		for Molecular BioSystems Society of Chemistry, 2007													
Supplementary Table 1. List o	of E. coli	netabolites identified in the literature.													
Pathway	CI	Metabolite	Abbreviation	KEGG ID ^b	Standard	Analytical	Soluvility			Form	nula		Molecular	m/z ^d	Description
Patilway	Class	metaboute	Abbreviation	KEGG ID	chemical	mode ^c	Soluvitity	C	H I	1 0	P S F	e Se Co	Cl weight	mız	Description
Acid fermentation	- 1	Acetaldehyde		C00084	+	Neutral	Hydrophilic	2	4	1			44.0262	-	Neutral and/or hydrophobic
Pyruvic acid oxidation	- 1	Acetic acid		C00033	+	Anion	Hydrophilic	2	4	2			60.0211	59.0139	Included in thebuffer solution
Short fatty acid degradation	II.	Acetoacetic acid		C00164	+	Anion	Hydrophilic	4	6	3			102.0317	101.0244	Unable to be detected in CE-MS
Short fatty acid degradation	ll ll	Acetoacetyl-CoA	i	C00332	+	Nucleotide	Hydrophilic	25	40	7 18	3 1		851.1363	850.1291	
Isoleucine biosynthesis	- 1	2-Aceto-2-hydroxybutyric acid	2A2HBA	_	-	Anion	Hydrophilic	6	10	4			146.0579	145.0506	
Acetoin biosynthesis	- 1	Acetoin	i	C00466	+	Neutral	Hydrophilic	4	8	2			88.0524	-	Neutral and/or hydrophobic
Valine biosynthesis	1	2-Acetolactic acid	2-Ac	C06010	-	Anion	Hydrophilic	5	8	4			132.0423	131.0350	
Pyruvic acid oxidation	- 1	Acetyl-CoA	AcCoA	C00024	+	Nucleotide	Hydrophilic	23	38	7 17	3 1		809.1258	403.5556	Detected as divalent ion in MS
Dihydrolipoic acid analog (in vitro)	VI	S-Acetyldihydrolipoamide		C01136	-	Cation	Hydrophilic	10	19	1 2	2		249.0857	250.0930	
Peptidoglycan turnover	ll ll	N-Acetyl-D-glucosamine	GlcNAc	C03000	-	Neutral	Hydrophilic	8	15	1 6			221.0899	_	Neutral and/or hydrophobic
			e1 111 B	60 1051									201 0512	200 0 100	

,	E. coli metabolites identified in the literature.		1 1	Standard	Analytical					Molecul	ar	
Pathway Acid fermentation	Class ^a Metabolite	Abbreviation	KEGG ID	chemical	mode ^c	Soluvility	СН	-	Fe Se Co	Cl weigh	. m/	Z ^d Description Neutral and/or hydrophobic
Pyruvic acid oxidation	I Acetic acid		C00084 C00033	+	Neutral Anion	Hydrophilic Hydrophilic	2 4	2		60.02	11 59	.0139 Included in thebuffer solution
Short fatty acid degradation Short fatty acid degradation	II Acetoacetic acid II Acetoacetyl-CoA		C00164 C00332	+	Anion Nucleotide	Hydrophilic Hydrophilic	25 40	7 18 3	1	102.03 851.13	63 850	.0244 Unable to be detected in CE-MS
Isoleucine biosynthesis Acetoin biosynthesis	I 2-Aceto-2-hydroxybutyric acid I Acetoin	2А2НВА	C00466	+	Anion Neutral	Hydrophilic Hydrophilic	6 10	2		146.05		.0506 Neutral and/or hydrophobic
Valine biosynthesis Pyruvic acid oxidation	I 2-Acetolactic acid I Acetyl-CoA	2-Ac AcCoA	C06010 C00024	-+	Anion Nucleotide	Hydrophilic Hydrophilic	5 8 23 38	7 17 3	1	132.04 809.12	23 131	.0350 .5556 Detected as divalent ion in MS
Dihydrolipoic acid analog (in vitro)	VI S-Acetyldihydrolipoamide		C01136	-	Cation	Hydrophilic	10 19	1 2	2	249.08	57 250	.0930
Peptidoglycan turnover UDP-N-acetylglucosamine biosynthesis	II N-Acetyl-D-glucosamine I N-Acetylglucosamine-1-phosphate	Glenae Glenae-P	C03000 C04256	+	Neutral Anion	Hydrophilic Hydrophilic	8 15 8 16	1 6 1 9 1		221.08 301.05	63 300	Neutral and/or hydrophobic
Glucosamine degradation Arginine biosynthesis	II N-Acetyl-D-glucosamine-6-phosphate I N-Acetylglutamatesemialdehyde	NACGLeNP N-AcGlu-semialdehyde	C00357 C01250	+	Anion Anion	Hydrophilic Hydrophilic	8 16 7 11	1 9 1		301.05 173.06		.0490
Arginine biosynthesis Arginine biosynthesis	I N-Acetyl-L-glutamic acid I N-Acetylglutamylphosphate	N-AcGlu N-AcGlu-P	C00624 C04133	+	Cation Anion	Hydrophilic Hydrophilic	7 11 7 12	1 5 1		189.06		.0710 .0228
Maltose assimilation	III Acetylmaltose		C02130	-	Neutral	Hydrophilic	14 24	12		384.12	68 -	Neutral and/or hydrophobic
Acetylglucosamine dissimilation Acetylglucosamine dissimilation	II N-Acetylmannosamine II N-Acetyl-D-mannosamine-6-phosphate	ManNAc ManNAc6P	C00645 C04257	+	Neutral Anion	Hydrophilic Hydrophilic	8 15 8 16	1 6		221.08 301.05	63 300	Neutral and/or hydrophobic
Peptideglycan biosynthesis Acetylglucosamine dissimilation	N-Acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminoheptane-D-alanyl-D-alaninediphosphoundeca N-Acetylneuraminic acid	orenol MurNAcAlaGludAHeAlaAdePPUn NeuNAc	C05897 C00270	+	Nucleotide Anion	Hydrophobic Hydrophilic	87 143 11 19	7 23 2		1715.97 309.10		.9638 Out of the MS range .0987
Arginine biosynthesis Pyruvic acid oxidation	I N-a-Acetylornithine I Acetylphosphate	N-AcOrn Ac-P	C00437	+	Cation Anion	Hydrophilic Hydrophilic	7 14 2 5			174.10	04 175	.1077
Cysteine biosynthesis	I O-Acetyl-L-serine	AcSer	C00979	+	Cation	Hydrophilic	5 9	1 4		147.05	32 148	.0604
Polyamine acetylation Polyamine acetylation	1 N¹-Acetylspermidine 1 N¹-Acetylspermine	N1AcSpermidine N1AcSpermine	C00612 C02567	+	Cation Cation	Hydrophilic Hydrophilic	9 21	3 1 4 1		187.16 244.22	63 245	.1757 .2336
TCA cycle trans-Aconitic acid metabolism	I cis-Aconitic acid III trans-Aconitic acid		C00417 C02341	+	Anion Anion	Hydrophilic Hydrophilic	6 6	6		174.01 174.01		.0092
Salvage of Ade, HypXan Purine biosynthesis	I Adenine I Adenine-5-phosphate	AMP	C00147 C00020	+	Cation Nucleotide	Hydrophilic Hydrophilic	5 5 10 14			135.05		.0618
Salvage of Ade, HypXan	I Adenosine		C00212	+	Cation	Hydrophilic	10 13	5 4		267.09	68 268	.1040
Sulfuric acid assimilation Purine biosynthesis	I Adenosine-3',5'-diphosphate I Adenosine-5'-diphosphate	pAp ADP	C00054 C00008	+	Nucleotide Nucleotide	Hydrophilic Hydrophilic	10 15 10 15	5 10 2 5 10 2		427.02 427.02		.0221 .0221
ADP-ribose degradation (putative) Sulfuric acid assimilation	VI Adenosinediphosphateribose I Adenosine-5'-phosphosulfate	AdePPRi APS	C01882 C00224	+ +	Nucleotide Nucleotide	Hydrophilic Hydrophilic	15 23 10 14	5 14 2 5 10 1	1	559.07 427.01		.0644
Purine biosynthesis Cobalamin biosynthesis	I Adenosine-5'-triphosphate IV Adenosylcobalamin-5'-phosphate	ATP AdeC	C00002	+	Nucleotide Nucleotide	Hydrophilic Hydrophobic	10 16 70 99	5 13 3 20 20 2		506.99		.9885 .5923 Out of the MS range
Cobalamin biosynthesis	IV Adenosylcobinamide IV Adenosylcobinamide phosphate		C06508	_	Cation	Hydrophobic	58 84	16 11	1	1237.56	81 1238	.5754 Out of the MS range
Cobalamin biosynthesis Cobalamin biosynthesis	IV Adenosylcobinamide-GDP	Adenosylcobinamide-P	C06510	_	Anion Nucleotide	Hydrophobic Hydrophobic	58 83 68 97	21 21 2	1	1315.51	19 1661	.5746 Out of the MS range
Proto- and siroheme biosynthesis Polyamine biosynthesis	I S-Adenosylhomocysteine I S-Adenosylmethioninamine	SAHC dAdoMet	C00021 C01137	+	Cation Cation	Hydrophilic Hydrophilic	14 20 14 23	6 5	1	384.12 355.15		.1289
SAM biosynthesis Biotin biosynthesis	I S-Adenosyl-L-methionine I S-Adenosyl-4-methylthio-2-oxobutanoic acid	SAM SA4MT2OBA	C00019 C04425	+	Cation Cation	Hydrophilic Hydrophilic	15 23 15 20		1	399.14 398.11		.1451 Including trinary sulfur .1134 Including trinary sulfur
Purine biosynthesis	I Adenylosuccinic acid	ASA	C03794	+	Nucleotide	Hydrophilic	13 16	5 11 1		449.05	84 448	.0511
Glycogen biosynthesis ADP-ribose degradation (putative)	I ADP-D-glucose VI ADP-ribose	ADP-Glc	C00498 C00301	+	Nucleotide Nucleotide	Hydrophilic Hydrophilic	16 25 15 23	5 15 2 5 14 2	Ш	589.08 559.07	17 558	.0750 .0644
Polyamine biosynthesis Pantothenic acid biosynthesis	I Agmatine I β-Alanine	β-Ala	C00179 C00099	+	Cation Cation	Hydrophilic Hydrophilic	5 14 3 7	1 2	+	130.12 89.04		.1291 .0550
Peptideglycan biosynthesis Alanine biosynthesis	I D-Alanine I L-Alanine	D-Ala Ala	C00133 C00041	+	Cation	Hydrophilic Hydrophilic	3 7	1 2	\mathbf{H}	89.04	77 90	.0550
Peptidoglycan turnover	II L-Alaninyl-γ-D-glutamyl- <i>meso</i> -diaminopimelyl-D-alanine	AlaGluDAPAla	_	-	Cation	Hydrophilic	16 27	5 9	+	433.18	09 434	.1882
Peptideglycan biosynthesis Peptidoglycan turnover	I D-Alanyl-D-alanine II L-Alanyl-γ-D-glutamic acid	AlaAla L-Ala-D-Glu	C00993	+	Cation Cation	Hydrophilic Hydrophilic	6 12 8 14	2 3		160.08 218.09	03 219	.0921 .0975 Multiple peaks were detected
Peptidoglycan turnover Peptideglycan biosynthesis	II L-Alanyl-y-D-glutamyldiaminopimelic acid I L-Alanyl-D-glutamyl- <i>meso</i> -A2pm	L-Ala-D-Glu-Dap AlaGluA2pm	-		Cation Cation	Hydrophilic Hydrophilic	13 19 15 26	5 4 4 8	+ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$ $+$	309.14 390.17		.1510
Allantoin degradation	III Allantoin		C00499	+	Anion	Hydrophilic	4 8	4 4	+	176.05	46 175	.0473 .0367
Allantoin degradation Lactose degradation	III Allolactose		C01551	-	Anion Neutral	Hydrophilic Hydrophilic	12 22	11	$\pm \pm \pm$	342.11	62 -	Neutral and/or hydrophobic
Allose degradtion Allose degradtion	III D-Allose III D-Allose-6-phosphate		C01487 C02962	+	Neutral Anion	Hydrophilic Hydrophilic	6 12 6 13	6 9 1	$\pm + \Box$	180.06 260.02		Neutral and/or hydrophobic
ItaE (in vitro) Allose degradtion	VI L-Allothreonine III D-Allulose-6-phosphate		C05519	+	Cation Anion	Hydrophilic Hydrophilic	4 9	1 3 9 1	H	119.05	82 120	.0655 .0224
Galacturonic acid degradation Taurine degradation	III D-Altronic acid		C00817		Anion	Hydrophilic	6 12	7	+	196.05	83 195	.0510
Threonine degradation	II Aminoacetone		C06735 C01888	-	Cation Cation	Hydrophilic Hydrophilic	3 7	1 1		73.05	28 74	.0600
Tetrahydrofolic acid biosynthesis Putrescine degradation	I p-Aminobenzoic acid II 4-Aminobutyraldehyde	PABA 4ABA	C00568	+	Cation Cation	Hydrophilic Hydrophilic	7 7	\rightarrow		137.0 ²		.0550
4-Aminobutyric acid degradation Tetrahydrofolic acid biosynthesis	III 4-Aminobutyric acid I 4-Amino-4-deoxychorismic acid	4-AB ADCA	C00334 C11355	+	Cation Cation	Hydrophilic Hydrophilic	4 9 10 11			103.06	33 104	.0706
Modification of lipid A	I 4-Amino-4-deoxy-L-arabinose	Ara4N	-		Cation	Hydrophilic	5 11	1 4		149.06	88 150	.0761
Polymyxin resistance Tetrahydrofolic acid biosynthesis	III 4-Amino-4-deoxy-L-arabinose-modified KDO2-Lipid A I 2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridinediphosphate	Ara4N-KOD2-Lipid A AHHMeDHPDP	C04807	-	Nucleotide Nucleotide	Hydrophobic Hydrophilic	7 11	4 45 2 5 8 2		2499.45 355.00		.4452 Out of the MS range .0010
Thiamine biosynthesis Fravin biosynthesis	I 4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate I 5-Amino-6-ribitylamino-2,4(1H,3H)-pyrimidinedione	4A5HMe2MePyrPP 5A6RbA2,4PD	C04752 C04732	_	Nucleotide Cation	Hydrophilic Hydrophilic	6 11 9 16	3 7 2		299.00		.0000
Purine biosynthesis Purine biosynthesis	I Aminoimidazole carboxamide ribonucleotide I 5-Aminoimidazoleribonucleotide	AICAR AIR	C04677 C03373	+	Nucleotide Nucleotide	Hydrophilic Hydrophilic	9 15	4 8 1		338.06	28 337	.0555
Proto- and siroheme biosynthesis	I 5-Aminolevulinic acid	AIR	C00430	+	Cation	Hydrophilic	5 9	1 3		131.05	82 132	.0655
YdfG Queuine biosynthesis (tRNA)	VI 2-Aminomalonatesemialdehyde I 7-(Aminomethyl)-7-deazaguanine	7AMe7DAGua	C11822 C01449		Anion Cation	Hydrophilic Hydrophilic	7 9	5 1		103.02		.0197 .0880 Modified tRNA
Threonine degradation Biotin biosynthesis	II 2-Amino-3-oxobutanoic acid I 8-Amino-7-oxononanoic acid	AOBA 8A7ONA	C03214 C01092	-	Cation Cation	Hydrophilic Hydrophilic	4 7 9 17	1 3		117.04		.0499
Fravin biosynthesis Fravin biosynthesis	I 5-Amino-6-(5'-phosphoribitylamino)uracil I 5-Amino-6-(5'-phosphoribosylamino)uracil	5A6-5'PRDAU 5A6-5'PRAU	C04454 C01268	-	Anion Anion	Hydrophilic Hydrophilic	9 17 9 15	4 9 1		356.07 354.05		.0660
Threonine degradation	II 1-Aminopropan-2-ol			+	Cation	Hydrophilic	3 9	1 1		75.06		.0757
		Apol	C03194							1100		
Pyridoxal-5'-phosphate biosynthesis Peptidoglycan turnover	I 1-Aminopropane-2-one-3-phosphate II Anhydro- <i>N</i> -acetylmuramic acid	Apol 1AP2O3P AHMurNAc	C03194 —	-	Anion Cation	Hydrophilic Hydrophilic	3 8 11 17	1 5 1		169.01 275.10		.1078
	I 1-Aminopropane-2-one-3-phosphate	1AP2O3P		- - + +				1 7			05 276 77 138	.0550
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion	1 -Aminopropane-2-one-3-phosphate	1AP2O3P AHMurNAc	- C00108 C00216 C00259	- + +	Cation Cation Neutral Neutral	Hydrophilic Hydrophilic Hydrophilic Hydrophilic	11 17 7 7 5 10 5 10	1 7 1 2 5		275.10 137.04 150.05	05 276 77 138 28 – 28 –	.1078 .0550 - Neutral and/or hydrophobic Neutral and/or hydrophobic
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport	I 1-Aminopropane-2-one-3-phosphate II Anhydro- <i>N</i> -acetylmuramic acid I Anthranitic acid III D-Arabinose III L-Arabinose I D-Arabinose-5-phosphate III Arbutin	1AP2O3P	C00108 C00216 C00259 C01112 C06186	- + + + + +	Cation Cation Neutral Neutral Anion Neutral	Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic	11 17 7 7 5 10 5 10 5 11 12 16	1 7 1 2 5 5 5 8 1 7		275.10 137.04 150.05 150.05 230.01 272.08	05 276 77 138 28 - 28 - 92 229 96 -	.1078 .0550 Neutral and/or hydrophobic Neutral and/or hydrophobic .0119 Neutral and/or hydrophobic
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis	1 - Aminopropane-2-one-3-phosphate	1AP2O3P AHMurNAc	- C00108 C00216 C00259 C01112	- + + + +	Cation Cation Neutral Neutral Anion	Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic	11 17 7 7 5 10 5 10 5 11	1 7 1 2 5 5 5 8 1 7 10 1		275.10 137.04 150.05 150.05 230.01	05 276 77 138 28 - 28 - 92 229 96 - 59 351	.1078 .0550 Neutral and/or hydrophobic Neutral and/or hydrophobic .0119
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport	I 1-Aminopropane-2-one-3-phosphate II Anhydro- <i>N</i> -acetylmuramic acid I Anthranilic acid III D-Arabinose III L-Arabinose I D-Arabinose	1AP2O3P AHMurNAc Ara5P	- C00108 C00216 C00259 C01112 C06186 C06187	- + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Anion	Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic	11 17 7 7 5 10 5 10 5 11 12 16 12 17	1 7 1 2 5 5 5 8 1 7 10 1		275.10 137.04 150.05 150.05 230.01 272.08 352.05	05 276 77 138 28 - 28 - 92 229 96 - 59 351 17 175 26 291	.1078 .0550 .Neutral and/or hydrophobic .Neutral and/or hydrophobic .0119 .Neutral and/or hydrophobic .0487
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation	1	AraSP Arg Arg Arguccinate		- + + + + + - + +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Cation Anion	Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic	11 17 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8	1 7 1 2 5 5 5 8 1 7 10 1 4 2 4 6 9 1 6 6		275.10 137.04 150.05 150.05 230.01 272.08 352.05 174.11 290.12 255.99	05 276 77 138 28 - 28 - 92 229 96 - 59 351 17 175 26 291 84 254 21 175	.1078 .0550 Neutral and/or hydrophobic Neutral and/or hydrophobic .0119 Neutral and/or hydrophobic .0487 .1190 .1299 .9911
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Asgranine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis	1	AraSP Arguccinate Asn AspSA	- C00108 C00216 C00259 C01112 C06186 C06187 C00062 C03406 C16186 C00072 C00152 C00441	- + + + + + - + + + - +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Cation Anion Cation Cation Cation Cation Cation Cation Cation	Hydrophilic	11 17 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7	1 7 1 2 5 5 5 8 1 7 7 10 1 4 2 4 6 9 1 6 2 3 1 3		275.10 137.0- 150.05 150.05 230.01 272.08 352.05 174.11 290.12 255.95 176.03	05 2766 77 1388 28 28 92 229 96 59 351 17 175 26 291 84 254 21 175 35 133 26 118	.1078 .0550 .Neutral and/or hydrophobic .Neutral and/or hydrophobic .0119 .Neutral and/or hydrophobic .0487 .1190 .1199 .9911 .0248 .0608 .0499
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Asgorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis D-Amino acids degradation Aspartic acid diegradation Aspartic acid biosynthesis	1	AraSP Arg ArgSuccinate Asn AspSA D-Asp Asp	- C00108 C00216 C00259 C01112 C06186 C06187 C00062 C03406 C03406 C00072 C00152 C00441 C00402 C00049	- + + + + + - + + +	Cation Cation Neutral Neutral Neutral Anion Neutral Anion Cation Cation Anion Cation	Hydrophilic	11 17 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8	1 7 1 2 5 5 5 8 1 7 10 1 4 2 4 6 9 1 6 2 3		275.10 137.0- 150.05 230.01 272.08 352.05 174.11 290.12 255.99 176.03 132.00 117.0- 133.03	05 276 77 138 28 28 92 229 96 55 351 17 175 26 44 254 21 175 35 133 26 118	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0119 . Neutral and/or hydrophobic .0487 .1190 .1299 .9911 .0248 .0408 .0499 .0448
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Argonic acid transport Ascorbic acid degradation Asparagine biosynthesis D-Amino acids degradation	1	AraSP Arg ArgSuccinate Asn AspSa D-Asp		- + + + + + - + + - - +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Cation Anion Anion Cation	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7	1 7 1 2 5 5 5 5 8 1 7 7 10 1 4 2 4 6 2 3 3 1 1 3 1 4 4		275.10 137.04 150.05 150.05 230.01 272.08 352.05 174.11 290.12 255.99 176.03 132.00 117.04	05	.1078 .0550 .Neutral and/or hydrophobic .Neutral and/or hydrophobic .0119 .Neutral and/or hydrophobic .0487 .1190 .1299 .9911 .0248 .0608 .0499
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arptinin biosynthesis Asgrorie acid transport Asgrinine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis D-Amino acids degradation Asparatic acid biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis	1	AraSP Arg ArgSuccinate Asn AspSA D-Asp Asp	C00108 C00216 C002259 C00112 C06186 C06187 C00626 C03406 C16186 C00052 C00072 C00072 C00072 C00072 C00072 C00079 C00079 C00079	- + + + + + + + + - - + + + + + + + +	Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Cation Anion Cation	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 7 4 7 4 7 4 7 4 8 5 11 5 11 5 11 5 11	1 7 1 2 5 5 5 5 8 8 1 7 7 100 1 4 4 6 9 9 1 6 6 2 2 3 1 1 3 1 1 4 4 1 1 7 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1	275.1(137.0- 150.00: 230.01 230.01 272.00: 352.00: 174.11 290.12 255.9- 176.00: 132.00: 133.00: 133.00: 133.00: 131.0	05	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0487 .1190 .1299 .9911 .0228 .0608 .0499 .0448 .0448 .0448 .0448 .0448 .0459 .0469 .0469 .0469 .0479 .0610 .0790 .0610ding quarternary amine
