Subsystems and scenarios used in reaction network generation

Category	Subsystem	Abbreviation	Scenario	*S. aureus*	*E. coli*	*H. pylori*	*L. lactis*
AminoAcids	Ammonia assimilation	NH3 assim	NH3 to Glutamine	x	x		
	Arginine Biosynthesis	Arginine	Arginine synthesis	x	x		
	Arginine Putrescine and 4-aminobutyrate degradation	ArgPut deg	Arginine to Proline	x			
			Arginine to Putrescine	x	x		
	Branched-Chain Amino Acid Biosynthesis	Branched AA	Isoleucine Leucine Valine synthesis	x	x		x
			Oxoisovalerate generation	x	x		x
	Chorismate Synthesis	Chorismate	Chorismate synthesis	x	x	x	x
	Glutamate, aspartate and asparagine biosynthesis	GluAspAsn	Asparagine synthesis	x	x		x
			Aspartate synthesis	x	x		
			Glutamate racemase	x	x	x	x
			Glutamate synthesis	x	x	x	
			Glutamine synthesis	x	x		x
	Histidine Biosynthesis	Histidine	Histidine synthesis	x	x		x
	Histidine Degradation	Hist deg	Histidine to Glutamate	x			
	Isoleucine degradation	Isoleu deg	Isoleucine to 2MethylbutyrylCoA	x			
			Isoleucine to PropanoylCoA	x			
	Leucine Degradation and HMG-CoA Metabolism	Leucine deg	Leucine to IsovalerylCoA	x			
	Lysine Biosynthesis DAP Pathway	Lysine	LL 2 6 Diaminoheptanedioate generation	x	x	x	x
			Lysine synthesis	x	x	x	
	Methionine Biosynthesis	Methionine	Methionine synthesis from homoserine	x	x		
			Methionine to Adenosyl Methionine	x	x	x	x
	Methionine Salvage	MethSalvage	*incomplete scenario*				
	Phenylalanine synthesis	Phenylalanine	Phenylalanine synthesis	x	x		
	Polyamine Metabolism	Polyamine	Putrescine to Spermine	x			
	Pyruvate Alanine Serine Interconversions	PyrAlaSer	Alanine Synthesis	x			
	Serine Biosynthesis	Serine	Glycine synthesis	x	x	x	x
			Serine synthesis	x	x		
	Threonine degradation	Threon deg	Threonine to Glycine and Acetaldehyde	x	x		
			Threonine to Oxobutanoate	x			x
	Threonine synthesis	Threonine	Homoserine generation	x	x	x	x
			Threonine synthesis	x	x	x	x
	Tryptophan synthesis	Tryptophan	Tryptophan synthesis	x	x	x	x
	Tyrosine synthesis	Tyrosine	Tyrosine synthesis	x	x		
	Valine degradation	Valine deg	Valine to IsobutyrylCoA	x			
	cysteine biosynthesis	cysteine	Cysteine synthesis	x	x		x
Carbohydrates	Embden-Meyerhof and Gluconeogenesis	EMP	Fructose16BP entry point	x	x		x
			Fructose6P entry point	x	x		x
			GAP entry point	x	x		x
			Gluconeogenesis		x	x	
			Glucose6P generation	x	x	x	x
			Glycerate3P generation	x	x		x
			GlyceroneP entry point	x	x		x
			GlyceroneP generation	x	x		x
			Glycolysis	x	x		x
			PEP generation	x	x		x
	Entner-Doudoroff Pathway	EntnerDoff	Gluconate to PhosphoDGluconate	x	x		x
	Fermentations: Lactate	FermLac	Bifidium precursors				x
			Heterofermentation precursors				x
			Homofermentation	x	x		x
	Fermentations: Mixed acid	FermMixed	PEP to Formate	x	x		
	Fructose utilization	Fructose	Fructose16BP generation	x	x		x
	Galactose degradation	Lactose	Lactose6P utilization	x			
	Glycerol and Glycerol-3-phosphate Uptake and Utilization	Glycerol	Glycerol3P and Glycerol to GlyceroneP	x	x		x
	Mannitol Utilization	Mannitol	Fructose6P generation	x	x		x
	Mannose Metabolism	Mannose	Fructose6P generation	x	x		x
	Pentose phosphate pathway	PPP	Erythrose4P generation	x	x		
			Glycolysis bypass	x	x		
			PRPP generation	x	x		x
			PhosphoDGluconate entry point	x	x		x
			Xylulose5P generation	x	x		x
	Pyruvate metabolism I: anaplerotic reactions, PEP	PyrMetab 1	PEP generation	x	x		
			PEP to TCA metabolites	x	x		
			Pyruvate generation	x	x		
			Pyruvate to TCA metabolites	x	x		
	Pyruvate metabolism II: acetyl-CoA, acetogenesis from pyruvat	PyrMetab II	Acetate to Acetaldehyde	x	x		x
			AcetylCoA generation	x	x		x
