.42]
rn:U0335	false	OASucc = AKG	isocitrate dehydrogenase [1.1.1.42]
rn:U0345	false	FAD(ex) + Succ = FADH2(ex) + Fum	succinate dehydrogenase [1.3.99.1]
rn:U0348	false	Sucrose_6-P = D-F + D-G_6-P	sucrose-6-phosphatehydrolase [3.2.1.26]
rn:U0358	false	cis-Acon = IsoCit	aconitate hydratase [4.2.1.3]
rn:U0359	false	Cit = cis-Acon	aconitate hydratase [4.2.1.3]
rn:U0360	false	D-F_16-BP = GA_P + Glycerone_P	fructose-bisphosphate aldolase [4.1.2.13]
rn:U0372	false	AKG + L-Gln + NADPH = 2 L-Glu + NADP+	glutamatesynthase [1.4.1.13]
rn:U0522	true	NH3(ex) = NH3	probabile ammonium transporter [2.A.49]
rn:U0534	false	D-G(ex) + PEP = D-G_6-P + PYR	glucose-specific PTS [2.7.1.69, 2.7.3.9]
rn:U0673	true	AKG + D-Ala = D-Glu + PYR	D-alanineaminotransferase [2.6.1.21]
rn:U0986	false	2 L-Glu + NADH = AKG + L-Orn + NAD+	EZComp_UreaOrnSyn [1.5.1.12, 2.6.1.13]
rn:U0987	false	2345-Tetrahydrodipicolinate + L-Glu + SuccCoA = AKG + CoA + L-Lys + Succ	EZComp_LysSyn [2.3.1.117, 2.6.1.17, 3.5.1.18, 5.1.1.7, 4.1.1.20]
rn:U0988	false	AKG + CoA + NAD+ = NADH + SuccCoA	EZComp_TCASuccinyl [1.2.4.2, 2.3.1.61, 1.8.1.4]
rn:U0989	false	2-(A-Hydroxyethyl)thiamine_diP + 2-Oxobutanoate + L-Glu + NADPH = AKG + L-Ile + NADP+ + Thiamin_diP	EZComp_Ile_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9, 2.6.1.42]
rn:U0990	false	2-(A-Hydroxyethyl)thiamine_diP + NADPH + PYR = 3-Methyl-2-oxobutanoate + NADP+ + Thiamin_diP	EZComp_Val_Meta [2.2.1.6, 1.1.1.86, 4.2.1.9]
rn:U0991	false	3-Methyl-2-oxobutanoate + Ac-CoA + L-Glu + NAD+ = AKG + CoA + L-Leu + NADH	EZComp_Leu_Meta [2.3.3.13, 4.2.1.33, 1.1.1.85, 2.6.1.42]
rn:U0993	false	L-Asp + L-Citrulline = Fum + L-Arg	EZComp_Fum_Asp [4.3.2.1, 6.3.4.5]
rn:U0994	false	CoA + NAD+ + PYR = Ac-CoA + NADH	EZComp_PyrAcetylCoA [1.2.4.1, 2.3.1.12, 1.8.1.4]
rn:U0995	false	Gly + NAD+ + THF = 510-MethyleneTHF + NADH + NH3	EZComp_GlySerThrMeta [2.1.2.10, 1.8.1.4, 1.4.4.2]
rn:U0996	false	Ac-CoA + L-Cys + L-HomoSer = Ac + CoA + L-HomoCys + NH3 + PYR	EZComp_MetMeta [2.3.1.31, 2.5.1.48, 4.4.1.8]
rn:U0997	false	AKG + L-Orn + NADH + 2 NADPH = 2 L-Pro + NAD+ + 2 NADP+	EZComp_UreaMeta [1.5.1.2, 1.5.1.12, 2.6.1.13]

Table 15: *S. epidermidis* network - Elementary Modes discussed in the results section¹

#	Flux	sum	Rev. ²	Length	Reactions ³	Net reaction
16	27	false	22	(1 m:E0019) (1 m:N02) (1 m:U0038) (1 m:U0061) (1 m:U0195) (2 m:U0238) (1 m:U0239) (2 m:U0255) (2 m:U0256) (1 m:U0260) (2 m:U0270) (1 m:U0276) (1 m:U0280) (1 m:U0297) (1 m:U0301) (1 m:U0302) (1 m:U0311) (1 m:U0360) (1 m:U0372) (1 m:U0522) (2 m:U0534) (1 m:U0990)	4 D-G(ex) + 6 NAD ⁺ + 5 NH ₃ (ex) = 2 Ala-tRNA(ex) + 6 NADH + Phe-tRNA(ex) + 2 Ser-tRNA(ex)	
17	148	false	25	(6 m:E0019) (6 m:U0038) (6 m:U0061) (6 m:U0195) (12 m:U0238) (5 m:U0239) (12 m:U0255) (12 m:U0256) (6 m:U0260) (5 m:U0269) (12 m:U0270) (5 m:U0276) (-2 m:U0295) (6 m:U0297) (6 m:U0301) (1 m:U0302) (2 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (5 m:U0360) (6 m:U0372) (6 m:U0522) (7 m:U0534) (6 m:U0990)	7 D-G(ex) + 12 NAD ⁺ + 6 NH ₃ (ex) = 12 NADH + 6 Val-tRNA(ex)	
18	221	false	30	(5 m:E0019) (4 m:N02) (5 m:U0038) (15 m:U0061) (10 m:U0089) (10 m:U0093) (5 m:U0195) (10 m:U0238) (4 m:U0239) (10 m:U0244) (10 m:U0246) (10 m:U0255) (10 m:U0256) (10 m:U0260) (10 m:U0270) (4 m:U0276) (4 m:U0280) (-2 m:U0295) (10 m:U0297) (10 m:U0301) (6 m:U0311) (4 m:U0314) (2 m:U0315) (-2 m:U0316) (4 m:U0360) (15 m:U0372) (5 m:U0522) (10 m:U0534) (5 m:U0990) (10 m:U0993)	2 D-G(ex) + 2 NAD ⁺ + NH ₃ (ex) = 2 NADH + Pyrimidine(ex) + Val-tRNA(ex)	
22	294	false	34	(5 m:E0012) (5 m:E0018) (6 m:N02) (5 m:U0047) (5 m:U0059) (15 m:U0061) (5 m:U0062) (10 m:U0093) (-5 m:U0106) (5 m:U0121) (5 m:U0138) (5 m:U0195) (15 m:U0238) (6 m:U0239) (10 m:U0244) (-10 m:U0245) (15 m:U0255) (15 m:U0256) (15 m:U0260) (15 m:U0270) (6 m:U0276) (6 m:U0280) (-3 m:U0295) (15 m:U0297) (15 m:U0301) (9 m:U0311) (6 m:U0314) (3 m:U0315) (-3 m:U0316) (6 m:U0360) (15 m:U0372) (10 m:U0522) (15 m:U0534) (5 m:U0989)	9 D-G(ex) + 13 NAD ⁺ + 11 NH ₃ (ex) = 9 Cys-tRNA(ex) + 13 NADH + 2 Phe-tRNA(ex) + Pyrimidine(ex)	

¹ complete list available from the authors on request² reversible³ reaction identifiers are taken from KEGG, for annotations see the reaction table