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis	1	AraSP AraSP Arg ArgSuccinate Asn AspSa D-Asp Asp Asp-P BlotinSul	C00108 C00216 C00216 C00217 C001192 C001192 C00186 C00186 C000187 C000087 C000182 C000182 C000182 C0007 C0	- + + + + + - + + - - + + + - - + + -	Cation Cation Neutral Neutral Anion Anion Cation Cation Anion Anion Cation	Hydrophitic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 11 5 11 6 10 6 14	1 7 1 2 5 5 5 5 5 5 5 6 8 1 7 7 100 1 4 2 4 6 6 9 9 1 6 6 2 3 3 1 3 1 4 4 1 7 1 1 2 1 1 1 2 2 1 1 1 1 2 2 3 3 2 3 3 2 4 4 6 6		275.10 137.0 137.0 150.00 230.01 250.01 272.08 352.00 174.11 290.12 255.99 176.00 133.00 117.00 102.06 240.00 260.00	05	.1078 .0550
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis D-Amino acids degradation Aspartic acid tionynthesis Homoserine biosynthesis Botaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin biosynthesis	1	Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00229 C01112 C00186 C00062 C03406 C16186 C00072 C00152 C00041 C00402 C00402 C00709 C00576 C00576 C00120 C00576 C00120 C00576 C0	- + + + + + + - + + - + + + + - - + + + + - - - +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 20 28 20 28	1 7 7 1 2 5 5 8 8 1 7 7 10 1 4 2 4 6 9 1 6 6 2 3 3 1 4 4 1 7 1 1 2 2 3 3 2 4 7 7 9 1 1 1 0 1 9 4	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.10 137.0 150.05 150.05 230.01 150.05 230.01 272.00 352.05 174.11 255.99 176.00 133.00 117.00 133.00 117.00 120.00 120.00 124.00 120.00 244.00 2573.1 2836.00	05	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0119 . Neutral and/or hydrophobic .0487 .1190 .9911 .0248 .0409 .0448 .0499 .0448 .9966 .0790 Including quarternary amine .0954 .0904 .0904 .1334
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arptinin biosynthesis Ascorbic acid transport Asginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis D-Amino acids degradation Asparatic acid biosynthesis Betaine biosynthesis	1	AraSP Arg ArgSuccinate Asn AspSa D-Asp Asp-P BiotinSul BiotinyL-AMP	C00108 C00216 C00226 C00229 C01112 C06186 C06187 C00622 C03406 C16186 C00152 C00072 C00072 C00072 C00072 C00072 C00072 C00072 C00072 C00072 C00720 C00720 C00720 C00720 C00921	- +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Cation Anion Cation Neutral	Hydrophilic Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 7 4 8 5 11 1 5 1 10 1 6 1 6 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7	1 7 1 2 5 5 5 8 8 1 7 7 10 1 4 2 4 6 6 9 9 1 1 6 6 1 1 3 1 4 1 7 1 1 2 3 1 2 2 4 7 9 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c 137.0c 150.0t 150.0t 230.0i 230.0i 352.0t 174.1i 255.99 117.0c	05	.1078 .0550 . Neutral and/or hydrophobic .0487 .1190 .0487 .0499 .9911 .0248 .0499 .0499 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .09966 .0910 .0910 .0910 .0910 .0910 .0910 .0910
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis D-Amino acids degradation Aspartic acid tolosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Botto biosynthesis Biotin oxidation Regulation of biotin biosynthesis AppppA biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis	1	Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00219 C01112 C06186 C06186 C06187 C00007 C00072 C00152 C00071 C00072 C00152 C00079 C00070 C0	- + + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Anion	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 8 4 8 4 7 4 7 4 7 4 8 5 11 10 16 20 28 20 28 20 28	1 7 7 1 1 2 5 5 8 8 1 7 7 1 1 0 1 1 4 2 6 6 2 3 3 1 1 3 1 4 4 1 7 1 1 1 2 2 3 3 2 4 4 7 7 9 1 1 10 19 4 1 1 12 1 2 2 8 1 1 2 2 8 1 1 2 2 8 1 1 2 2	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.10 137.0 150.05 150.05 230.01 150.05 230.01 174.11 255.99 176.03 131.00 117.00 131.00 117.00 120.00 1244.00 1244.00 1244.00 1255.39 127.00	005	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0119 . Neutral and/or hydrophobic .0487 .1190 .1299 .9911 .0248 .0608 .0499 .0448 .0448 .0448 .0448 .0448 .0448 .0449 .0449 .0449 .0440 .0450 .0440 .0450
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis D-Amino acids degradation Asparatic acid biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Lysine degradation Lysine degradation	1	Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00226 C00229 C01112 C06186 C06187 C006187 C00062 C03406 C16186 C0007 C007 C0		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Cation C	Hydrophilic Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 8 4 7 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 20 28 20 28 34 66 12 11 7 15 22 5 5 14	1 7 7 1 2 5 5 8 8 1 7 7 1 0 1 4 2 6 6 2 3 1 1 4 1 1 1 2 1 1 1 2 2 4 4 7 9 1 1 1 1 2 2 8 1 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 7 3 2 1 1 3 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c 137.0c 150.0t 150.0t 230.0t 150.0t 230.0t 174.1t 255.99 1776.0t 117.0c	005	.1078 .0550 . Neutral and/or hydrophobic .0487 .1190 .0487 .0499 .9991 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0449 .05906 .0790 .0790 .01cluding quarternary amine .0950 .0951 .0954 .0956 .0960 .0960 .0960 .1176 .0180 .1176 .2155
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Asginine biosynthesis Ascorbic acid transport Ascorbic acid transport Ascorbic acid transport Ascorbic acid transport Ascorbic acid segradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis LiaC (in vitro) Carnitine degradation Carnitine degradation Cyanic acid degradation Pyrimidine biosynthesis	1	AraSP Arg Arg ArgSuccinate Asn AspSa D-Asp Asp Asp Asp-P BiotinyLAMP ApppA BHMyrGcIP Carbamoyl-Asp	C00108 C00216 C00216 C00216 C00216 C01112 C06186 C06187 C006186 C06187 C00072 C00152 C00072 C00152 C00071 C00072 C00152 C00071 C00075 C00071 C00077 C00120 C00402 C00402 C00402 C0077 C00576 C0120 C01		Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Anion Nucleotide Cation Nucleotide Cation	Hydrophilic	11 17 7 7 7 5 10 5 10 12 16 6 14 10 18 6 9 6 8 4 7 4 7 4 7 4 8 5 11 15 12 10 16 10 16 10 16 20 28 20 28 20 28 34 66 12 11 7 28 55 5 11 1 2 17 1 3 16 1 3 16	1 7 7 1 1 2 5 5 8 8 1 7 7 1 1 0 1 1 4 4 6 6 6 2 3 1 1 3 1 1 4 1 1 7 1 1 1 2 3 1 1 1 1 1 2 2 4 4 7 9 1 1 1 1 1 2 2 8 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c	05	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0119 . Neutral and/or hydrophobic .0487 .1190 .1299 .9911 .0248 .0608 .0499 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0449 .05966 .0590 .0691 .0790 .0790 .0810
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Cyanic acid degradation Dyrimidine biosynthesis Purine biosynthesis	1 -Aminopropane-2-one-3-phosphate Anhydro-N-acetylmuramic acid	Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp.P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P	C00108 C00216 C00216 C00216 C0029 C01112 C06186 C00062 C03406 C16186 C00072 C00152 C00041 C00402 C00049 C0072 C00150 C0072 C00150 C0072 C0072 C0072 C00740 C0072 C		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Nucleotide	Hydrophitic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 20 28 20 28 20 28 21 21 21 15 28 50 5 14 1 2 28 50 5 14 1 2 28 50 5 14 1 3 28 50 5 14 1 3 28 50 6 8 7 12 1 12 1 12 1 12 1 12 1 12 1 12 1 12	1 7 7 1 1 2 5 5 5 6 8 8 1 7 7 7 7 9 1 1 1 2 1 2 1 2 1 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 2 2 2 5 5 1 1 3 3 9 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.10 137.0 150.05 150.05 230.01 150.05 230.01 174.11 255.99 176.03 131.00 117.04 131.00 117.04 131.00 141.01 141.01 150.05 160.00 171.4.1 171.01 17	005	.1078 .0550 . Neutral and/or hydrophobic . Neutral and/or hydrophobic . Neutral and/or hydrophobic . Neutral and/or hydrophobic .0487 .1190 .9911 .0248 .0499 .9911 .0248 .0499 .0448 .0499 .0448 .0996 .0190 .0101 .010
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis D-Amino acids degradation Aspartic acid biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Blotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis	1	Ara5P Arg Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P	C00108 C00216 C00216 C00216 C00216 C01112 C06186 C06187 C006186 C06187 C00072 C00152 C00072 C00152 C00071 C00072 C00152 C00071 C00075 C00071 C00077 C00120 C00402 C00402 C00402 C0077 C00576 C0120 C01		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Anion Cation Cation Cation Cation Anion Cation Cation Cation Anion Cation Cation Anion Cation Anion Cation Anion Cation Anion	Hydrophilic Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 8 4 7 4 7 4 7 4 7 4 7 4 7 4 7 1 10 16 5 11 5 12 10 16 20 28 34 66 12 17 10 16 20 28 34 66 12 17 17 15 28 50 5 11 7 15 8 5 10 10 16 10	1 7 7 1 1 2 5 5 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c 137.0c 150.0t 150.0t 230.0t 150.0t 230.0t 174.1t 255.99 1776.0t 117.0c	05	.1078 .0550 . Neutral and/or hydrophobic .0487 .1190 .0487 .0499 .9911 .0248 .0499 .0499 .0499 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0440 .0596 .0790 including quarternary amine .0950 .0950 .0910 .
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Lysine degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis	1	Ara5P Arg Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P	C00108 C00216 C00216 C00226 C00259 C01112 C06186 C006187 C00062 C03406 C16188 C00072 C00152 C00152 C00152 C00402 C00402 C00402 C00719 C00576 C00120 C	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide	Hydrophitic	11 17 7 7 7 5 10 5 10 5 11 12 16 12 17 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 20 28 20 28 20 28 34 66 11 7 15 28 50 5 14 1 7 15 28 50 5 14 1 7 15 28 50 5 14 1 7 15 28 50 5 14 1 7 15 28 50 6 14 1 7 15 28 50 1 7 15 5 12 5 14 1 7 15 5 12 5 14 1 7 15 5 14 1 7 15 5 12 5 14 1 7 15 5 14 1 7 15 5 12 5 14 1 7 15 5 14 1 7 15 1 7	1 7 7 1 2 5 5 8 8 1 7 7 1 0 1 4 2 1 4 6 6 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(1) 137.0 150.00 1	05	.1078 .0550
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis D-Amino acids degradation Aspartic acid biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Arginine biosynthesis Purine biosynthesis Carnitine metabolism Carnitine metabolism Carnitine metabolism	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Carbamoyl-Asp Carbamoyl-P N5-CAIR	C00108 C00216 C00216 C00216 C0029 C01112 C06186 C006186 C006187 C006186 C00062 C03406 C16188 C00072 C00152 C00402 C00402 C00402 C00402 C00402 C00402 C00402 C00576 C00120 C00576 C01563 C00677 C01563 C00677 C01563 C00666 C01302 C01302 C01302 C01302 C003666 C01302 C01302 C01502 C003666 C01302 C01502 C00379		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Anion Cation Cation Cation Cation Cation Cation Nucleotide Cation Anion Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 10 16 10 16 10 16 11 10 16 11 10 16 12 12 16 12 16 13 16 14 17 16 15 17 16 16 17 16 17 16 16 17 16 16 17 16 16 18 17 16 18 18 17 16 18 17 17 17 17 17 17 17 17 17 17 17 17 17	1 7 7 1 1 2 5 5 1 8 8 1 7 7 1 1 2 1 1 2 1 1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c 137.0c 130.0t 150.0t 230.0t 150.0t 230.0t 174.1t 255.99 1776.0t 131.0c	005	.1078 .0550 . Neutral and/or hydrophobic .0487 .1190 .0248 .0499 .0911 .0248 .0499 .0448 .0499 .0448 .0996 .0090 .0101
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Asgorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparatic acid biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Apppab biosynthesis ElaC (in vitro) Carrittine degradation Cyanic acid degradation Cueo Tryptophan biosynthesis Purine biosynthesis Purine metabolism Carrittine metabolism Carrittine metabolism Carrittine metabolism	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Carbamoyl-Asp Carbamoyl-P N5-CAIR	C00108 C00216 C00216 C00216 C00217 C00119 C00119 C00119 C00119 C0016 C0016 C0007 C0007 C0015 C0007 C0007 C0015 C0007 C0007 C0015 C0007 C00	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Anion Cation Cation Cation Cation Cation Nucleotide Cation Cation Nucleotide Cation C	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 9 6 8 4 7 4 7 4 7 4 7 4 7 4 8 5 11 5 12 10 16 10 18 6 20 28 20 28 34 66 12 11 7 15 5 12 10 16 12 12 10 16 12 12 10 16 12 12 10 16 10 1	1 7 7 1 1 2 5 5 1 1 5 1 1 3 1		275.1(2) 137.0(2) 137.0(2) 137.0(2) 137.0(2) 130.0(2) 130.0(2) 130.0(2) 130.0(2) 132	05	.1078 .0550 . Neutral and/or hydrophobic
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Carnitine degradation Carnitine degradation Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Phenylpropionic acid degradation Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Carbamoyl-Asp Carbamoyl-P N5-CAIR	C00108 C00216 C00216 C00216 C00226 C01112 C06186 C06187 C06187 C00628 C03406 C01002 C00102 C0		Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Nucleotide Cation Anion Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide Cation Nucleotide Cation Nucleotide	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 8 5 11 5 12 10 16 10 16 20 28 20 28 20 28 34 66 12 11 5 12 10 16 20 28 20 18 21 10 16 20 28 20 19 31 46 20 19 31 46 20 19 31 46 31 46 31 46 31 46 31 46 31 46 31 46 31 46 31 57	1 7 7 1 1 2 5 5 8 8 1 7 7 1 1 0 1 1 4 4 6 6 6 1 1 2 2 4 7 9 1 1 1 2 2 3 1 2 4 7 9 1 1 1 2 2 8 1 1 2 2 8 1 1 2 2 5 1 1 5 1 1 2 2 3 3 9 1 1 1 2 2 8 1 1 2 3 3 9 1 1 1 2 3 3 8 1 8 3 8 1 8 3 8 1 8 3 1	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0(2) 137.0(2) 137.0(2) 150	005	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Apppab biosynthesis ElaC (in vitro) Carrittine degradation Cyanic acid degradation Cyanic acid degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Purine biosynthesis Purine biosynthesis Arginine biosynthesis Arginine biosynthesis Carrittine metabolism	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Carbamoyl-Asp Carbamoyl-P N5-CAIR	C00108 C00216 C00216 C00216 C00217 C00119 C00119 C00119 C00118 C0018 C0018 C0007 C0007 C0007 C0007 C0007 C0007 C0007 C0007 C00152 C0040 C0007 C0		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide	Hydrophilic	11	1 7 7 1 1 2 5 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	275.1(2) 137.0c 137.0c 150.00c 220.00c 230.00c 230.00c 230.00c 230.00c 240.00c 150.00c 177.0c	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ApppaA biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Phenylpropionic acid degradation Cuel Carnitine metabolism Carnitine m	1	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-P N5-CAIR CPADRP	C00108 C00216 C00216 C00216 C00216 C001112 C06188 C06188 C06188 C00072 C00120 C00102 C00102 C0002 C000	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Nucleotide Cation Anion Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide Cation Cation Nucleotide Neutral Cation Nucleotide Cation Nucleotide	Hydrophilic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 9 6 8 4 8 4 7 4 7 4 7 4 8 5 11 5 11 5 12 10 16 20 28 20 28 34 66 12 11 5 12 10 16 20 28 20 28 31 66 28 10 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 17 15 28 50 5 14 27 7 6 12 12 16 7 15 7 15 28 50	1 7 7 1 1 2 1 5 5 5 8 8 1 7 7 1 1 0 1 1 4 4 6 6 1 1 2 1 1 1 2 2 4 7 9 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 8 1 1 1 2 2 1 1 1 1		275.1(2) 137.0(2) 137.0(2) 137.0(2) 150	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Carnitine degradation Lysine degradation Dyrimidine biosynthesis Purine biosynthesis Purine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism C	I	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-P N5-CAIR CPADRP	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00062 C03406 C15186 C00072 C00152 C0041 C00041 C00040 C00041 C00040 C00719 C00576 C00120 C0120 C04824 C03779 C01563 C00486 C01300 C01563 C00486 C01300 C15025 C01674 C00307 C00185 C00185		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Nucleotide Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide Nucleotide Nucleotide Neutral Cation Nucleotide	Hydrophitic	11 17 7 7 7 5 10 5 10 5 11 12 16 6 14 10 18 6 8 4 8 4 7 4 7 4 7 4 7 4 7 4 7 4 7 4 7 1 2 1 2 1 2 1 2 1 3 1 3 1 3 1 3 1 3 1 3 1 3 1 3 1 3 1 3	1 7 7 1 1 2 5 5 1 1 3 1 4 4 1 1 7 1 1 2 2 3 1 1 3 1 1 4 1 1 1 1 1 1 1 1 1 1 1 1 1		275.1(2) 137.0c 130.01 150.05 230.01 150.05 230.01 174.11 255.90 1774.01 133.00 117.00 133.00 117.00	055	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis D-Amino acids degradation Aspartic acid biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Purine biosynthesis Purine biosynthesis Purine biosynthesis Carnitine metabolism Carnitine metaboli	1	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-P N5-CAIR CPADRP	C00108 C00216 C00216 C00216 C00216 C00217 C001112 C00188 C00018 C0018 C00		Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Anion Cation Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide	Hydrophilic	11	1 7 7 1 1 2 5 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6		275.1(2) 137.0c 137.0c 130.01 150.05 230.01 150.05	05	.1078 .0550 . Neutral and/or hydrophobic