	Sucrose Metabolism	Sucrose	Sucrose6P and Glucose to Glucose6P	x	x	x	x
			UDPglucose generation	x	x		
	TCA Cycle	TCA	Fumarate entry point	x	x	x	
			Oxaloacetate to Succinate	x	x	x	
			Oxoglutarate generation	x		x	
			SuccinylCoA entry point	x	x		
			TCA cycle	x	x		
	Trehalose Uptake and Utilization	Trehalose	Trehalose6P to Glucose and Glucose6P	x	x		
Cell Wall	Peptidoglycan Biosynthesis	Peptidogly	UDP N acetyl muramate generation	x	x	x	x
	Sialic Acid Metabolism	Aminosugars	D glucosamine1P	x	x	x	x
			N acetyl D glucosamine1P generation	x	x	x	x
			UDP N acetyl D galactosamine generation	x	x	x	x
			UDP N acetyl D glucosamine generation	x	x	x	x
			UDP N acetyl D mannosamine generation	x	x		x
	Teichoic and lipoteichoic acids biosynthesis	(Lipo)teich	CDPglycerol generation	x			x
			Diglucosyl diacylglycerol generation	x			
Lipids	Fatty Acid Biosynthesis FASII	FattySynth	Malonyl CoA generation	x	x	x	
	Glycerolipid and glycerphospholipid metabolism	Glyc(P)lipids	CDP diacylglycerol generation	x	x		
			Cardiolipin synthesis	x	x		
			Diacylglycerol synthesis	x	x		
			For 3 D Glucosyl 1 2 diacylglycerol generation	x	x	x	x
			Phosphatidylethanolamine synthesis	x	x		
			Phosphatidylglycerol generation	x	x		
			Phosphatidylserine synthesis	x	x		
	fatty acid metabolism	FattyMetab	Hexadecanoate to AcetylCoA	x	x		
Nitrogen Metabolism	Nitrate and nitrite ammonification	Nitra/ite	Nitrite to Ammonia reduction	x	x		

Category	Subsystem	Abbreviation	Scenario	*S. aureus*	*E. coli*	*H. pylori*	*L. lactis*
Nucleotide metabolism	De Novo Purine Biosynthesis	IMP	AICAR to IMP	x	x		x
			IMP synthesis	x	x		x
	De Novo Pyrimidine Synthesis	UMP	UMP synthesis from CarbamoylP	x	x	x	x
			UMP synthesis from Glutamine	x	x	x	x
	Purine conversions	Purines	ADP generation	x	x	x	x
			AMP generation	x	x	x	x
			Adenine to AMP	x	x	x	x
			AdenosinePP to AMP	x	x	x	x
			GDP generation	x	x	x	x
			GMP generation	x	x	x	x
			GTP generation	x	x	x	x
			dAMP generation	x	x	x	x
			dGMP generation	x	x	x	x
	Ribonucleotide reduction	RiboReduc	dADP generation	x	x	x	x
			dCTP generation	x	x		x
			dGDP generation	x	x	x	x
	Ribose and deoxyribose phosphate metabolism	(Deoxy)Rib	Deoxyribose1P generation	x	x		x
			Ribose5P generation	x	x		x
	pyrimidine conversions	Pyrimidines	CMP generation	x	x		
			CTP generation	x	x	x	
			dCMP generation	x			
			dTMP generation	x	x		x
One Carbon	Glycine cleavage system	Gly cleavage	Glycine cleavage	x	x		
	One-carbon metabolism by tetrahydropterines	One carbon	Formyltetrahydrofolate generation	x			x
			Methylenetetrahydrofolate generation	x			x
			Methyltetrahydrofolate generation	x	x		x
			Tetrahydrofolate generation	x	x	x	
Redox	Dehydrogenase complexes	Dehydro	*no scenario*				
	F0F1 type ATP synthase	ATP	*no scenario*				
	Formate hydrogenase	Formate	Formate dehydrogenase	x	x		
	Respiratory dehydrogenases 1	RespDH	NADH ubiquinone oxidation	x	x		x
	Succinate dehydrogenase	FAD dehydro	FADH2 ubiquinone oxidation	x	x	x	
Sulfur	Inorganic Sulfur Assimilation	Sulfide	Sulfate to Sulfide	x	x		
Vitamins and Cofactors	Coenzyme A Biosynthesis	CoA	CoA synthesis	x	x	x	
	FMN and FAD biosynthesis	FMN/FAD	FAD synthesis	x			
	Folate Biosynthesis	Folate	Dihydrofolate to Tetrahydrofolate	x	x		x
			Tetrahydrofolate generation	x			x
	Isoprenoid Biosynthesis	FarnesylPP	DOXP pathway		x		
			Mevalonate pathway	x			x
	NAD and NADP cofactor biosynthesis global	NAD/NADP	De novo from Trp and Asp		x		
			Nicotinamide to NAD	x	x		x
			Nicotinamide to NADP	x	x		x
	Porphyrin, Heme, and Siroheme Biosynthesis	Heme	Heme synthesis	x			
			Siroheme synthesis	x	x		