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ROD biosynthesis ElaC (in vitro) Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Phenylorpoinoic acid degradation CueO Tryptophan biosynthesis Phenylorpoinoic acid degradation Curol Tryptophan biosynthesis Carnitine metabolism Carnitine me	I	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00186 C001112 C00186 C00062 C03406 C116186 C00072 C00152 C00402 C00041 C00402 C00049 C00719 C00576 C00120 C0120 C00185 C00185 C00120 C00121		Cation Cation Neutral Anion Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Neutral Anion Anion Anion Anion	Hydrophitic	11 17 7 7 15 10 10 16 12 12 16 16 12 17 15 12 11 15 12 12 17 16 12 12 16 12 18 16 19 18 18 18 18 18 18 18 18 18 18 18 18 18	1		275.1(2) 137.0 150.00 1	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Lysine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Purine biosynthesis Purine biosynthesis Carnitine metabolism Carnitine degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis	I Anhydro-M-acetylmuramic acid III Anhydro-M-acetylmuramic acid III D-Arabinose III A-Arabinose III Arbutin-6-phosphate III Arbutin-6-phosphate III L-Argininosuccinic acid III L-Asgorbic acid L-Asgorbic acid L-Asparagine L-Asparagine L-Asparagine L-Asparagine L-Asparatesemialdehyde III D-Aspartic acid III L-Aspartic acid III Betaine IIII Betaine IIII Betaine IIII Betaine IIII Biotin-d-sulfoxide III Biotin-d-sulfoxide III Biotin-d-sulfoxide III Biotin-d-sulfoxide III Biotin-d-sulfoxide III Biotin-d-sulfoxide III P(II),P(I)-Bis(S-adenosyl)tetraphosphate III P(II),P(I)-Bis(S-adenosyl)tetraphosphate III P-Butyrobetaine III P-Butyrobetaine III P-Butyrobetaine III Carbamoyl-I-aspartic acid III Carbamoyl-I-aspartic acid III Carbamoyl-I-aspartic acid III Carbamoyl-I-aspartic acid III Carbamoyl-I-osphosphate III Carbamoyl-I-osphosphate III P-Butyrobetaine III Carbamoyl-I-osphosphate III P-Garmitine III Carbamoyl-I-osphosphate III P-Garmitine III C-Garmitine III C-Garmitine III C-Garmitine Carbamoyl-I-osphosphate III C-Garmitine III C-Garmitine III C-Garmitine III C-Garmitine III C-I-ochoxynehrylamino)-I'-deoxyribulose-5'-phosphate III C-I-ochoxynehrylamino)-I'-deoxyribulose-5	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP ApppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00018 C00018 C00018 C00018 C00019 C00019 C00019 C00019 C00019 C00019 C00019 C00019 C00100 C00000 C00100 C000000 C0000000 C00000000		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Anion Nucleotide Cation Anion Nucleotide Neutral Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Cation Nucleotide Neutral Cation Cation Cation Cation Cation Nucleotide Neutral Anion Nucleotide Cation Anion Nucleotide Cation Nucleotide Cation	Hydrophilic	11	1		275.1(2) 137.0c 137.0c 137.0c 130.01 150.05 230.01 150.05 230.01 150.05	05	.1078 .0550 . Neutral and/or hydrophobic
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis LiaC (in vitro) Carnitine degradation Carnitine degradation Lysine degradation Cyanic acid degradation Pyrimidine biosynthesis Phenylpropionic acid degradation Cueo Tryptophan biosynthesis Phenylpropionic acid degradation Cueo Tryptophan biosynthesis Carnitine metabolism Carnit	1	AraSP Arg ArgSuccinate Asn AspSa D-Asp Asp Asp-P BiotinSul BiotinyI-AMP AppppA BHMyrGc1P CarbamoyI-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA COA	C00108 C00216 C00216 C00216 C00216 C001112 C06186 C06186 C06187 C00062 C03406 C01007 C00120 C00041 C00042 C00042 C00076 C00120 C0042 C00048 C00077 C00576 C0120 C0		Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Cation Nucleotide Cation Anion Cation Cation Anion Cation Anion Cation Cation Anion Cation Cation Anion Nucleotide Neutral Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.00 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Botanie biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Regulation of biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Cyanic acid degradation Pyrimidine biosynthesis Purine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Phenylpropionic acid degradation Carnitine metabolism Carnitine me	1	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C0029 C01112 C06186 C006187 C006187 C00062 C03406 C16188 C00072 C00152 C00152 C00152 C00152 C00402 C00049 C00576 C00160 C001674 C00695 C00114 C00695 C00774 C00106		Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Neutral Anion Cation Nucleotide	Hydrophilic	11	1		275.1(2) 137.0 150.00 1	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Lysine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Purine biosynthesis Purine biosynthesis Carnitine metabolism Carnitine degradation TCA cycle Arginine biosynthesis Cholainnin biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00117 C00186 C0017 C00186 C00012 C00186 C00012 C00186 C00012 C00186 C00012 C00186 C00012 C00120 C00		Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Anion Nucleotide Cation Cation Nucleotide Cation Cation Cation Cation Nucleotide Cation Cati	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.0(2)	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis AppppA biosynthesis ElaC (in vitro) Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Phenylpropionic acid degradation CueCO Tryptophan biosynthesis Carnitine metabolism Ca	1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00062 C03406 C0117 C000152 C00152 C	+ + + + + + + + + + + + + + + + + + +	Cation Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Anion Nucleotide Neutral Cation Nucleotide Nucleotide Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Nucleotide Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide	Hydrophitic	11	1		275.1(2) 137.0 150.00 1	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion (L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Carnitine degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Carnitine biosynthesis Cholaismin biosynthesis Cholaismin biosynthesis Cholaismin biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Phenylpropionic acid degradation Cac (gutative) Acs (putative) Carnitine metabolism	1	Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00187 C00062 C03406 C116186 C00072 C00187 C00041 C00041 C00040 C00041 C00041 C0040 C0		Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Anion Cation Nucleotide Cation Anion Nucleotide Cation Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Anion Anion Anion Anion Anion Nucleotide Cation Cation Nucleotide	Hydrophitic	11	1		275.10 137.0 150.01 150	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arginine biosynthesis Asgoribic acid transport Asgoribic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Lysine degradation Lysine degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Cobalamin biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation Acs (putative) Cobalamin biosynthesis Phenylpropionic acid degradation Acs (putative) Carnitine metabolism	1 1-Aminopropane-2-one-3-phosphate 1	Ara5P Arg Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00062 C03406 C0117 C000152 C00152 C	+ + + + + + + + + + + + + + + + + + +	Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Anion Nucleotide Neutral Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Neutral Cation Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Nucleotide Neutral Anion Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.01 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion (L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ROD biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimdine biosynthesis Phenylorpolonic acid degradation Cyanic acid degradation Cyanic acid degradation Cyanic acid messamplesis Phenylorpolonic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Carnitine biosynthesis Chotosiom caid degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Phenylpropionic acid degradation Acs (putative) Carlotine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism Cobalamin biosynthesis Phenylpropionic acid degradation Cacs (putative) Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism Cobalamin biosynthesis Phenylpropionic acid degradation Cacs (putative) Callotiose transport Chitobiose transport C	1	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp Asp Asp	C00108 C00216 C00216 C00216 C00226 C001112 C00186 C00117 C00186 C00022 C00108 C00022 C00108 C00022 C00108 C00022 C00108 C00022 C00108 C00022 C00108 C	+ + + + + + + + + + + + + + + + + + +	Cation Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Cation Cation Nucleotide Cation Cation Nucleotide Neutral Cation Cation Cation Nucleotide Neutral Cation Cation Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide	Hydrophitic	11	1		275.1(2) 137.0 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 150.0(3) 174.1(1) 174.1(1) 174.1(1) 175.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 133.0(3) 134.0(3) 135.0(3) 136.0(3) 136.0(3) 137.0(3) 137.0(3) 138.0(3) 138.0(3) 138.0(3) 138.0(3) 138.0(3) 138.0(3) 148.0(3) 148.0(3) 148.0(3) 159.1(05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Asgorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Robio biosynthesis Biotin oxidation Regulation of biotin biosynthesis Robio biosynthesis ElaC (in vitro) Carritine degradation Cyanic acid degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Purine biosynthesis Purine biosynthesis Purine degradation Cueo Tryptophan biosynthesis Carritine metabolism Carritine in biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis	1 - 1-Aminopropane 2-one 3-phosphate 1 Anthraniic acid 1 Anthraniic acid 1 Anthraniic acid 1 D-Arabinose 1 D-Arabino	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManQA CoA CoB12 CoPorgen III	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00112 C00186 C00172 C00187 C000187 C000187 C000187 C000187 C000187 C00187 C00187 C0160187 C000185	+ + + + + + + + + + + + + + + + + + +	Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Anion Cation Nucleotide Cation Anion Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.01 15	05	.1078 .0550 .0550 .0550 .0550 .0550 .0550 .0550 .0550 .0550 .0550 .0550 .0687 .0687 .0991 .0248 .0499 .0491 .0248 .0499 .0498 .0499 .0499 .0491 .0591 .0790 .0591 .0790 .0591 .0790 .0591 .0790 .0591 .0790
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Apppa biosynthesis BiaC (in vitro) Carnitine degradation Lysine degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Phenylpropionic acid degradation Carnitine metabolism Carnitine diosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation Acs (putative) Cobalamin biosynthesis Phenylpropionic acid degradation Acs (putative) Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine metabolism Carnitine biosynthesis Phenylpropionic acid degradation Acs (putative) Carnitine metabolism Car	1 1-Aminopropane'-2-one'-3-phosphate	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 CoPorgen III CAMP CGMP CGMP CGMP CCYS Cys	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00186 C001112 C006187 C00062 C03406 C01012 C0012 C0013 C00	+ + + + + + + + + + + + + + + + + + +	Cation Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Cation Cation Nucleotide Cation Cation Cation Nucleotide Nucleotide Nucleotide Neutral Cation Cation Nucleotide Cation	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.00 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Appopa biosynthesis Biotin oxidation Regulation of biotin biosynthesis Contintine degradation Lysine degradation Carritine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Phenyloropionic acid degradation CueO Tryptophan biosynthesis Phenyloropionic acid degradation Carritine metabolism Carritine acid biosynthesis Phenyloropionic acid degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis Cobalamin biosynthesis Phenyloropionic acid degradation ACS (putative) Acs (putative) Acs (putative) Acs (putative) Carritine metabolism Carritine metabolism Carritine metabolism Carritine metabolism Cobalamin biosynthesis Phenyloropionic acid degradation ACS (putative) Acs (puta	1 Anthropropane 2-one 3-phosphate Anthranitic acid Anthranitic acid	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManQA CoA CoB12 CoPorgen III CAMP CGMP CGMP CAMP CGMP	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00186 C00187 C00188 C0	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Neutral Anion Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Nucleotide Neutral Anion Anion Nucleotide Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Cation Cation Cation Cation Cation Cation Cation Cation	Hydrophilic	11	1		275.1(2) 137.0 150.00 1	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Apppap biosynthesis Biocompaniesis Biocompani	1 1-Aminopropane 2-one 3-phosphate 1 Anthranitic acid 1 D-Arabinose	Ara5P Ara5P Ara5P Arg ArgSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 CoPorgen III CAMP CAMP CAMP CAMP CAMP CAMP CAMP CCys Cys Cys	C00108 C00216 C00216 C00216 C00216 C00216 C00217 C0018 C0018 C00117 C0018 C0018 C0018 C0018 C0018 C0018 C0018 C0019 C0018 C0019 C0018 C001		Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Cation Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Nucleotide Nucleotide Neutral Cation Cation Nucleotide Cation Anion Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Cat	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.00 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis AppppA biosynthesis ElaC (in vitro) Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Purine biosynthesis Purine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Carnitine biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation Acs (putative) Caclobiamin biosynthesis Phenylpropionic acid degradation CACS (putative) Carnitine metabolism Cannitine metabolism Cannitine metabolism Cannitine metabolism Cannitine metabolism Cannitine metabolism Cannitine metabolism Cobalamin biosynthesis Phenylpropionic acid degradation Cysteine diosynthesis Phenylpropionic acid degradation Cysteine diosynthesis Phenylpropionic acid degradation Cysteine diosynthesis Dobalamine biosynthesis Phenylpropionic acid degradation Cysteine diosynthesis Dobalamine biosynthesis Dobalamine biosynthesis Dobalamine biosynthesis Dobalamin	1 - Aminopropane 2-one 3-phosphate 1 - Anthranilic acid 1 - An	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyi-AMP AppppA BHMyrGc1P Carbamoyi-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 COPorgen III CAMP CAMP CAMP CAMP CAMP CAMP CAMP CAM	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C0018 C001112 C006186 C00012 C006187 C00062 C03406 C16188 C00072 C00152 C00411 C00402 C00402 C00402 C00402 C00719 C00576 C00120 C0120 C0120 C04824 C03779 C05921 C01620 C04824 C03779 C05921 C01620 C04824 C03779 C01672 C01563 C00438 C00186 C01674 C00695 C00114 C00695 C00777 C001470 C00777		Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Nucleotide Neutral Cation Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide	Hydrophilic	11	1		275.1(2) 137.0(2) 137.0(2) 137.0(2) 150	05	.1078 .0550 .0550 .0550 .0550 .0687 .0887 .0887 .0999 .9911 .0228 .0608 .0499 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .0448 .05966 .0999 .0910 .0110
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion (L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Arginine biosynthesis Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis KDO biosynthesis ElaC (in vitro) Carnitine degradation Carnitine degradation Lysine degradation Lysine degradation Lysine degradation Pyrimidine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Cobalamin biosynthesis Carnitine metabolism Carnitine metabolism Carnitine metabolism	1 - Aminopropane 2-one -3-phosphate 1 - Anthranilis acid 1 Anthranilis acid 1 Anthranilis acid 1 Anthranilis acid 1 D-Arabinose D-Arabin	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyi-AMP AppppA BHMyrGc1P Carbamoyi-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 COPorgen III CAMP CAMP CAMP CAMP CAMP CAMP CAMP CAM	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C00117 C00186 C00018 C00018 C00018 C00018 C00018 C00018 C00018 C00018 C00018 C0018 C00		Cation Cation Neutral Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Cation Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Cation Cation Anion Nucleotide Cation Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Ca	Hydrophitic	11	1		275.10.177.00.15	05	.1078 .0550
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Appppa biosynthesis Biod (in vitro) Carritine degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation CueO Tryptophan biosynthesis Carritine metabolism Carritine diosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation Acs (putative) Cellobiose transport Cell	1 - Aminopropane 2-one 3-phosphate 1 - Anthranilic acid 1 An	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyi-AMP AppppA BHMyrGc1P Carbamoyi-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 COPorgen III CAMP CAMP CAMP CAMP CAMP CAMP CAMP CAM	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C001112 C00186 C0017 C00187 C00187 C00018 C00018 C00018 C00018 C00018 C00018 C00018 C0018 C008 C00		Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Neutral Cation Cation Nucleotide Cation Anion Nucleotide Cation Cation Nucleotide Cation Cat	Hydrophilic Hydrop	11	1		275.1(2) 137.0 137.0 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 174.11 174.11 174.11 175.00 176.00 17	05	
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Asgrinine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis AppppA biosynthesis Biotin oxidation Carnitine degradation Carnitine degradation Cyanic acid degradation Cyanic acid degradation Pyrimdine biosynthesis Phenylorpoinoic acid degradation Pyrimdine biosynthesis Phenylorpoinoic acid degradation CueO Tryptophan biosynthesis Carnitine metabolism Ca	1 - Aminopropone 2-one-3-phosphate 1 - Anthranilic acid 1 An	AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp Asp-P BiotinSul Biotinyi-AMP AppppA BHMyrGc1P Carbamoyi-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA CoA CoB12 COPorgen III CAMP CAMP CAMP CAMP CAMP CAMP CAMP CAM	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00186 C00187 C00187 C00015 C00112 C00186 C00017 C00186 C00017 C00186 C00187 C00187 C00187 C00188	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Anion Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Neutral Anion Nucleotide Neutral Anion Nucleotide Neutral Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide	Hydrophilic	11	1		275.1(2) 137.0 137.0 150.00 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid transport Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin oxidation Regulation of biotin biosynthesis ROD biosynthesis ElaC (in vitro) Carnitine degradation Cyanic acid degradation Lysine degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation Cueo Tryptophan biosynthesis Carnitine metabolism Carnitine biosynthesis Cholamin biosynthesis Cholamin biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis Phenylpropionic acid degradation Custeine biosynthesis Cobalamin biosynthesis Phenylpropionic acid degradation Custeine biosynthesis Cobalamine biosynthesis Phenylpropionic acid degradation Galactonic acid degradation Custeine biosynthesis Salvage of pyrimidine Pyrimidine cacid biosynthesis Salvage of pyrimidine Py	I - Anthropropane 2- one 3-phosphate I - Anthropropane 3- one 3-phosphate I - Anthropropane 3- one 3-phosphate I - Anthropose I - An	AraSP AraSP AraSP Arg ArgSuccinate Asn AspSA D-Asp Asp Asp. BiotinSul BiotinSul Biotinyl-AMP AppppA BHMyrGc1P Carbamoyl-Asp Carbamoyl-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA COA COB12 COPorgen III CAMP CAMP COPP CMP CTP CTP	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00186 C00117 C00187 C00187 C00187 C000187 C000187 C000187 C000187 C00187 C00187 C0160187 C000187 C0160187 C000187 C0160187 C000187 C00		Cation Cation Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Neutral Cation Nucleotide Neutral Cation Nucleotide Cation Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Cation Anion	Hydrophilic Hydrop	11	1		275.1(2) 137.0 137.0 150.00 15	05	.1078
Peptidoglycan turnover Tryptophan biosynthesis D-Arabinose degradtion L-Arabinose degradtion KDO biosynthesis Arbutin transport Arbutin transport Arbutin transport Arginine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Ascorbic acid degradation Asparagine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Homoserine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Betaine biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin biosynthesis Biotin degradation Carnitine degradation Carnitine degradation Carnitine degradation Cyanic acid degradation Cyanic acid degradation Cyanic acid degradation Pyrimidine biosynthesis Arginine biosynthesis Phenylpropionic acid degradation Cueo Tryptophan biosynthesis Phenylpropionic acid degradation Cueo Tryptophan biosynthesis Carnitine metabolism Carnitine diosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Phenylpropionic acid degradation TCA cycle Arginine biosynthesis Cobalamin biosynthesis Phenylpropionic acid degradation Acs (putative) Carnitine metabolism CAMP biosynthesis Cobalamin biosynthesis Denoisynthesis Cobalamin biosynthesis Denoisynthesis Cobalamine biosynthesis Denoisynthesis	1 Anthronitic acid	AraSP AraSP AraSP AraSuccinate Asn AspSA D-Asp Asp Asp Asp Asp.P BiotinSul Biotinyi-AMP AppppA BHMyrGc1P Carbamoyi-Asp Carbamoyi-P N5-CAIR CPADRP Cellobiose6P Citrulline CMP-DManOA COA COB12 COPorgen III CAMP CGMP D-Cys Cys Cys CTP	C00108 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C00216 C0018 C001112 C006186 C00002 C03406 C16188 C00072 C00152 C00146 C000152 C00041 C00041 C00041 C00041 C00041 C00160	+ + + + + + + + + + + + + + + + + + +	Cation Cation Neutral Neutral Anion Neutral Anion Neutral Anion Cation Nucleotide Anion Nucleotide Cation Cation Cation Nucleotide Cation Cation Nucleotide Neutral Cation Nucleotide Cation Cation Nucleotide Neutral Cation Nucleotide Cation Cation Nucleotide Cation Cation Nucleotide	Hydrophilic	11	1		275.1(2) 137.0 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 150.00 174.11 174.11 174.11 175.01 176.00 177.00 1	05	.1078

								I I I	
Menaquinone biosynthesis Ubiquinone biosynthesis	Demethylmenaquinone-8 3-Demethylubiquinone-8	dMMeQ-8	C05815 -	Neutral Anion	Hydrophobic		4	702.5376 712.5431	- Neutral and/or hydrophobic 711.5358 Neutral and/or hydrophobic
NudB (in vitro) Purine biosynthesis	VI Deoxyadenine-5'-phosphate I Deoxyadenine-5'-triphosphate	dAMP dATP	C00360 + C00131 +	Cation Nucleotide		10 16 5 1		331.0682 491.0008	332.0754 489.9936
Purine biosynthesis	Deoxyadenosine Deoxyadenosine-5'-diphosphate	dAdenosine dADP	C00559 + C00206 +	Cation Nucleotide	Hydrophilic Hydrophilic	10 15 5	9 2	251.1018 411.0345	252.1091 410.0272
Chorismic acid biosynthesis Pyrimidine biosynthesis	1 3-Deoxy-D-arabinoheptulosonate-7-phosphate 1 Deoxycitidine-5-diphosphate	3DAH7P dCDP	C04691 – C00705 +	Anion Nucleotide	Hydrophilic Hydrophilic	9 15 3 1	10 1	288.0246 387.0233	287.0174 386.0160
NudB (in vitro)	Deoxycytidine Deoxycytidine-5-phosphate	dCyt dCMP	C00881 + C00239 +	Cation Nucleotide	Hydrophilic Hydrophilic	9 14 3	7 1	227.0906 307.0569	228.0979 306.0497
Pyrimidine biosynthesis Salvage of Gua, Xan	1 Deoxycytidine-5'-triphosphate 1 Deoxyguanosine	dCTP dGuanosine	C00458 + C00330 +	Nucleotide Cation	Hydrophilic Hydrophilic	10 13 5	13 3	469.0053 267.0968	467.9980 268.1040
NudB (in vitro) Purine biosynthesis	VI Deoxyguanosine-5'-phosphate I Deoxyguanosine-5'-triphosphate	dGMP dGTP	C00362 + C00286 +	Nucleotide Nucleotide	Hydrophilic Hydrophilic	10 15 5 1		347.0631 505.9879	346.0558 504.9807
Purine biosynthesis Salvage of Ade, HypXan	Deoxyguanosone-5'-diphosphate Deoxyinosine	dGDP dInosine dIMP	C00361 + C05512 +	Nucleotide Cation	Hydrophilic Hydrophilic	10 12 4	10 2	427.0294 252.0859	426.0221 253.0931
ITP, XTP dephosphorelation ITP, XTP dephosphorelation KDO biosynthesis	V Deoxyinosine-5'-phosphate V Deoxyinosine-5'-phosphate 3-Deoxy-D-mannooctulosonate-8-phosphate	dITP DManOP	C06196 + C01345 + C04478 -	Nucleotide Nucleotide Anion	Hydrophilic Hydrophilic Hydrophilic	10 15 4 1	7 1 13 3	332.0522 491.9849 318.0352	331.0449 490.9776 317.0279
KDO biosynthesis	1 3-Deoxy-D-manno-octulosonic acid	DManOA dR1P	C01187 – C00672 +	Anion	Hydrophilic	8 14	8	238.0689 214.0242	237.0616 213.0170
Salvage of Gua, Xan Ribosephosphate degradation Pyrimidine biosynthesis	Deoxyribose-1-phosphate Deoxyribose-5-phosphate Deoxythymidine-5-phosphate	dR5P dTMP	C00673 + C00364 +	Anion Anion Nucleotide	Hydrophilic Hydrophilic Hydrophilic	5 11	7 1 7 1 8 1	214.0242 214.0242 322.0566	213.0170 213.0170 321.0493
Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis	Deoxythymidine-5-triphosphate Deoxythymidine-5-triphosphate	dTTP dTDP	C00364 + C00459 + C00363 +	Nucleotide Nucleotide	Hydrophilic Hydrophilic		14 3	481.9893 402.0229	480.9820 401.0157
Salvage of pyrimidine Pyrimidine biosynthesis	Deoxyuridine Deox	dUri dUDP	C00526 + C01346 +	Cation Nucleotide	Hydrophilic Hydrophilic		5	228.0746 388.0073	229.0819 387.0000
Pyrimidine biosynthesis Pyrimidine biosynthesis	Deoxyuridine-5-phosphate Deoxyuridine-5-triphosphate Deoxyuridine-5-triphosphate	dUMP dUTP	C00365 + C00460 +	Nucleotide Nucleotide	Hydrophilic Hydrophilic		8 1	308.0410 467.9736	307.0337 466.9663
1-Deoxy-D-xylulose assimilation Pyridoxal-5'-phosphate biosynthesis	1-Deoxy-D-xylulose 1-Deoxy	dXylulose 1DX5P	C06257 – C11437 –	Neutral Anion	Hydrophilic Hydrophilic	5 10	4 7 1	134.0579 214.0242	Neutral and/or hydrophobic 213.0170
CoA biosynthesis Biotin biosynthesis	Dephospho-CoA Detholotin	dePCoA	C00882 + C01909 +	Nucleotide Cation		21 35 7 1	13 2 1	687.1489 214.1317	686.1416 215.1390
Acetoin biosynthesis	Diacetyl	Diacetylchitobiose6P	C00741 +	Neutral Anion	Hydrophilic Hydrophilic		2	86.0368 520.1306	Neutral and/or hydrophobic 519.1233
Fravin biosynthesis Biotin biosynthesis	2,5-Diamino-6-(ribosylamino)-4-(3H)-pyrimidinone-5'-phosphate	2,5DA6RA4P5P 7,8DANA	C01304 — C01037 —	Anion	Hydrophilic	9 16 5	8 1	353.0737 188.1525	352.0664 189.1598
Lysine biosynthesis	L,L-Diaminopimelatic acid meso-Diaminopimelatic acid	DPA meso-DPA	C00666 + C00680 -	Anion	Hydrophilic Hydrophilic	7 14 2	4	190.0954 190.0954	189.0881 189.0881
Lysine biosynthesis YgeX Enterobactin biosynthesis	Misso-Galininophinetic acid 2,3-Dihaminopropionic acid V 2,3-Dihaminopropionic acid	IIIeso-DPA	C06393 + C04171 -	Anion Cation Anion	Hydrophilic Hydrophilic Hydrophilic	3 8 2	2 4	104.0586 156.0423	105.0659 155.0350
	v Z_2>-Uniyuro_2,3-uniyuroxyoetizoic acid i.cis-Diihydrodiol derivative of phenylacetyl-CoA 1 L_2,3-Dihydrodipicolinic acid	2,3-DPA	C03340 -	Nucleotide Anion		29 44 7 1	19 3 1	919.1626 169.0375	918.1553 168.0302
Tetrahydrofolic acid biosynthesis	7,8-Dihydrofolic acid	DHFA	C00415 +	Cation	Hydrophilic	19 21 7	6	443.1553	444.1626
	VI Dihydrolipoamide III Dihydrolipoic acid	DHLA	C00579 – C02147 +	Cation	Hydrophilic Hydrophilic	8 16	1 2 2	207.0752	208.0824 207.0519
Tetrahydrofolic acid biosynthesis Tetrahydrofolic acid biosynthesis	Dihydromonapterin-3'-triphosphate 7,8-Dihydromeopterin	DHMPTP DHN	C04874 +	Nucleotide Cation	Hydrophilic Hydrophilic		4	494.9958 255.0968	493.9885 256.1040
Tetrahydrofolic acid biosynthesis Tetrahydrofolic acid biosynthesis	Dihydroneopterinphosphate 7,8-Dihydroneopterin-3'-triphosphate	DHNPMP DHNPTP	C05925 – C04895 –	Nucleotide Nucleotide	Hydrophilic Hydrophilic	9 16 5 1		335.0631 494.9958	334.0558 493.9885
	U 6,7-Dihydropteridine		C00337 + C05649 -	Anion Cation	Hydrophilic Hydrophilic	6 6 4	4	158.0328 134.0592	157.0255 135.0665
Tetrahydrofolic acid biosynthesis YeiA, YeiT, YgfK (putative)	1 7,8-Dihydropteroic acid VI Dihydrouracil	DHPA	C00921 – C00429 +	Cation Neutral	Hydrophilic Hydrophilic		2	314.1127 114.0429	315.1200 Neutral and/or hydrophobic
Glycolysis (Embden-Meyerhof-Parnas)	III Dihydroxyacetone I Dihydroxyacetonephosphate	DHAP	C00184 + C00111 +	Neutral Anion	Hydrophilic Hydrophilic	3 7	3 6 1	90.0317 169.9980	- Neutral and/or hydrophobic 168.9908
	V 2,3-Dihydroxybenzoic acid V (2,3-Dihydroxybenzoyl)adenylic acid		C00196 + C04030 -	Anion Anion	Hydrophilic Hydrophilic	17 18 5 1	4 10 1	154.0266 483.0791	153.0193 482.0719
Enterobactin degradation	V 2,3-Dihydroxybenzoylserine I 3,4-Dihydroxy-2-butanone-4-phosphate	2,3DHBSer 3,4D2B4P	C04204 — C15556 —	Anion Anion		10 11 1	6 1	241.0586 184.0137	240.0514 183.0064
Valine biosynthesis Isoleucine biosynthesis	2,3-Dihydroxyisovaleric acid 2,3-Dihydroxy-3-methylvaleric acid	2,3-DIV 2,3DH3MVA	C04039 — C04104 —	Anion Anion	Hydrophilic Hydrophilic	5 10	4 4	134.0579 148.0736	133.0506 147.0663
Menaquinone biosynthesis HdhA (in vitro)	1 1,4-Dihydroxy-2-naphthoic acid VI 3-α,12-α-Dihydroxy-7-oxo-5-β-cholanic acid	1,4DHNaphA	C03657 + C04643 -	Anion Anion	Hydrophilic	11 8	4 5	204.0423	203.0350 405.2646
Phenylpropionic acid degradation Ketogluconic acid metabolism	3-(2,5-Dihydroxyphenyl)propionic acid		C04044 — C02780 —	Anion Anion	Hydrophilic Hydrophilic	9 10 6 8	4 7	182.0579 192.0270	181.0506 191.0197
YiaK Anaerobic respiration	VI 2,3-Diketo-L-gulonic acid VI Dimethyl sulfide		C04575 — C00580 +	Anion Neutral	Hydrophilic Hydrophilic	6 8 2 6	7	192.0270 62.0190	191.0197 - Neutral and/or hydrophobic
Isopentenyldiphosphate biosynthesis Cobalamin biosynthesis	I Dimethylallylpyrophosphate V Dimethylallylpyrophosphate	DMAProP	C00235 + C03114 +	Anion	Hydrophilic Hydrophilic		7 2	246.0058 146.0844	244.9986 147.0917
Fravin biosynthesis	6,7-Dimethyl-8-(1-D-ribityl)lumazine VI 2,4-Dinitrophenyl-5-glutathione	6,7D81RbL	C04332 - C11175 -	Anion	Hydrophilic Hydrophilic		6	326.1226 475.1009	325.1154 474.0936
Glycolysis (Embden-Meyerhof-Parnas)	I 1,3-Diphosphateglyceric acid	1,3-DPG	C01159 +	Anion	Hydrophilic	3 8 1	10 2	265.9593	264.9520
Isopentenyldiphosphate biosynthesis Isopentenyldiphosphate biosynthesis	4-Diphosphocytidyl-2- C-methylerythritol 4-Diphosphocytidyl-2- C-methylerythritol-2-phosphate	PPCytMeEry PPCytMeEryP	C11435 – C11436 –	Nucleotide Nucleotide	Hydrophilic Hydrophilic	14 26 3 1	14 2 17 3	521.0812 601.0475	520.0739 600.0402
Common antigen biosynthesis dTDP-rhamnose biosynthesis	I dTDP-4-acetamido-4,6-dideoxy-D-galactose I dTDP-4-dehydro-6-deoxy-D-glucose	dTDP-AADDGal dTDP-DDGlc	C11907 —	Nucleotide Nucleotide	Hydrophilic Hydrophilic	16 24 2 1		589.1074 546.0652	588.1001 545.0579
dTDP-rhamnose biosynthesis Common antigen biosynthesis	dTDP-4-dehydro-6-deoxy-L-mannose dTDP-D-fucosamine	dTDP-DDMan dTDP-FAN	C00688 –	Nucleotide Nucleotide		16 24 2 1 16 27 3 1	14 2	546.0652 547.0968	545.0579 546.0896
dTDP-rhamnose biosynthesis	I dTDP-D-glucose I dTDP-α-L-rhamnose	dTDP-Glc dTDP-Rhm	C00842 + C03319 -	Nucleotide Nucleotide	Hydrophilic Hydrophilic		15 2	564.0758 548.0808	563.0685 547.0736
-	5-Enolpyruvylshikimate-3-phosphate Enterobactin	5EPS3P	C01269 – C05821 –	Anion Cation		30 27 3 1	10 1	324.0246 669.1442	323.0174 670.1515
Histidine biosynthesis	(((2,3-Epoxy-4,5-cis-dihydroxycyclopent-1-yl)amino)methyl)-7-deazaguanosine D-Erythroimidazoleglycerolphosphate	EpodHCycPenylAM-deazaGua EIGP	C04666 -	Cation Nucleotide	Hydrophilic Hydrophilic	6 11 2	6 1	426.1625 238.0355	427.1698 Modified tRNA 237.0282
Pyridoxal-5'-phosphate biosynthesis Pentose phosphate pathway (non-oxidative)	I Erythronate-4-phosphate D-Erythrose-4-phosphate	Ery4P E4P	C03393 - C00279 +	Anion Anion	Hydrophilic Hydrophilic	4 9	8 1 7 1	214.9957 200.0086	213.9884 199.0013
	Ethanol Ethanolamine		C00469 – C00189 +	Neutral Cation	Hydrophilic Hydrophilic	- ' '	1	46.0419 61.0528	- Neutral and/or hydrophobic 62.0600
Repair of alkylated DNA/RNA DkgA (in vitro)	III 1-Ethyladenine VI Ethyl-2-methylacetoacetic acid			Cation Anion	Hydrophilic Hydrophilic	7 9 5 7 12	3	163.0858 144.0786	164.0931 143.0714
DkgA (in vitro) Isoprenoid biosynthesis	VI Ethyl-(2R)-methyl-(3S)-hydroxybutanoic acid I trans, trans-Farnesyl diphosphate	FPP	 C00448 +	Anion Nucleotide	Hydrophilic Hydrophobic	15 28	7 2	146.0943 382.1310	145.0870 381.1238 Neutral and/or hydrophobic
Fravin biosynthesis	Flavinadeninedinucleotide (oxidized form) Flavinadeninedinucleotide (reduced form)	FAD FADH₂	C00016 + C01352 -	Nucleotide Nucleotide	Hydrophilic	27 35 9 1	15 2 15 2	785.1571 787.1728	391.5713 Detected as divalent ion in MS 786.1655
Fravin biosynthesis	Flavinmononucleotide (oxidized form) Flavinmononucleotide (reduced form)	FMN FMNH₂	C00061 + C01847 -	Nucleotide Nucleotide	Hydrophilic Hydrophilic	17 23 4	9 1	456.1046 458.1203	455.0973 457.1130
Alkylated DNA repair YgiU (putative)	III Formaldehyde VI Formamide		C00067 + C00488 +	Neutral Neutral	Hydrophilic Hydrophilic		1	30.0106 45.0215	 Neutral and/or hydrophobic Neutral and/or hydrophobic
Acid fermentation Oxalic acid degradation	I Formic acid III Formyl-CoA		C00058 + C00798 -	Anion Nucleotide	Hydrophilic Hydrophilic		2 17 3 1	46.0055 795.1101	44.9982 Out of the MS range 794.1029
FrmA (in vitro) Tetrahydrofolic acid biosynthesis	VI S-Formylglutathione I N ¹⁰ -Formyl-THF	N10F-THF	C01031 – C00234 –	Anion Cation		11 17 3 20 23 7	7 1 7	335.0787 473.1659	334.0714 474.1732
Fructose transport Glycolysis (Embden-Meyerhof-Parnas)	III D-Fructose I D-Fructose-1,6-diphosphate	F1,6P	C01496 – C00354 +	Neutral Anion	Hydrophilic Hydrophilic		6 12 2	180.0634 339.9961	- Neutral and/or hydrophobic
Fructoselysine degradation Fructoselysine degradation	III Fructoselysine III Fructoselysine-6-phosphate	Fructoselysine6P		Cation Anion			7 10 1	307.1505 387.1169	308.1578 386.1096
Fructose transport Glycolysis (Embden-Meyerhof-Parnas)	III D-Fructose-1-phosphate I D-Fructose-6-phosphate	Fructose1P F6P	C01094 + C00085 +	Anion Anion	Hydrophilic Hydrophilic		9 1 9 1	260.0297 260.0297	259.0224 259.0224
	III Fructuronic acid III L-Fucose		C00905 — C01019 —	Anion Neutral	Hydrophilic Hydrophilic	- 12	5	194.0427 164.0685	193.0354 Neutral and/or hydrophobic
Fucose degradation	III L-Fuculose III D-Fuculose-1-phosphate	Fuculose1P	C01721 – C01099 –	Neutral Anion	Hydrophilic Hydrophilic	6 12	5 8 1	164.0685 244.0348	- Neutral and/or hydrophobic 243.0275
TCA cycle	Funaric acid D-Galactaric acid		C00122 + C01807 +	Anion Anion	Hydrophilic Hydrophilic		4 8	116.0110 210.0376	115.0037 209.0303
Galactitol degradation Galactitol degradation	D-Galactitol D-Ga	Galactitol1P	C01697 + C06311 -	Neutral Anion	Hydrophilic Hydrophilic	6 14	6 9 1	182.0790	Neutral and/or hydrophobic 261.0381
Galactonic acid degradation		and the second s	C00311	Ailloil	and the second of the second		7	262.0454	
Dgd (putative)	D-Galactonic acid VI D-Galactono-1,4-lactone		C00880 + C03383 +	Anion Neutral	Hydrophilic Hydrophilic		6	196.0583 178.0477	195.0510 - Neutral and/or hydrophobic
Colanic acid biosynthesis		D-Galactose	C00880 +	Anion		6 10 6 12		196.0583	
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis	VI D-Galactono-1,4-lactone I α-D-Galactose	D-Galactose Gal1P	C00880 + C03383 + C00984 -	Anion Neutral Neutral	Hydrophilic Hydrophilic	6 10 6 12 6 12 6 13	6	196.0583 178.0477 180.0634	 Neutral and/or hydrophobic Neutral and/or hydrophobic
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis	D-Galactono-1,4-lactone α-D-Galactose	Gal1P GDP-DDMan	C00880 + C03383 + C00984 - C00124 + C00446 + C00333 + C01222 -	Anion Neutral Neutral Neutral Anion Anion Nucleotide	Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic Hydrophilic	6 10 6 12 6 12 6 13 6 10 16 23 5 1	6 6 6 9 1 7 1 15 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666	Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 193.0354 586.0593
Colanic acid biosynthesis Lactose degradation (holanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis	D-Galactono-1,4-lactone	Gal1P	C00880 + C03383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Nucleotide Nucleotide	Hydrophilic	6 10 6 12 6 13 6 10 16 23 5 1 16 25 5 1	6 6 6 9 1 7 7 7 1 1 1 1 5 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.093 586.093 604.0699
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis	D-Galactono-1,4-lactone α-D-Galactose β-D-Galactose α-D-Galactose α-D-Galactose α-D-Galactose α-D-Galactose-1-phosphate Galacturonic acid GDP-4-dehydro-6-deoxy-D-mannose GDP-I-fucose GDP-I-monose GDP-mannose Geranyldiphosphate D-Glucaric acid	Gal1P GDP-DDMan GDP-fucose GDP-Man	C00880 + C03383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 +	Anion Neutral Neutral Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Anion	Hydrophilic	6 10 6 12 6 13 6 10 16 23 5 1 16 25 5 1 10 20 6 10	6 6 6 9 1 7 1 15 2 15 2 15 2	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation	D-Galactono-1,4-lactone	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton	C00880 + C03383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 + C00257 + C00198 +	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Neutral	Hydrophilic	6 10 6 12 6 13 6 10 16 23 5 1 16 25 5 1 10 20 6 10 6 10 6 10 6 10 6 10 6 10 6	6 6 6 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0334 586.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport	D-Galactono-1,4-lactone α-D-Galactose β-D-Galactose α-D-Galactose α-D-Fannose α-D-Fannose α-D-Fannose α-D-Fannose α-D-Fannose α-D-Fannose α-D-Galactose α-D-Galacto	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P	C00880 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 + C00257 + C00198 + C001236 - C001236 - C00329 +	Anion Neutral Neutral Neutral Neutral Anion Anion Anion Nucleotide Anion Anion Anion Cation	Hydrophilic	6 10 6 12 6 12 6 10 16 23 5 1 16 25 5 1 10 20 6 10 6 11 2 6 10 6 11 6 6 11 6 6 11 6 6 11 1 6 13 1 1	6 6 6 9 1 9 1 9 1 1 15 2 15 2 16 2 7 2 9 1 1 7 7 6 6 9 9 1 1 9 1 5 5 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 193.0354 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Sisperencial biosynthesis Isoprencial degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis	VI D-Galactono-1,4-lactone 1 α-D-Galactose 11 β-D-Galactose 12 α-D-Galactose 13 β-D-Galactose 14 α-D-Galactose 15 α-D-Galactose-1-phosphate 16 α-D-4-dehydro-6-deoxy-D-mannose 17 α-D-1-drose 18 α-D-1-drose 19 α-D-1-drose 19 α-D-1-drose 19 α-D-1-drose 10 α-D-1-drose 10 α-D-1-drose 11 α-D-1-drose 12 α-D-1-drose 13 α-D-1-drose 14 α-D-1-drose 15 α-D-1-drose 16 α-D-1-drose 17 α-D-1-drose 18 α-D-1-drose 19 α-D-1-drose 10 α-	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P	C00880 + C03383 + C03383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C0096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00329 + C00329 + C00329 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Anion	Hydrophilic	6 10 6 12 6 13 6 10 10 20 6 10 20 6 10 6 12 6 10 6 11 6 25 5 11 6 25 6 10 6 10 6 11 6 11 6 11 1 6 11 1 1 6 11 1 1 1	6 6 6 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycoglys (Embden-Meyerhof-Parnas) Glycogen biosynthesis	VI D-Galactono-1,4-lactone 1 α-D-Galactose 11 β-D-Galactose 11 Ga-D-Galactose 11 Ga-D-Galactose 12 Ga-D-Galactose 13 GDP-4-deplydro-6-deoxy-D-mannose 14 GDP-4-flydro-6-deoxy-D-mannose 15 GDP-1-flydro-6-deoxy-D-mannose 16 GDP-1-flydro-6-deoxy-D-mannose 17 GDP-1-flydro-6-deoxy-D-mannose 18 GDP-1-flydro-6-deoxy-D-mannose 19 Gerany(diphosphate 10 Gluconic acid 11 Gluconic acid 12 Gluconic α-lactone 13 Gluconic α-lactone 14 D-Glucosamine 15 D-Glucosamine-1-phosphate 16 D-Glucosamine-6-phosphate 17 D-Glucosamine-6-phosphate 18 α-D-Glucosamine-6-phosphate 19 α-D-Glucosamine-6-phosphate 10 α-D-Glucosamine-6-phosphate	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00986 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C01236 - C00329 + C00325 + C00329 + C00325 + C00326 + C0031 + C00031 +	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Anion	Hydrophilic	6 10 6 12 6 12 6 13 6 10 10 10 20 10 10 10 10 10 10 10 10 10 10 10 10 10	6 6 6 9 9 1 7 7 2 8 8 7 7 7 6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0727 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 259.0457 259.0457	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 6604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 258.0384 - Neutral and/or hydrophobic 259.0224
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Soprenoid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation Glucose degradation UDP-Nacetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas)	D-Galactono-1,4-lactone α-D-Galactose	Gal1P GDP-DDMan GDP-fucose GDPMan GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P	C00880 + C0383 + C0383 + C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C0096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00329 + C00329 + C00352 + C00031 + C00031 + C00103 + C00103 + C00103 + C00103 + C00104 + C00104 + C00109 + C00101 +	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Neutral Anion Neutral Anion Anion Anion Anion Neutral Anion Anion Neutral Anion Anion Anion Anion Anion	Hydrophilic	6 10 12 6 12 6 13 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	6 6 6 9 1 9 1 1 9 1 9 1 9 1 9 1 9 1 9 1	196,0583 178,0477 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 210,0376 2178,0477 258,0141 179,0794 259,0457 180,0634 260,0297 194,0427	- Neutral and/or hydrophobic - Neutral and/or hydrophobic Neutral and/or hydrophobic 259,0224 193,0354 586,0750 604,0699 313,0612 Neutral and/or hydrophobic 209,0303 195,0510 - Neutral and/or hydrophobic 257,0068 180,0867 258,0384 - Neutral and/or hydrophobic 259,0224 193,0354
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Protine biosynthesis Proto- and siroheme biosynthesis	D-Galactono-1,4-lactone α-D-Galactose β-D-Galactose β-D-Galactose α-D-Galactose α-D-Galactose α-D-Galactose-1-phosphate Galacturonic acid GDP-4-dehydro-6-deoxy-D-mannose GDP-1-fucose GDP-3-dehydro-6-deoxy-D-mannose GDP-3-deoxy-D-mannose GDP-3-deoxy-D-mannose GDP-3-deoxy-D-mannose GDP-3-deoxy-D-mannose GDP-3-deoxy-D-mannose GP-3-deoxy-D-mannose GP-3-deoxy-D-mannose Geranyldiphosphate Gluconic acid Glucono-Δ-lactone D-Glucoso-Δ-lactone D-Glucosamine D-Glucosamine D-Glucosamine D-Glucosamine D-Glucose-1-phosphate α-D-Glucose-1-phosphate α-D-Glucose-1-phos	Gal1P GPP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu-5-P Glu5A	C00880 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00988 + C03517 - C00818 + C00257 + C00198 + C00329 + C00352 + C00352 + C00035 + C00090 + C00010	Anion Neutral Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Neutral Anion Anion Neutral Anion Cation	Hydrophilic	6 10	6 6 6 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196,0583 178,0477 180,0634 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 259,0457 259,0457 260,0297 194,0427 260,0297 194,0427 27,0195 131,0582	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 259.0224 259.0224 193.0354 226.0122 132.0655
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid biosynthesis Galacturonic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycogn biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Protine biosynthesis	D-Galactono-1,4-lactone I a-D-Galactose II a-D-Galactose II β-D-Galactose II β-D-Galactose II β-D-Galactose II β-D-Galactose II Galactose	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu-5-P Glu-semialdehyde D-Glu	C00880 + C0383 + C0383 + C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C00986 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C01236 - C00329 + C00327 + C00327 + C00327 - C00191 + C03287 - C033287 - C033741 - C01165 - C00151	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Anion Anion Neutral Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Cation Cation Cation	Hydrophilic	6 10 10 12 12 13 16 16 12 15 16 11 15 16 11 15 16 11 15 15 16 11 15 15 19 11 15 15 19 11 15 15 19 11 15 15 19 11 15 15 19 11 15 19 11 15 19 11 15 19 1	6 6 6 9 9 1 7 7 2 8 8 7 7 7 6 6 9 9 1 9 1 9 9 1	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 259.0457 260.0297 260.0297 260.0297 194.0427 227.0195 131.0582 131.0582 147.0532	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 6604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 258.0384 - Neutral and/or hydrophobic 259.0224 259.0224 259.0224 193.0354 226.0122 132.0655 148.0665
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Glucanic acid degradation Ketogluconic acid metabolism Glucose degradation Ketogluconic acid metabolism Glucose degradation Fentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Florional biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Potto- and siroheme biosynthesis Glytanic acid biosynthesis Glutamic acid biosynthesis	D-Galactono-1,4-lactone	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P G1C-5P G1C-	C00880 + C0383 + C0383 + C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C0096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00352 + C00031 + C00031 + C00092 + C00352 + C00014 + C00027 + C00191 + C00027 + C00191 + C0	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Neutral Anion Anion Neutral Anion Anion Anion Anion Anion Cation Anion Anion Cation	Hydrophilic	6 10 10 12 10 10 10 10 10 10 10 10 10 10 10 10 10	6 6 6 9 1 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196,0583 178,0477 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 10,0376 210,0376 210,0376 258,0141 179,0794 259,0457 258,0141 179,0794 259,0457 180,0634 260,0297 194,0427 227,0195 131,0582 131,0582 131,0582 147,0532 147,0532 147,0532	- Neutral and/or hydrophobic - Neutral and/or hydrophobic Neutral and/or hydrophobic 259,0224 193,0354 586,0750 604,0699 313,0612 Neutral and/or hydrophobic 209,0303 195,0510 - Neutral and/or hydrophobic 257,0068 180,0867 258,0384 - Neutral and/or hydrophobic 259,0224 259,0224 193,0354 226,0122 132,0655 148,0604 147,0764
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid biosynthesis Galacturonic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Soprenoid biosynthesis Glucaric acid degradation Retogluconic acid degradation Glucaric acid degradation Retogluconic acid metabolism Glucosed degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Glucamic acid biosynthesis Glucamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutathione biosynthesis Glutathione biosynthesis	VI D-Galactono-1,4-lactone 1 a-D-Galactose 11 β-D-Galactose 12 β-D-Galactose 13 Galactoronic acid 14 GDP-4-dehydro-6-deoxy-D-mannose 15 GDP-1-fucose 16 GDP-1-fucose 17 GDP-1-fucose 18 GDP-annose 19 G-Gucaric acid 10 Gluconic acid 11 Glucono-A-lactone-6-phosphate 11 Glucono-A-lactone-6-phosphate 12 G-Glucosamine-1-phosphate 13 G-Glucosamine-1-phosphate 14 a-D-Glucose-1-phosphate 15 a-D-Glucose-1-phosphate 16 a-D-Glucose-1-phosphate 17 a-D-Glucose-1-phosphate 18 Glucamine-1-phosphate 19 G-Glucose-1-phosphate 10 a-D-Glucose-1-phosphate 11 a-D-Glucose-1-phosphate 12 a-D-Glucose-1-phosphate 13 a-D-Glucose-1-phosphate 14 a-D-Glucose-1-phosphate 15 Glutamate-5-phosphate 16 Glutamate-5-phosphate 17 Glutamate-5-phosphate 18 Glutamate-1-semialdehyde 19 Glutamic acid 10 L-Glutamic acid 10 L-Glutamic acid 11 L-Glutamic acid 11 L-Glutamic acid 12 L-Glutamic acid 13 L-Glutamic acid 14 L-Glutamic acid 15 L-Glutamic-1-gl	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlicnL6P Glic-1P Glic-6P D-Glucose G1P G6P Glu-5-P Glu-5-P Glu-5-P Glu-5-B Glu-5-P Glu-5-B Glu-5-P Glu	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00068 + C03517 - C00818 + C01236 - C00329 + C00352 + C00035 + C00031 + C00191 + C00191 + C03267 - C032741 - C032741 - C032741 - C01165 - C00217 + C00025 + - C00025 + - C00025 + - C00026 + - C00025 + C00069 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Anion Cation	Hydrophilic	6 10	6 6 6 9 9 1 7 7 1 1 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	196,0583 178,0477 180,0634 180,0634 180,0634 190,0637 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 259,0457 259,0457 180,0634 260,0297 194,0427 227,0195 131,0582 131,0582 147,0532 147,0532 146,0691 146,0691	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 259.0224 193.0354 259.0224 193.0354 226.0122 132.0655 132.0655 132.0655 148.0604 148.0604 147.0764 147.0764 147.0764
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Isoprenoid biosynthesis IDP-N-acetylglucosamine biosynthesis IDP-N-acetylglucosamine biosynthesis IDP-N-acetylglucosamine biosynthesis ISOprolysis (Embden-Meyerhof-Parnas) Isoprenoid Biosynthesis Isoproline biosynthesis Isop	VI	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semaldehyde D-Glu Glu Glu Glu Glu Glu Glu Glu Glu Glu	C00880 + C03883 + C03883 + C03884 - C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C00986 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C01236 - C00329 + C00327 + C00191 + C00127 + C00191 + C00287 - C003287 - C03741 - C00051 + C00064 + C00069 + C00064 + C000669 + C00064 + C00061 + C000127 + C000127 + C00064 + C00064 + C00064 + C00064 + C00061 + C000127 + C000127 + C000127 + C00064 + C00064 + C000669 + C000127 + C000	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Cation	Hydrophilic	6 10 10 12 16 17 18 18 18 18 18 18 18 18 18 18 18 18 18	6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196.0583 178.0477 180.0634 260.0297 194.0427 587.0666 589.0822 690.0727 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 259.0457 260.0297 260.0297 260.0297 131.0582 147.0532 147.0532 147.0532 146.0691 250.0623 307.0838	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 6604.0699 313.0612 - Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 258.0384 - Neutral and/or hydrophobic 259.0224 259.0224 259.0224 129.0255 148.0605 148.0604 148.0604 147.0764 147.0764 147.0764 147.0764 251.0696 307.0833 Detected as divalent ion in MS
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylgucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycomic degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Peptideglycan biosynthesis Peptideglycan biosynthesis Glycaline acid biosynthesis Glycaline acid biosynthesis Glycaline acid biosynthesis Glycaline acid biosynthesis Glycaline glycaline metabolism Glycolysis (Embden-Meyerhof-Parnas)	VI D-Galactono-1,4-lactone 1	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton Glcnl6P Glc-1P Glc-6P D-Glucose G1P G6P G1U-5-P G1U-5-P G1U-5-Q	C00880 + C0383 + C0383 + C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C0096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00352 + C00031 + C00191 + C0	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Neutral Anion Anion Anion Neutral Anion Anion Cation Anion Anion Cation	Hydrophilic	6 10 6 112 6 13 6 10 16 12 6 13 6 10 16 12 6 10 6 11	6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9	196.0583 178.0477 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 180.0634 260.0297 260.0297 194.0427 227.0195 131.0582 131.0582 147.0532 147.0532 146.0691 146.0691 146.0691 146.0691	- Neutral and/or hydrophobic - Neutral and/or hydrophobic Neutral and/or hydrophobic 259,0224 193,0354 586,0750 604,0699 313,0612 Neutral and/or hydrophobic 209,0303 195,0510 - Neutral and/or hydrophobic 257,0068 180,0867 258,0384 - Neutral and/or hydrophobic 259,0224 191,0354 259,0224 193,0354 226,0122 132,0655 148,0604 147,0764 147,0764 1251,0696 307,0833 Detected as divalent ion in MS
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid biosynthesis IDP-N-acetylglucosamine biosynthesis IDP-N-acetylglucosamine biosynthesis IDP-N-acetylglucosamine biosynthesis Isoprenoid bio	VI D-Galactono-1,4-lactone 1 a-D-Galactose 1 ii B-D-Galactose 1 iii B-D-Galactose 1 iii B-D-Galactose 1 iii Galactoronic acid 1 iii GDP-4-delydro-6-deoxy-D-mannose 1 iii GDP-4-delydro-6-deoxy-D-mannose 1 iii GDP-3-delydro-6-deoxy-D-mannose 2 iii GDP-3-delydro-6-deoxy-D-mannose 3 iii GB-3-delydro-6-deoxy-D-mannose 4 iii Gluconic acid 5 iii Gluconic acid 6 iii Gluconic A-lactone 7 iii Gluconic A-lactone 8 iii Gluconic A-lactone 9 iii Gluconic A-lactone 1 iii Gluconic A-lactone 1 iii Glucosamine 1 p-Glucosamine-1-phosphate 1 iii Glucosamine-6-phosphate 1 iii Glucosamine-6-phosphate 1 iii Glucose-6-phosphate 1 iii Glucose-6-phosphate 1 iii Glucose-6-phosphate 1 iii Glucoronic acid 1 iii Glucoronic acid 1 iii Glucoronic acid 1 iii Glutamate-7-phosphate 3 iii Glutamate-1-semialdehyde 1 iii Glutamate-1-semialdehyde 1 iii Glutamate-1-semialdehyde 1 iii Glutamine 1 iii Glutathione (oxidized form) 1 iii Glutathione (reduced form) 1 iii Glutathione (reduced form) 1 iii Glutathione (reduced form) 1 iiii Glutathione (reduced form)	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlicnL6P Glic-1P Glic-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semialdehyde D-Glu Glu Glu Gli Glu GSSG GSSG GSSH	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00066 + C03517 - C00818 + C00257 + C00198 + C00329 + C00352 + C000352 + C000352 + C00092 + C00191 + C00191 + C03267 - C032741 - C032741 - C01165 - C00177 + C00025 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Anion Cation	Hydrophilic	6 10 10 12 16 17 18 18 18 18 18 18 18 18 18 18 18 18 18	6 6 6 9 9 1 1 9 15 2 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9	196,0583 178,0477 180,0634 180,0634 180,0634 190,0637 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 259,0457 250,0297 194,0427 227,0195 131,0582 147,0532 147,0532 146,0691 146,0691 146,0691 250,0623 141,0582 147,0532 146,0691 146,0691 146,0691 146,0691 146,0691 150,0623 1612,1520 170,0838 17	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 258.0384 - Neutral and/or hydrophobic 259.0224 193.0354 2259.0224 193.0354 226.0122 132.0655 132.0655 132.0655 148.0604 148.0604 147.0764 251.0696 307.0833 Detected as divalent ion in MS 308.0911 435.2384
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Soprenoid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Peptideglycan biosynthesis Peptideglycan biosynthesis Glutathione diosynthesis Glutathione diosynthesis Glutathione diosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolic acid degradation Glycerol degradation Glycerol degradation Glycerol degradation	D-Galactono-1,4-lactone In -D-Galactose In -Galactose In -Gal	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlicnL6P Glic-1P Glic-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semialdehyde D-Glu Glu Glu Gli Glu GSSG GSSG GSSH	C00880 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00066 + C03517 - C00818 + C00257 + C00198 + C00329 + C00329 + C00329 + C00329 + C00329 + C00320 + C00320 +	Anion Neutral Neutral Neutral Neutral Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Cation	Hydrophilic	6 10	6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196,0583 178,0477 180,0634 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 180,0634 260,0297 260,0297 194,0427 227,0199 131,0582 147,0532 147,0532 147,0532 146,0691	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 6604.0699 313.0612 - Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - See Neutral and/or hydrophobic 259.0224 259.0224 259.0224 259.0224 132.0655 148.0604 148.0604 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 148.0693 105.0193
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic biosynthesis Glutathione biosynthesis Glutathionelyspermidine metabolism Glycolis acid degradation Glycord degradation Glycord degradation Glycord degradation Glycore degradation Glycore degradation Glycore degradation Glycore degradation Glycore degradation Glycore biosynthesis	VI D-Galactono-1,4-lactone 1 a-D-Galactose 11 ig-D-Galactose 12 ig-D-Galactose 13 ig-D-Galactose 14 ig-D-Galactose 15 ig-D-Galactose-1-phosphate 16 ig-D-4-delydro-6-deoxy-D-mannose 17 ig-D-Galactose-1-phosphate 18 ig-D-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 11 ig-Galactose-1-phosphate 12 ig-Galactose-1-phosphate 13 ig-Galactose-1-phosphate 14 ig-Galactose-1-phosphate 15 ig-Galactose-1-phosphate 16 ig-Galactose-1-phosphate 17 ig-Galactose-1-phosphate 18 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 11 ig-Galactose-1-phosphate 12 ig-Galactose-1-phosphate 13 ig-Galactose-1-phosphate 14 ig-Galactose-1-phosphate 15 ig-Galactose-1-phosphate 16 ig-Galactose-1-phosphate 17 ig-Galactose-1-phosphate 18 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 11 ig-Galactose-1-phosphate 12 ig-Galactose-1-phosphate 13 ig-Galactose-1-phosphate 14 ig-Galactose-1-phosphate 15 ig-Galactose-1-phosphate 16 ig-Galactose-1-phosphate 17 ig-Galactose-1-phosphate 18 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 11 ig-Galactose-1-phosphate 12 ig-Galactose-1-phosphate 13 ig-Galactose-1-phosphate 14 ig-Galactose-1-phosphate 15 ig-Galactose-1-phosphate 16 ig-Galactose-1-phosphate 17 ig-Galactose-1-phosphate 18 ig-Galactose-1-phosphate 19 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 10 ig-Galactose-1-phosphate 11 ig-Galactos-1-phosphate 11 ig-Galactos-1-phosphate 12 ig-Galactos-1-phosphate 13 ig-Galactos-1-phosphate 14 ig-Galactos-1-phosphate 15 ig-Galactos-1-phosphate 16 ig-Galactos-1-phosphate 17 ig-Galactos-1-phosphate 18 ig-Galactos-1-phosphate 19 ig-Galactos-1-phosphate 10 ig-Galactos-1-phosphate 10 ig-Galactos-1-phosph	Gal1P GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu-5-P Glu-5-B Glu-5	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 + C00257 + C01236 - C00329 + C00352 + C00096 + C00191 +	Anion Neutral Neutral Neutral Anion Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Anion Neutral Anion Anion Anion Anion Cation	Hydrophilic	6 10	6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9	196.0583 178.0477 180.0634 180.0634 180.0634 190.0637 194.0427 587.0666 589.0822 605.0772 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 260.0297 194.0427 227.0195 131.0582 147.0532 147.0532 146.0691 146.0691 146.0691 146.0691 149.9890 169.9890 169.9890 169.9890 169.9890 169.9890 169.0297 179.0437 179	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259,0224 193,0354 586,0750 604,0699 313,0612 Neutral and/or hydrophobic 209,0303 195,0510 - Neutral and/or hydrophobic 257,0068 180,0867 258,0384 - Neutral and/or hydrophobic 259,0224 193,0354 - Neutral and/or hydrophobic 259,0224 193,0354 226,0122 132,0655 132,0655 148,0604 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 147,0764 148,0908 105,013 08,0911 148,5908 105,019 - Neutral and/or hydrophobic 171,0064 171,0064 171,0064 171,0064
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Soprenoid biosynthesis Isoprenoid biosynthesis IUDP-N-acetylglucosamine biosynthesis IUDP-N-acetylglucosamine biosynthesis IUDP-N-acetylglucosamine biosynthesis Isoprenoid bios	VI D-Galactono-1,4-lactone 1 a-D-Galactose 11 β-D-Galactose 11 β-D-Galactose 11 Galactose-1-phosphate 11 Galactoronic acid 1 GDP-4-delydro-6-deoxy-D-mannose 1 GDP-1-fucose 1 GDP-1-fucose 1 GDP-3-delydro-6-deoxy-D-mannose 1 GDP-1-fucose 1 GDP-3-delydro-6-deoxy-D-mannose 1 GDP-1-fucose 1 GE-anyldiphosphate 1 Geranyldiphosphate 1 Geranyldiphosphate 1 Gluconic acid 1 Gluconic acid 1 Glucosamine-1-phosphate 1 Glucosamine-1-phosphate 1 D-Glucosamine-1-phosphate 1 D-Glucosamine-6-phosphate 1 a-D-Glucose-1-phosphate 1 a-D-Glucose-1-phosphate 1 a-D-Glucose-1-phosphate 1 Gluconic acid 1 Glucoronic acid 1 Glutarmate-1-semialdehyde 1 L-Glutarmate-3-phosphate 1 D-Glutarmic acid 1 Glutarmic acid 1	Gal1P GP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semlaldehyde D-Glu Glu Gln Gln GluCys GSSG GSH GSH-spermidine G3P GIP GJP GJP GJP GJP GJP GJP GJP GJP GJP GJ	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00066 + C03517 - C00818 + C01236 - C00329 + C00352 + C00352 + C00352 + C00352 + C00198 + C011236 - C00352 + C00352 + C00352 + C00352 + C00352 +	Anion Neutral Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Anion Cation Neutral	Hydrophilic	6 10 12 6 12 6 13 6 10 7 7 7 7 7 7 7 7 7	6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196,0583 178,0477 180,0634 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 259,0457 259,0457 259,0457 180,0634 260,0297 194,0427 227,0195 131,0582 131,0582 147,0532 146,0691 146,0691 146,0691 146,0691 150,9380 160,0266 172,038 172,037 172,0137 172,0137 175,0320 166,0266 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320 175,0320	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 258.0384 - Neutral and/or hydrophobic 259.0224 193.0354 2259.0224 193.0354 122.0655 132.0655 143.0655 144.0604 147.0764 147.0764 147.0764 147.0764 147.0764 151.0696 307.0833 Detected as divalent ion in MS 308.0911 435.2384 168.9908 105.0193 - Neutral and/or hydrophobic 171.0064 258.1107 Including quarternary amine 76.0393 - Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Soprenoid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Protine biosynthesis Protine biosynthesis Potline biosynthesis Glutamine acid biosynthesis Glutamine acid biosynthesis Glutamine biosynthesis Glutathione biosynthesis Glucalid degradation PldC (in vitro) Glycic acid degradation Flat (in vitro) Glycic acid degradation	VI D-Galactono-1,4-lactone 1 a-D-Galactose 11 B-D-Galactose 11 Ga-D-Galactose 11 Ga-D-Galactose 11 Gap-4-delydro-6-dexy-D-mannose 1 GDP-1-fucose 1 GDP-3-delydro-6-dexy-D-mannose 1 GDP-1-fucose 1 Geranyldiphosphate 1 Geranyldiphosphate 1 Gluconic acid 1 Gluconic acid 1 Gluconic A-lactone 1 D-Glucosamine 1 D-Glucosamine-1-phosphate 1 D-Glucosamine-1-phosphate 1 D-Glucosamine-6-phosphate 1 D-Glucosamine-6-phosphate 1 D-Glucose-6-phosphate 1 G-Glucose-1-phosphate 1 G-Ucose-6-phosphate 1 Glucamate-1-pensphate 1 Glucamate-1-semialdehyde 1 L-Glutamate-1-semialdehyde 1 L-Glutamate-y-semialdehyde 1 L-Glutamine 1 L-Glutamine 1 L-Glutamine 1 L-Glutamine 1 L-Glutamine 1 L-Glutamine 1 Glutathione (reduced form) 1 Glutathione (roddiced form) 1 Glyceric acid 1 Glycero-3-phosphocholine 1 Glycogen 1 Glycoladehyde 1 D-Glycogen 1 Glycoladehyde 1 Glycoladehyde 1 Glycoladehyde	Gal1P GP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semlaldehyde D-Glu Glu Gln Gln GluCys GSSG GSH GSH-spermidine G3P GIP GJP GJP GJP GJP GJP GJP GJP GJP GJP GJ	C00880 + C0383 + C0383 + C0383 + C00984 - C00124 + C00466 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00329 + C00329 + C00329 + C00329 + C00110 + C00025 + C00031 + C00032 + C00031 + C00032 + C00031 + C00032 + C00033 + C00034 + C00066 + C00025 + C00066 + C00025 + C00066 + C000258 + C00116 + C00039 + C00066 + C00039 + C00031 + C00030 + C00061 + C00030 + C00031 + C00040 + C0004	Anion Neutral Neutral Neutral Neutral Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Neutral Anion Anion Anion Anion Anion Cation Anion Anion Neutral Neutral Neutral Neutral	Hydrophilic	6 10	6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196.0583 178.0477 180.0634 260.0297 194.0427 587.0666 589.0822 695.0727 314.0684 210.0376 196.0583 178.0477 258.0141 179.0794 259.0457 180.0634 260.0297 260.0297 260.0297 140.0376 147.0532 147.0532 147.0532 147.0532 146.0691 146.06	- Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic - Neutral and/or hydrophobic 259.0224 193.0354 586.0750 664.0669 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 - Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 259.0224 193.0354 - Neutral and/or hydrophobic 193.0354 226.0122 132.0655 148.0604 148.0604 148.0604 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 147.0764 148.06091 148.060
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation Glucose degradation Glucose degradation Fentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycoghs (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Protone and siroheme biosynthesis Protone and siroheme biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutathione biosynthesis Glycolic acid degradation Glycerol degradation Glycerol degradation Tetrahydrofolic acid biosynthesis Glycolic acid degradation Tetrahydrofolic acid biosynthesis Glycolic acid degradation Glycolic acid degradation Tetrahydrofolic acid biosynthesis Glycolic acid degradation	VI D-Galactono-1,4-lactone 1	Gal1P GP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semlaldehyde D-Glu Glu Gln Gln GluCys GSSG GSH GSH-spermidine G3P GIP GJP GJP GJP GJP GJP GJP GJP GJP GJP GJ	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00096 + C03517 - C00818 + C00257 + C00198 + C01236 - C00329 + C00352 + C00032 + C00352 + C00031 + C00131 + C00131 + C00105 - C00352 + C00352 + C00352 + C00352 + C00352 + C00191 + C0027 + C00191 + C0027 + C00191 + C0027 + C00191 + C0028 + C00191 + C00069 + C00191 + C000691 + C00	Anion Neutral Neutral Neutral Anion Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Anion Neutral Anion Cation Anion Cation Anion Anion Anion Neutral Anion Cation	Hydrophilic	6 10	6 6 6 9 1 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1	196.0583 178.0477 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 178.0477 258.0141 179.0794 259.0457 180.0634 260.0297 194.0427 227.0195 131.0582 147.0532 146.0691 146.0691 146.0691 146.0691 146.0691 147.0532	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 159,0224 193,0354 586,0750 604,0699 331,0612 Neutral and/or hydrophobic 209,0303 195,0510 - Neutral and/or hydrophobic 257,0068 180,0867 258,0384 258,0384 - Neutral and/or hydrophobic 259,0224 199,0224 191,0355 148,0604 147,0764 148,0609 148,0609 149,0609 148,0609 148,0609 148,0609 148,0609 148,0609 148,0609 149,0764 149,0764 140,0764 140,0764 141,0764 141,0764 141,0764 141,0764 142,0764 1435,2384 168,9908 105,0193 - Neutral and/or hydrophobic 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 171,0064 172,0381 173,0381
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Soprenoid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Retogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycogne biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Glutamic biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutathione prosynthesis	VI D-Galactono-1,4-lactone 1	Gal1P GP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlicnL6P Glic-1P Glic-6P D-Glucose G1P G6P Glu-5-P Glu-	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00066 + C03517 - C00818 + C00257 + C00198 + C00329 + C00329 + C00329 + C00329 + C00329 + C00329 + C00352 + C00191 + C00191 + C00257 + C0196 + C0197 + C00057 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Cation Neutral Anion Anion Cation Neutral	Hydrophilic	6 10	6 6 6 6 7 7 7 2 8 8 7 7 6 6 6 7 7 2 8 8 8 7 7 8 8 8 1 8 1 8 1 8 1 8 1 8 1 8	196,0583 178,0477 180,0634 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 259,0457 259,0457 180,0634 260,0297 194,0427 227,0195 131,0582 131,0582 147,0532 146,0691 146,0691 146,0691 146,0691 159,9980 160,0297 172,0195 172,0195 172,0195 175,0320 666,2219 175,0320 666,2219 175,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320 660,0211 75,0320	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 259.0224 193.0354 586.0593 588.0750 604.0699 313.0612 Neutral and/or hydrophobic 209.0303 195.0510 Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 258.0384 - Neutral and/or hydrophobic 259.0224 193.0354 2259.0224 193.0354 226.0122 132.0655 143.0655 143.0655 144.0604 147.0764 148.0604 147.0764 148.0604 147.0764 151.0969 307.0833 Detected as divalent ion in MS 308.0911 435.2384 168.9908 1105.0193 - Neutral and/or hydrophobic 171.0064 258.1107 Including quarternary amine 76.0393 - Neutral and/or hydrophobic
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Cholanic acid biosynthesis Isoprenoid	VI D-Galactono-1,4-lactone 1 α-D-Galactose 11 α-D-Galactose 12 α-D-Galactose 13 α-D-Galactose-1-phosphate 14 GDP-4-dehydro-6-deoxy-D-mannose 15 GDP-1-tucose 16 GDP-1-tucose 17 GDP-1-tucose 18 Galacturonic acid 19 Gucono-A-lactone 10 Gucono-A-lactone 10 Gucono-A-lactone 11 Glucono-A-lactone 11 G-Gucono-A-lactone 11 D-Glucose-1-phosphate 12 D-Glucose-1-phosphate 13 α-D-Glucose-1-phosphate 14 α-D-Glucose-1-phosphate 15 α-D-Glucose-1-phosphate 16 α-D-Glucose-1-phosphate 17 α-D-Glucose-1-phosphate 18 Glucunoric acid 19 L-Glucose-1-phosphate 10 L-Glutamate-9-phosphate 10 L-Glutamate-9-phosphate 11 L-Glutamate-9-phosphate 12 L-Glutamate-9-phosphate 13 L-Glutamate-9-phosphate 14 L-Glutamate-9-phosphate 15 L-Glutamic acid 16 L-Glutamic acid 17 L-Glutamic acid 18 Glucamide 19 L-Glutamic acid 10 L-Glutamic acid 11 Glutamine 10 L-Glutamic acid 11 Glutathion (reduced form) 11 Glutathionylspermidine 10 L-Glutamine 11 L-Glutamic (reduced form) 11 Glutathionylspermidine 12 Glucathionylspermidine 13 Glucathionylspermidine 14 Glucathionylspermidine 15 Glucerol-3-phosphate 16 Glycorol 17 Glycorol 18 Glycorol 19 Glycoladehyde 10 Glycorol 11 Glycorol 11 Glycorol 12 Glycorol 13 Glycoladenyde 14 Glycorol 15 Glycorol 16 Glycosphate 17 Glycosphate 18 Glyconie-3-diphosphate 19 Guanosine-3-diphosphate 5'-phosphate	Gal1P GPP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu5A Glu-semlaldehyde D-Glu Glu Glu Glu Gln GluCys GSSG GSH GSH-spermidine G3P Gly3P Gly3P GDP ppGpp ppGpp	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C000818 + C00257 + C00182 - C00329 + C00329 + C00329 + C00329 + C00329 + C00352 + C00031 + C00032 + C00352 + C00352 +	Anion Neutral Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Cation Neutral	Hydrophilic	6 10	6 6 6 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	196,0583 178,0477 180,0634 180,0634 180,0634 260,0297 194,0427 587,0666 589,0822 605,0772 314,0684 210,0376 196,0583 178,0477 258,0141 179,0794 259,0457 180,0634 260,0297 260,0297 194,0427 227,0199 131,0582 147,0532 147,0532 146,0691 146,0691 146,0691 146,0691 146,0691 146,0691 146,0691 146,0691 175,0320 175	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 193.0354 193.0354 1956.0593 188.0750 1956.0593 195.0510 Neutral and/or hydrophobic 209.0303 195.0510 Neutral and/or hydrophobic 257.0068 180.0867 1258.0384 1258.0384 1258.0384 1258.0384 1259.0224 132.0655 148.0604 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 148.06064 159.0764 169.0764 170.0764
Colanic acid biosynthesis Lactose degradation Cholanic acid biosynthesis Galacturonic acid degradation Cholanic acid biosynthesis Isoprenoid biosynthesis Glucaric acid degradation Ketogluconic acid metabolism Glucose degradation Pentose phosphate pathway (oxidative) Glucose degradation Pentose phosphate pathway (oxidative) Glucosamine transport UDP-N-acetylgucosamine biosynthesis Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas) Glucuronide degradation Proline biosynthesis Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis Peptideglycan biosynthesis Peptideglycan biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutamic acid biosynthesis Glutathione biosynthesis Glutathione biosynthesis Glutathione biosynthesis Glutathione biosynthesis Glutathione phosynthesis Glycolic acid degradation Glycerol degradation FldC (in vitro) Glycoric acid degradation Glycoric acid biosynthesis	VI D-Galactono-1,4-lactone 1	GaltP GDP-DDMan GDP-fucose GDP-Man GPP Gluconolacton GlcnL6P Glc-1P Glc-6P D-Glucose G1P G6P Glu-5-P Glu-5-P Glu-5-B Glu-5	C00880 + C0383 + C0383 + C00984 - C00124 + C00446 + C00333 + C01222 - C00325 + C00066 + C03517 - C00818 + C00257 + C00198 + C00329 + C00329 + C00329 + C00329 + C00329 + C00329 + C00352 + C00191 + C00191 + C00257 + C0196 + C0197 + C00057 +	Anion Neutral Neutral Neutral Anion Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Anion Neutral Anion Cation Cation Cation Cation Cation Cation Cation Neutral Anion Cation Neutral	Hydrophilic	6 10	6 6	196.0583 178.0477 180.0634 180.0634 180.0634 260.0297 194.0427 587.0666 589.0822 605.0772 314.0684 179.0794 259.0457 180.0583 178.0477 258.0141 179.0794 259.0457 180.0634 260.0297 194.0427 227.0195 131.0582 147.0532 146.0691 146.0691 146.0691 146.0691 150.0297 175.0320 160.0297 175.0320 160.0297 175.0320 175	- Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic 193.0354 193.0354 1958.0750 604.0699 133.0612 Neutral and/or hydrophobic 209.0303 195.0510 Neutral and/or hydrophobic 257.0068 180.0867 258.0384 - Neutral and/or hydrophobic 258.0384 - Neutral and/or hydrophobic 259.0224 193.0334 2258.0384 - Neutral and/or hydrophobic 193.0354 125.0655 132.0655 143.0655 1448.0604 147.0764 147.0764 147.0764 147.0764 147.0764 1417.0764 151.0968 307.0933 Detected as divalent ion in MS 308.0911 145.2384 168.9908 1105.0193 - Neutral and/or hydrophobic 171.0064 258.1107 Including quarternary amine 76.0393 - Neutral and/or hydrophobic

	V Guanosine-3-phosphate 5'-phosphate I Guanosine-5-triphosphate	pGp GTP	- + Nucleotide C00044 + Nucleotide		11 2 443.0243 442.0171 Catalytic enzyme is unidentified 14 3 522.9907 521.9834
	I H ₂ O I HCO ₃		C00001 C00288 + Anion	- 2 Hydrophilic 1 1	1 18.0106 — Solvent 3 60.9926 59.9853 Volatile
Proto- and siroheme biosynthesis	Heme 0 L-Histidinal	Histidinal	C15672 – Anion C01929 – Cation	Hydrophobic 49 58 4 Hydrophilic 6 9 3	5 1 836.3600 835.3527 Neutral and/or hydrophobic 1 139.0746 140.0818 Intermediate of rection
Histidine biosynthesis	L-Histidine L-Histidinol	His Histidinal	C00135 + Cation C00860 + Cation		2 155.0695 156.0768 1 141.0902 142.0975
Histidine biosynthesis	L-Histidinolphosphate I Homocysteine	Histidinol-P HomoCys	C01100 Nucleotide C05330 Cation	Hydrophilic 6 12 3	4 1 221.0565 220.0493 2 1 135.0354 136.0427
Homoserine biosynthesis	Introduction L-Homoserine L-Ho	HomoSer	C00263 + Cation Cation	Hydrophilic 4 9 1	3 119.0582 120.0655 2 101.0477 102.0550
Sulfuric acid assimilation	I Hydrogen sulfide		C00283 – Cation	Hydrophilic 2	1 33.9877 34.9950 Out of the MS range
Ubiquinone biosynthesis	III 3-Hydroxyadipyl-CoA I p-Hydroxybenzoic acid	PHBA	C00156 + Anion	Hydrophilic 7 6	20 3 1 911.1575 910.1502 3 138.0317 137.0244
	I 4-Hydroxybenzylalcohol III 2-Hydroxydeoxyadenosine-5-triphosphate	4Hben-ol	Neutral	Hydrophilic 10 16 5	2 124.0524 - Neutral and/or hydrophobic 13 3 506.9958 505.9885
2-Oxoglutaric acid reduction (in vitro)	III 8-Hydroxydeoxyguanosine-5'-triphosphate VI (R)-2-Hydroxyglutaric acid		Nucleotide C01087 - Anion	Hydrophilic 5 8	14 3 522.9907 521.9834 5 148.0372 147.0299
	III (S)-2-Hydroxyglutaric acid L-4-Hydroxy-2-ketoglutaric acid		C02630 – Anion C01127 – Anion		5 148.0372 147.0299 6 162.0164 161.0092
71.1	2-Hydroxy-6-ketonona-2,4-diene-1,9-dicarboxylic acid 4-Hydroxy-2-ketovaleric acid 4-Hydroxy-2-ketovaleric acid		C04479 – Anion C03589 – Anion		6 214.0477 213.0405 4 132.0423 131.0350
	1-Hydroxy-2-methyl-2-(<i>E</i>)-butenyl-4-diphosphate Hydroxymethylbilane	HMeBuPP HMB	C11811 – Anion C01024 – Anion		8 2 262.0007 260.9935 17 854.2858 853.2785
	1 6-Hydroxymethyldehydropterin VI S-Hydroxymethylglutathione	HMeDHP	C01300 – Cation C14180 – Cation		2 195.0756 196.0829 7 1 337.0944 338.1017
manine biosynthesis	Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate	HMePyr HMePyrP	C01279 – Cation C04556 – Anion	Hydrophilic 6 9 3 Hydrophilic 6 10 3	1 139.0746 140.0818 4 1 219.0409 218.0336
Phenylpropionic acid degradation	III 3-(2-Hydroxyphenyl)propionic acid III 3-(3-Hydroxyphenyl)propionic acid	3HPP	C01198 – Anion C11457 – Anion	Hydrophilic 9 10	3 166.0630 165.0557 3 166.0630 165.0557
HyuA (in vitro)	VI Hydroxyphenylhydantoin	HPP	Cation C01179 + Anion	Hydrophilic 9 8 2	3 192.0535 193.0608
Pyridoxal-5'-phosphate biosynthesis	P-Hydroxyphenylpyruvic acid 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid	ЗН4РНКВА	Anion	Hydrophilic 4 6	8 1 212.9800 211.9728
Salvage of Ade, HypXan	III Hydroxypyruvic acid I Hypoxanthine		C00168 + Anion C00262 + Cation	Hydrophilic 5 4 4	4 104.0110 103.0037 1 136.0385 137.0458
Histidine degradation	III L-idonic acid III Imidazole lactic acid	Im-lactate	C00770 — Anion C05568 — Cation		7 196.0583 195.0510 3 156.0535 157.0608
modeline biodynericsis	II Imidazoleacetolphosphate II Imidazolepyruvic acid	IM-pyruvic acid	C01267 – Nucleotide C03277 – Cation		5 1 220.0249 219.0176 3 154.0378 155.0451
NAD biosynthesis Tryptophan biosynthesis	I Iminoaspartic acid I Indole		C05840 – Cation C00463 + Cation	Hydrophilic 4 5 1 Hydrophilic 8 7 1	4 131.0219 132.0291 117.0578 118.0651
Tryptophan biosynthesis	I Indole-3-glycerolphosphate I Inosine	IG-P	C03506 - Nucleotide C00294 + Cation	Hydrophilic 11 14 1	6 1 287.0559 286.0486 5 268.0808 269.0880
Purine biosynthesis	I Inosine-5'-phosphate	IMP ITP	C00130 + Nucleotide	Hydrophilic 10 13 4	8 1 348.0471 347.0398
Inositol utilization (SuhB)	IV Inosine-5'-triphosphate VI Impolential VI Impolential VI IV IV IV IV IV IV I		C00081 + Nucleotide C00137 + Neutral	Hydrophilic 6 12	14 3 507.9798 506.9725 6 180.0634 - Neutral and/or hydrophobic
Phytic acid degradation	III myo-Inositolhexakisphosphate		C01204 + Nucleotide C04579 - Nucleotide	Hydrophilic 6 17	24 6 659.8614 658.8541 21 5 579.8951 578.8878
Inositol utilization (SuhB)	III D-myo-inositol-1,2,4,5,6-pentakisphosphate VI 1L-myo-inositol-1-phosphate		C04563 – Nucleotide C04006 – Anion	Hydrophilic 6 13	21 5 579.8951 578.8878 9 1 260.0297 259.0224
	VI 1D- <i>myo</i> -Inositol-1-phosphate III D- <i>myo</i> -Inositol-2,3,4,5-tetraphosphate		C01177		9 1 260.0297 259.0224 18 4 499.9287 498.9214
Phytic acid degradation	III D-myo-Inositol-2,4,5-triphosphate I Isochorismic acid		Nucleotide C00885 - Anion	Hydrophilic 6 15	15 3 419.9624 418.9551 6 226.0477 225.0405
TCA cycle	I Isocitric acid L-Isoleucine	Ile	C00311 + Nucleotide C00407 + Cation	Hydrophilic 6 8	7 192.0270 191.0197 2 131.0946 132.1019
Isopentenyldiphosphate biosynthesis	I \(\Delta 3-Isopentenyldiphosphate \)	IPPP 2IPMA	C00129 – Anion	Hydrophilic 5 12	7 2 246.0058 244.9986
Leucine biosynthesis	1 2-Isopropylmalic acid 1 3-Isopropylmalic acid	3IPMA	C04411 – Anion	Hydrophilic 7 12	5 176.0685 175.0612 5 176.0685 175.0612 6 176.0685 175.0612
AidA (in vitro)	2-Isopropyl-3-oxosuccinic acid Isovaleryl-CoA	2IP3OSA	Anion C02939 - Nucleotide	Hydrophilic 26 44 7	5 174.0528 173.0455 17 3 1 851.1727 850.1655
LipidA biosynthesis LipidA biosynthesis	I KDO2-(lauroyl)-lipid IVA I KDO2-lipid A	KDO2-Lau-lipid IVA	C06251 — Nucleotide C06026 — Nucleotide	Hydrophobic 110 202 2	38 2 2027.1376 2026.1304 Out of the MS range 39 2 2237.3360 2236.3287 Out of the MS range
LipidA biosynthesis KDO biosynthesis	I KD02-lipid A, cold adapted I KD02-lipid IVA	KDO2-lipid A (cold)	Nucleotide C06025 - Nucleotide	7	39 2 2291.3830 2290.3757 Out of the MS range 37 2 1844.9706 1843.9633 Out of the MS range
LipidA biosynthesis KDO biosynthesis	I KD02-(palmitoleoyl)-lipid IVA I (KD0)-lipid IV(A)	KDO2-Pal-lipid IVA	Nucleotide		38 2 2081.1846 2080.1773 Out of the MS range 37 2 1844.9706 1843.9633 Out of the MS range
Phenylacetic acid degaradation	III B-Ketoadipyl-CoA III 5-Keto-4-deoxy-D-glucaric acid		C02232 – Nucleotide C00679 – Anion	Hydrophilic 27 42 7	20 3 1 909.1418 908.1346 7 192.0270 191.0197
Entner-Doudoroff pathway	2-Keto-3-deoxy-6-phosphogluconic acid	KDPGlcA	C04442 – Anion	Hydrophilic 6 11	9 1 258.0141 257.0068
Ascorbic acid degradation	III 3-Keto-L-gulonate-6-phosphate		C01062 — Anion C14899 — Anion	Hydrophilic 6 11	7 194.0427 193.0354 10 1 274.0090 273.0017
			C15673 – Anion C00618 – Anion	Hydrophilic 6 10	7 194.0427 193.0354 7 194.0427 193.0354
Leucine biosynthesis Valine biosynthesis	2-Ketoisocaproic acid 2-Ketoisovaleric acid	2KICA 2-KIV	C00233 + Anion C00141 + Anion	,	3 130.0630 129.0557 3 116.0473 115.0401
Isoleucine biosynthesis Methylglyoxal pathway	2-Keto-3-methylvaleric acid D-Lactaldehyde	2K3MVA Lactaldehyde	C03465 + Anion C00424 - Neutral	Hydrophilic 6 10 Hydrophilic 3 6	3 130.0630 129.0557 2 74.0368 - Neutral and/or hydrophobic
Methylglyoxal pathway	D-Lactic acid L-Lactic acid	Lactic acid	C00256 + Anion C01432 - Anion	Hydrophilic 3 6	3 90.0317 89.0244 3 90.0317 89.0244
Lactose degradation	III Lactose I S-Lactoylglutathione	SL-GSH	C00243 + Neutral C03451 + Cation	Hydrophilic 12 22	11 342.1162 — Neutral and/or hydrophobic 8 1 379.1049 380.1122
Leucine biosynthesis	I L-Leucine	Leu	C00123 + Cation	Hydrophilic 6 13 1	2 131.0946 132.1019
122 2337.111111	I Lipid A disaccharide I Lipid IV(A)	Lipid A dSc	C04919 – Nucleotide	Hydrophobic 68 130 2	20 1 1324.8876 1323.8804 Out of the MS range 23 2 1404.8540 1403.8467 Out of the MS range
	VI Lipoamide III Lipoic acid		C00248 + Neutral C00725 + Anion	Hydrophilic 8 14	2 2 206.0435 205.0362
Lyxose transport	L-Lysine D-Lyxose D-Lyxose L-Lysine L-Lysine D-Lyxose L-Lysine L-Lysine	Lys	C00047 + Cation C00476 + Neutral	Hydrophilic 5 10	2 146.1055 147.1128 5 150.0528 - Neutral and/or hydrophobic
	L-Lyxose		C01508 + Neutral C00497 - Anion	Hydrophilic 5 10 Hydrophilic 4 6	5 150.0528 - Neutral and/or hydrophobic 5 134.0215 133.0142
Fatty acid biosynthesis Glycerol degradation	I Malonyl-CoA III Maltose		C00083 + Nucleotide C00208 + Neutral	Hydrophilic 24 38 7 Hydrophilic 12 22	19 3 1 853.1156 403.5556 Detected as acetyl-CoA in MS 11 342.1162 - Neutral and/or hydrophobic
Glycerol degradation	III Maltotetraose III Maltotriose		C02052 + Neutral C01835 + Neutral	Hydrophilic 24 42	21 666.2219 — Neutral and/or hydrophobic 16 504.1690 — Neutral and/or hydrophobic
Mannitol degradation	D-Mannitol D-M	Mant1P	C00392 + Neutral C00644 + Anion	Hydrophilic 6 14	6 182.0790 — Neutral and/or hydrophobic 9 1 262.0454 261.0381
Glucuronide degradation	D-Mannonic acid	Marieri	C00514 – Anion	Hydrophilic 6 12	7 196.0583 195.0510
Cholanic acid biosynthesis	III D-Mannose I D-Mannose-1-phosphate	Man1P	C00159 + Neutral C00636 + Anion	Hydrophilic 6 12 Hydrophilic 6 13	6 180.0634 - Neutral and/or hydrophobic 9 1 260.0297 259.0224
	D-Mannose-6-phosphate III 2-O-α-Mannosyl-D-glyceric acid	Man6P ManGlycerate	C00275 + Anion C11544 - Anion	Hydrophilic 9 16	9 1 260.0297 259.0224 9 268.0794 267.0722
Oxidation of menadiol (in vitro)			C05402 + Neutral C07126 - Neutral	Hydrophilic 11 10	11 342.1162 — Neutral and/or hydrophobic 2 174.0681 — Neutral and/or hydrophobic
	VI Menadione IV Menaquinol		C05377 + Neutral C05819 - Neutral		2 172.0524 — Neutral and/or hydrophobic 2 720.5845 — Neutral and/or hydrophobic
	V Menaquinone-6 V Menaquinone-7		Neutral		2 648.4906 — Neutral and/or hydrophobic 2 716.5532 — Neutral and/or hydrophobic
Menaquinone biosynthesis	I Menaquinone-8 V Menaquinone-9	MeQ-8	C00828 - Neutral - Neutral	Hydrophobic 51 72	2 716.5532 - Neutral and/or hydrophobic 2 852.6784 - Neutral and/or hydrophobic
3-Mercaptopyruvic acid assimilation	III 3-Mercaptopyruvic acid	MercPyr	C00957 + Anion	Hydrophilic 3 4	3 1 119.9881 118.9808
Formyltetrahydrofolic acid biosynthesis	III Methanol I 5,10-Methenyl-THF	5,10Me-THF	C00445 – Cation	Hydrophilic 20 23 7	6 457.1704 457.1704 Including quarternary amine
Methionine biosynthesis	III D-Methionine I L-Methionine	D-Met Met	C00855 — Cation C00073 + Cation	Hydrophilic 5 11 1	2 1 149.0511 150.0583 2 1 149.0511 150.0583
Thiamine biosynthesis	I L-Methionine sulfoxide I 4-Methyl-5-(β-hydroxyethyl)thiazole	MetSFX 4Me5BHEthThiazole	C02989 + Cation C04294 + Cation	Hydrophilic 6 9 1	3 1 165.0460 166.0532 1 1 1 143.0405 144.0478
	4-Methyl-5-(β-hydroxyethyl)thiazolephosphate 2-Methyl-c/is-aconitic acid	4Me5BHEthThiazoleP	C04327 – Anion C04225 – Anion	Hydrophilic 7 8	4 1 1 223.0068 221.9995 6 188.0321 187.0248
	III N¹-Methyladenine 1 5-Methylaminomethyl-2-selenouridine	5-MeAMe-2-SeUri	Cation _ Cation	Hydrophilic 6 8 5 Hydrophilic 11 17 3	5 1 351.0333 352.0406 Modified tRNA
Selenouridine biosynthesis (tRNA) Methylcitric acid cycle	I 5-Methylaminomethyl-2-thiouridine III 2-Methylcitric acid	5-MeAMe-2-thioUri	Cation C02225 - Anion		5 1 303.0889 304.0962 Modified tRNA 7 206.0427 205.0354
AidA (in vitro)	3-Methylcrotonyl-CoA		C03069 — Nucleotide — — Cation		7 3 1 849.1571 848.1498 1 126.0667 127.0740
Formyltetrahydrofolic acid biosynthesis	I 5,10-Methylene-THF	5,10MeL-THF	C00143 – Cation	Hydrophilic 20 23 7	6 457.1710 458.1783
	CMethyl-D-erythritol-2,4-cyclodiphosphate CMethyl-D-erythritol-4-phosphate	MeEry2,4CP MeEry4P	C11453 — Anion C11434 — Anion	Hydrophilic 5 12 Hydrophilic 5 13	9 2 277.9957 276.9884 7 1 216.0399 215.0326
Methylglyoxal pathway	I M²-Methyl-L-glutamine I Methylglyoxal	N5-methyl-Gln	C03153 — Cation C00546 + Neutral	7. 7	3 160.0848 161.0921 Modified protein 2 72.0211 - Neutral and/or hydrophobic
Methylmalonyl pathway	III Methylisocitric acid II D-Methylmalonyl-CoA	D-MeMal-CoA	C04593 – Anion C02557 + Nucleotide		
Methylmalonyl pathway	II L-Methylmalonyl-CoA III S-Methyl-methionine	L-MeMal-CoA	C01213 - Nucleotide C03172 - Cation	Hydrophilic 25 40 7	19 3 1 867.1313 432.5584 Detected as divalent ion in MS
Methionine biosynthesis	5-Methyltetrahydropteroyltri-L-glutamic acid 5-Methyl-THF	5MTHTGlu Me-THF	C04489 - Cation C00440 + Cation	Hydrophilic 25 36 8	12 640.2453 641.2525
Polyamine biosynthesis	I 5'-Methylthioadenosine	MTA	C00170 + Cation	Hydrophilic 11 15 5	3 1 297.0896 298.0968
Molybdopterin biosynthesis	VI M-Methyttryptophan I Molybdopterin Multipaterin form	Mol form A	C02983 — Cation C05924 — Anion	Hydrophilic 10 14 5	6 1 2 395.0123 394.0050
Molybdopterin biosynthesis	I Molybdopterin formA I Molybdopterin formA-GMP	Mol-form A-GMP	Anion - Nucleotide		13 2 671.0765 670.0692
	III Molybdopteringuaninedinucleotide III Monomethyl-ester-of-trans-aconitic acid	MolGDN	Nucleotide C11514 - Anion	Hydrophilic 7 8	6 188.0321 187.0248
	I Nicotinamide I Nicotinamideadeninedinucleotide (oxidized form)	NADH	C00153 + Cation C00004 + Nucleotide	Hydrophilic 6 6 2	
	Nicotinamideadeninedinucleotide (reduced form) Nicotinamideadeninedinucleotidephosphate (oxidized form)	NAD* NADPH	C00003 + Nucleotide C00005 + Nucleotide	Hydrophilic 21 28 7	14 2 664.1164 662.1019 Including quarternary amine 17 3 745.0911 371.5383 Detected as divalent ion in MS
NAD biosynthesis NAD biosynthesis	Nicotinamideademinedinucleotidephosphate (oxidized form) Nicotinamide-Dribonucleotide Nicotinamide-Dribonucleotide	NADP* NicRN	C00005 + Nucleotide C00006 + Nucleotide C00455 + Anion	Hydrophilic 21 29 7	17 3 744.0827 742.0682 Including quarternary amine
NAD biosynthesis NAD biosynthesis		rical)	C01185 + Nucleotide	Hydrophilic 11 15 1	9 1 336.0484 334.0339 Including quarternary amine
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis	Nicotinatenucleotide Nicotinic acid		C00253 + Cation C00870 + Anion		2 122.0242 123.0315 3 139.0269 138.0197
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro)	I Nicotinic acid VI p-Nitrophenol		C02340	116.00000000000000000000000000000000000	6 1 218.9933 217.9860
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro) Lipoic acid biosynthesis	Nicotinic acid Nicotinic acid P-Nitrophenol P-Nitrophenol		C03360 + Anion C06423 + Anion	Hydrophilic 8 16	2 144.1150 143.1078
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro) ElaC (in vitro)	Nicotinic acid P-Nitrophenol P-Nitrophenylphosphate P-Nitrophen	OPrPP 3Oct4HBA		Hydrophilic 8 16	2 144.1150 143.1078 72 722.4440 721.4368 Neutral and/or hydrophobic 3 682.5325 681.5252 Neutral and/or hydrophobic
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro) Lipoic acid biosynthesis Lipoic acid biosynthesis Lipoic acid biosynthesis Ubiquinone biosynthesis Ubiquinone biosynthesis	Nicotinic acid Nicotinic acid P-Nitrophenol P-Nitrophenol P-Nitrophenol P-Nitrophenol	3Oct4HBA 2Oct6Hphe	C06423 + Anion C04146 - Nucleotide C05809 - Anion C05811 - Neutral	Hydrophilic 8 16 Hydrophobic 40 68 Hydrophobic 47 70 Hydrophobic 46 70	7 2 722.4440 721.4368 Neutral and/or hydrophobic 3 682.5325 681.5252 Neutral and/or hydrophobic 2 654.5376 Neutral and/or hydrophobic
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro) ElaC (in vitro) Lipoic acid biosynthesis Ubiquinone biosynthesis Ubiquinone biosynthesis Ubiquinone biosynthesis Ubiquinone biosynthesis Ubiquinone biosynthesis	Nicotinic acid	3Oct4HBA 2Oct6Hphe 2Oct6Meth1,4BQ 2Oct6MethPhe	C06423 + Anion C04146 - Nucleotide C05809 - Anion C05811 - Neutral C05813 - Neutral C05812 - Neutral	Hydrophilic 8 16	7 2 722.4440 721.4368 Neutral and/or hydrophobic 682.5325 681.5252 Neutral and/or hydrophobic 692.5376 Neutral and/or hydrophobic Neutral and/or hydrophobic 654.5376 Neutral and/or hydrophobic
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycting NAD biosynthesis Pyridine nucleotide with side of the side of th	Nicotinic acid V P-Nitrophenol D Politrophenol D Politrophenol D Politrophenol D D Politrophenol D D D D D D D D D	3Oct4HBA 2Oct6Hphe 2Oct6Meth1,4BQ 2Oct6MethPhe 2Oct3Me6Meth1,4BQ 2OctPhe	C06423 + Anion C04146 - Nucleotide C05809 - Anion C05811 - Neutral C05813 - Neutral C05812 - Neutral C05814 - Neutral C05810 - Neutral	Hydrophilic 8 16	7 2 72.4440 721.4368 Neutral and/or hydrophobic 682.5325 681.5252 Neutral and/or hydrophobic 682.5325 — Neutral and/or hydrophobic 682.5325 — Neutral and/or hydrophobic 682.5325 — Neutral and/or hydrophobic 668.5332 — Neutral and/or hydrophobic 683.5427 — Neutral and/or hydrophobic 693.5427 — Neutral and/or hydrophobic
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling NAD biosynthesis Pyridine nucleotide cycling ElaC (in vitro) ElaC (in vitro) Lipoic acid biosynthesis Ubiquinone biosynthesis	Nicotinic acid Nicotinic acid Pittrophenol Pittrophenol Pittrophenol Octanoic acid Octaprenyldiphosphate Octaprenyldiphosphate Octaprenyldiphosphate 3-Octaprenyl-4-hydroxybenzoic acid 2-Octaprenyl-6-hydroxyphenol 2-Octaprenyl-6-methoxy-1,4-benzoquinone 2-Octaprenyl-6-methoxy-hydroxyphenol 2-Octaprenyl-3-methyl-6-methoxy-1,4-benzoquinone 2-Octaprenyl-3-methyl-6-methoxy-1,4-benzoquinone 1-Orotic acid Orotic acid Orotic acid	3Oct4HBA 2Oct6Hphe 2Oct6Meth1,4BQ 2Oct6MethPhe 2Oct3Me6Meth1,4BQ 2OctPhe Ornithine	C06423 + Anion C04146 - Nucleotide C05809 - Anion C05811 - Neutral C05813 - Neutral C05812 - Neutral C05814 - Neutral C05814 - Neutral C05810 - Neutral C05810 - Neutral C05910 + Anion	Hydrophilic 8 16	7 2
NAD biosynthesis NAD biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling ElaC (in vitro) ElaC (in vitro) Lipoic acid biosynthesis Ubiquinone biosynthesis Upiquinone biosynthesis Upiquinone biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis	Nicotinic acid Nicotinic acid Nitrophenol	3Oct4HBA 2Oct6Hphe 2Oct6Meth1,4BQ 2Oct6MethPhe 2Oct3Me6Meth1,4BQ 2OctPhe	C06423 + Anion C04146 - Nucleotide C05809 - Anion C05811 - Neutral C05813 - Neutral C05814 - Neutral C05814 - Neutral C05810 - Neutral C00077 + Cation	Hydrophilic 8 16	7 2

Property								
March Marc								
Mathematical Math								
Company Comp								
Mate	CoA biosynthesis	I Pantetheine-4'-phosphate	1	C01134 – Nucleotide	Hydrophilic 1	11 23 2 7 1 1	358.0964	357.0891
Company	Pantothenic acid biosynthesis	I Pantothenic acid	Tancoic dela	C00864 + Anion	Hydrophilic	9 17 1 5	219.1107	218.1034
Mathematical Math	Phenylethylamine degradation	III Phenylacetaldehyde		C00601 + Neutral	Hydrophilic	8 8 1	120.0575	Neutral and/or hydrophobic
Section	Phenylacetic acid degaradation	III Phenylacetyl-CoA	D. Div.	C00582 + Nucleotide	Hydrophilic 2	29 42 7 17 3 1	885.1571	884.1498
March Marc	Phenylalanine biosynthesis	I L-Phenylalanine		C00079 + Cation	Hydrophilic	9 11 1 2	165.0790	166.0863
Company	HyuA (in vitro)	VI Phenylhydantoin		Cation	Hydrophilic	9 8 2 2	176.0586	177.0659
Company Comp	Phenylalanine biosynthesis	I Phenylpyruvic acid		C00166 + Anion	Hydrophilic	9 8 3	164.0473	163.0401
Martin		, , ,						
Mary			6-PG					
Mary								
Manual Property	Gph (in vitro)	VI 2-Phosphoglycolic acid		C00988 – Anion	Hydrophilic	2 5 6 1	155.9824	
Martin	Serine biosynthesis	I 3-Phosphohydroxypyruvic acid	3PHPA	C03232 – Anion	Hydrophilic	3 5 7 1	183.9773	182.9700
Company Comp	CoA biosynthesis	I D-4'-Phosphopantothenic acid	4'PPA	C03492 – Nucleotide	Hydrophilic	9 18 1 8 1	299.0770	298.0697
Visit	Purine biosynthesis	I 5-Phosphoribosylamine	PRA	C03090 – Nucleotide	Hydrophilic	5 12 1 7 1	229.0351	228.0279
Martin M	Tryptophan biosynthesis	I N-(5'-Phosphoribosyl)anthranilic acid	PRAnth	C04302 - Nucleotide	Hydrophilic 1	12 16 1 9 1	349.0563	348.0490
Manual	Purine biosynthesis	I 5'-Phosphoribosyl-4-carboxy-5-aminoimidazole	CAIR	C04751 – Nucleotide	Hydrophilic	9 14 3 9 1	339.0468	338.0395
March Marc	Purine biosynthesis	I Phosphoribosylformamidocarboxamide	FAICAR	Nucleotide	Hydrophilic 1	10 15 4 9 1	366.0577	365.0504
SCHOOL STATE OF THE PROPERTY O								
March Marc								
Management 1 Mana								
Description 1	Serine biosynthesis	I 3-Phosphoserine	3PSer	C01005 + Anion	Hydrophilic	3 8 1 6 1	185.0089	184.0017
Description	Biotin biosynthesis	I Pimeloyl-CoA		C01063 – Nucleotide	Hydrophilic 2	28 46 7 19 3 1	909.1782	908.1709
Modern of the property of the	Proto- and siroheme biosynthesis	I Precorrin-1		C15527 – Anion	Hydrophilic 4	41 46 4 16	850.2909	849.2836
March Marc	Molybdopterin biosynthesis	I Precursor-Z	Precousor-Z	Cation	Hydrophilic 1	10 12 5 7 1	345.0474	346.0547
Team Programs	Proline biosynthesis	L-Proline	Pro	C00148 + Cation	Hydrophilic	5 9 1 2	115.0633	116.0706
Company	Threonine degradation	II Propionic acid		C00163 + Anion	Hydrophilic	3 6 2	74.0368	73.0295
Marchester 1	Threonine degradation	II Propionyl-CoA	Propionyl-P	C00100 + Nucleotide	Hydrophilic 2	24 40 7 17 3 1	823.1414	822.1342
March Marc	Proto- and siroheme biosynthesis	I Protoheme IX	Por IX	C00032 – Anion	Hydrophilic 3	34 32 4 4 1	614.1616	613.1544 Detected as divalent ion in MS
Marchestand	Proto- and siroheme biosynthesis	I Protoporphyrinogen IX		C01079 – Anion	Hydrophilic 3	34 40 4 4	564.2737	563.2664
Control Cont	Polyamine biosynthesis	I Putrescine	, acudoUJF	C00134 + Cation	Hydrophilic	4 12 2	88.1000	89.1073
TREAL PROMESSAME NO. 1000 1000 1000 1000 1000 1000 1000 10				Cation	Hydrophilic	5 4 2 2	124.0273	125.0346
Column C			Pyr5'P		Trydropintic	0 7 1 3		
Part			PX5'P					
Processor Proc			Pvn5'P					
Separate Propose Pro	Inorganic metabolite	I Pyrophosphate	PPi	C00013 + Anion	Hydrophilic	4 7 2	177.9432	176.9360
Septembrown	Quinones (pathway unknown)	V Pyrroloquinolinequinone	 	C00113 + Anion	Hydrophilic 1	14 6 2 8	330.0124	329.0051
Teach	Queuine biosynthesis (tRNA)	I Queuine		Cation	Hydrophilic 1	12 15 5 3	277.1175	278.1248 Modified tRNA
	Rhamnose degradation	III L-Rhamnose		C00507 + Neutral	Hydrophilic	6 12 5	164.0685	Neutral and/or hydrophobic
Company Comp								
Company Comp			Ribazole5'P					
March Marc		I Riboflavin		C00255 + Cation	Hydrophilic 1			
March State	PRPP biosynthesis	I D-Ribose-1,5-diphosphate		C01151 – Nucleotide	Hydrophilic	5 12 11 2	309.9855	308.9782
Section personne 1 Section 1 Secti	Pentose phosphate pathway (non-oxidative)	I D-Ribose-5-phosphate	R5P	C00117 + Anion	Hydrophilic	5 11 8 1	230.0192	229.0119
Processor Proc	D-Arabinose degradtion	III D-Ribulose	RibHomoCys	C00309 + Neutral	Hydrophilic	5 10 5	150.0528	Neutral and/or hydrophobic
1	D-Arabinose degradtion	D-Ribulose-1-phosphate		Anion	Hydrophilic	5 11 8 1	230.0192	229.0119
Mary			Ru5P					
Marchen Marc		-						
Control of Control o	Salicin degradation	III Salicin-6-phosphate	S7P	C06188 – Anion	Hydrophilic 1	13 19 10 1	366.0716	365.0643
Contact processing 1 Processing	Selenouridine biosynthesis (tRNA)	I Selenide		C01528 – Anion	Hydrophilic	2 1	81.9322	80.9249 Modified tRNA
Seminary 1 Semina	Selenouridine biosynthesis (tRNA)	I Selenophosphate		C05172 – Anion	Hydrophilic	3 31 1	161.8985	160.8912 Modified tRNA
Common and statements	Serine biosynthesis	I L-Serine		C00065 + Cation	Hydrophilic	3 7 1 3	105.0426	106.0499
1. Survive 1.	Chorismic acid biosynthesis	I Shikimate-3-phosphate	S3P	C03175 – Anion	Hydrophilic	7 11 8 1	254.0192	253.0119
Section 1								
Pages of temporals								
Name								
Company Comp	Polyamine acetylation	I Spermine		C00750 + Cation	Hydrophilic 1	10 26 4	202.2157	203.2230
Processor Proc	TCA cycle	I Succinic acid	ΣΔΚΡΔ	C00042 + Anion	Hydrophilic	4 6 4	118.0266	117.0193
1 1 2 Control Principal Control Contro	Arginine degradation	II N ² -Succinyl-L-arginine	N2SucArg	C03296 – Cation	Hydrophilic 1	10 18 4 5	274.1277	275.1350
Dec	Menaquinone biosynthesis	I O-Succinylbenzoyl-CoA	OSucB-CoA	C03160 – Nucleotide	Hydrophilic 3	32 44 7 20 3 1	971.1575	970.1502
Seminary	Lysine biosynthesis	I N-Succinyl-L,L-2,6-diaminopimelic acid		C04421 – Anion	Hydrophilic 1	11 18 2 7	290.1114	
Name	Arginine degradation	II N²-Succinylglutamate-5-semialdehyde		C05932 – Cation	Hydrophilic	9 15 1 6	233.0899	234.0972
Mary to Age patients		I O-Succinyl-L-homoserine	SucHomoSer	C01118 + Cation	Hydrophilic	8 13 1 6	219.0743	220.0816
Secure Sequence Bi				C05817 – Anion	Hydrophilic 1			
Suffer and commissions 1 Martine Codi definitions 1 Martine Codi definitions 1 Martine Codi definitions 1 Martine Coding Suffer and Suffering Coding Suffering C	Sucrose transport	III Sucrose		C00089 + Neutral	Hydrophilic 1	12 22 11	342.1162	Neutral and/or hydrophobic
Column C	Sulfuric acid assimilation	I Sulfite		C00094 + Anion	Hydrophilic	2 3 1	81.9725	80.9652 Inorganic metabolite
Second Fig. Company	Galactitol degradation	III D-Tagatose-1,6-diphosphate		C03785 – Nucleotide	Hydrophilic	6 14 12 2	339.9961	338.9888
Suppose Control of Suppose	Galacturonic acid degradation	III D-Tagaturonic acid	- agatoscor	C00558 – Anion	Hydrophilic		194.0427	193.0354
1	Glycolic acid degradation	III Tartronatesemialdehyde		C01146 – Anion	Hydrophilic		104.0110	103.0037
Tetrahydrotics and bosynthesis 1 Tetrahydr	Lysine biosynthesis	I L-2,3,4,5-Tetrahydrodipicolinic acid		C03972 – Anion	Hydrophilic	7 9 1 4	171.0532	170.0459
	Tetrahydrofolic acid biosynthesis	I Tetrahydrofolic acid		C00101 + Anion	Hydrophilic 1	19 23 7 6	445.1710	444.1637 Unstable in aqueous solution
Maerobic repiration M. Festalysofrolity plane Sample Sam	Methionine biosynthesis	I Tetrahydropteroyltri-L-glutamic acid		C04144 – Cation	Hydrophilic 2	24 34 8 12	626.2296	627.2369
Thanne blowymbres 1 Thanne plowymbres	Anaerobic respiration	IV Tetrahydrothiophene-1-oxide		Neutral	Hydrophilic	4 8 1 1	104.0296	Neutral and/or hydrophobic
American Ministration Ministra	Thiamine biosynthesis	Thiaminediphosphate		C00068 + Nucleotide	Hydrophilic 1	12 19 4 7 2 1	425.0450	423.0304 Including quarternary amine
Definition acids degradation III Definition Defin	4-Mercaptopyruvic acid assimilation	III Thiocyanic acid		C01755 – Anion	Hydrophilic	1 1 1 1	58.9830	57.9757
Salvage of pyrimidine 1 Thymidine C00214	D-Amino acids degradation	III D-Threonine		C00820 – Cation	Hydrophilic	4 9 1 3	119.0582	120.0655
Quinones (pathway unknown)	Salvage of pyrimidine	1 Thymidine	ihr	C00214 + Cation	Hydrophilic 1	10 14 2 5	242.0903	243.0975
Trehalose biosynthesis	Quinones (pathway unknown)	V Topaquinone		Neutral	Hydrophobic	9 9 1 5	211.0481	Neutral and/or hydrophobic
Anaerobic respiration IV Trimethylamme TmeAla C0055 + Cation Hydrophilic 3 9 1 1 0 59,0736 60,0808	Trehalose biosynthesis	I Trehalose	Tre6P	C01083 + Neutral	Hydrophilic 1	12 22 11	342.1162	Neutral and/or hydrophobic
Citric acid llase activation 1 2-(5-Triphosphoribosyl)-3-dephospho-CoA PRIDP-CoA - Nucleotide Hydrophilic 1 1 1 2 2 1 0 1057.0745 1056.0672 Out of the MS range Tryptophan biosynthesis 1 L-Tryptophan L-Tryptophan L-Tryptophan Tryptophan Tryptop	Anaerobic respiration	IV Trimethylamine	TMeAla	C00565 + Cation	Hydrophilic	3 9 1	59.0735	60.0808
Tyrosine biosynthesis		I 2'-(5"-Triphosphoribosyl)-3'-dephospho-CoA	PRiDP-CoA	- Nucleotide	Hydrophilic 2	26 44 7 26 5 1	1057.0745	1056.0672 Out of the MS range
Quinones (pathway unknown) V Ubiquinol-1 CQH		. _—	Tyr	C00082 + Cation	Hydrophilic	9 11 1 3	181.0739	182.0812
Quinones (pathway unknown) V Ubiquinol-3 CoQH3 — Neutral Hydrophobic 29 44 4 I 456,3240 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-15 CoQH4 — Neutral Hydrophobic 34 52 4 I 524,3866 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-5 — Neutral Hydrophobic 39 60 4 I 524,3866 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-6 CoQH6 — Neutral Hydrophobic 4 68 4 I 660.5118 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-6 CoQH7 — Neutral Hydrophobic 49 76 4 I 72,35,744 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-9 CoQH8 — Neutral Hydrophobic	Tryptophan biosynthesis Tyrosine biosynthesis		In Torre	Cation	nyarophilic	וו 1 1 1 1 1 1 1 1		
Quinones (pathway unknown) V Ubiquinol-5 CoQH5 — Neutral Hydrophobic 39 60 4 0 592.4492 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-6 CoQH6 — Neutral Hydrophobic 44 68 4 0 620.5118 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-19 Neutral Hydrophobic 49 76 4 0 730.5794 — Neutral and/or hydrophobic Ubiquinoles (pathway unknown) V Ubiquinol-19 CoQH8 — — Neutral Hydrophobic 49 78 4 0 730.5790 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-8 CoQH9 — Neutral Hydrophobic 4 0 864.6996 — Neutral and/or hydrophobic	Tryptophan biosynthesis Tyrosine biosynthesis D-Amino acids degradation Quinones (pathway unknown)	D-Tyrosine	CoQH1	Neutral				
Quinones (pathway unknown) V Ubiquinol-6 CoQH6 — Neutral Hydrophobic 44 68 4 I 660.5118 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-7 — Neutral Hydrophobic 49 76 4 I 78.5744 — Neutral and/or hydrophobic Ubiquinones (pathway unknown) I Ubiquinol-8 CoQH8 — — Neutral Hydrophobic 49 78 4 I 78.5794 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-9 — Neutral Hydrophobic 49 78 4 I 78.5794 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-9 — Neutral and/or hydrophobic - Neutral and/or hydrophobic	Tryptophan biosynthesis Tyrosine biosynthesis D-Amino acids degradation Quinones (pathway unknown) Quinones (pathway unknown) Quinones (pathway unknown)	D-Tyrosine V Ubiquinol-1 V Ubiquinol-2 V Ubiquinol-3 V V V V V V V V V	CoQH1 CoQH2 CoQH3	Neutral - Neutral - Neutral - Neutral	Hydrophobic 2 Hydrophobic 2	24 36 4 29 44 4 4	388.2614 456.3240	Neutral and/or hydrophobic Neutral and/or hydrophobic
Ubiquinone biosynthesis I Ubiquinol-8 CoQH8 — Neutral Hydrophobic 49 78 4 0 730.5900 — Neutral and/or hydrophobic Quinones (pathway unknown) V Ubiquinol-9 CoQH9 — Neutral Hydrophobic 59 92 4 0 864.6996 — Neutral and/or hydrophobic	Tryptophan biosynthesis Tyrosine biosynthesis D-Amino acids degradation Quinones (pathway unknown) Quinones (pathway unknown) Quinones (pathway unknown) Quinones (pathway unknown)	D-Tyrosine	CoQH1 CoQH2 CoQH3 CoQH4	Neutral Neutral Neutral Neutral Neutral	Hydrophobic 2 Hydrophobic 2 Hydrophobic 3	24 36 4 29 44 4 334 52 4	388.2614 456.3240 524.3866	Neutral and/or hydrophobic Neutral and/or hydrophobic Neutral and/or hydrophobic
	Tryptophan biosynthesis Tyrosine biosynthesis D-Amino acids degradation Quinones (pathway unknown)	III D-Tyrosine V Ubiquinol-1 V Ubiquinol-2 V Ubiquinol-3 V Ubiquinol-3 V Ubiquinol-4 V Ubiquinol-5 V Ubiquinol-5 V Ubiquinol-6 V Ubiquinol-6 V Ubiquinol-6 V Ubiquinol-6 V V V V V V V V V	CoQH1 CoQH2 CoQH3 CoQH4 CoQH5 CoQH6	Neutral Neutral Neutral Neutral Neutral - Neutral - Neutral - Neutral	Hydrophobic 2 Hydrophobic 2 Hydrophobic 3 Hydrophobic 3 Hydrophobic 4	24 36 4 29 44 4 4 34 52 4 39 60 4 4 4 4 68 4 4 5 4 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6	388.2614 456.3240 524.3866 592.4492 660.5118	- Neutral and/or hydrophobic
	Tryptophan biosynthesis Tyrosine biosynthesis Tyrosine biosynthesis D-Amino acids degradation Quinones (pathway unknown) Ubiquinone biosynthesis	III	CoQH1 CoQH2 CoQH3 CoQH4 CoQH5 CoQH6 CoQH7 CoQH7 CoQH8	- Neutral	Hydrophobic 2 Hydrophobic 3 Hydrophobic 3 Hydrophobic 4 Hydrophobic 4 Hydrophobic 4 Hydrophobic 4	24 36 4 99 44 4 9 9 44 4 9 9 44 4 9 9 44 4 9 9 44 4 9 9 9 60 4 9 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 4 9 9 7 8 9 9 7 8 9 9 7 8 9 9 7 8 9 9 9 7 8 9 9 9 7 8 9 9 9 7 8 9 9 9 7 8 9 9 9 7 8 9 9 9 9	388.2614 456.3240 524.3866 592.4492 660.5118 728.5744 730.5900	Neutral and/or hydrophobic

uinones (pathway unknown)	V Ubiquinone-2	CoQ2	_	-	Neutral	Hydrophobic	24	34	4 '		386.2457	- '	Neutral and/or hydrophobic
rinones (pathway unknown)	V Ubiquinone-3	CoQ3	_	-	Neutral	Hydrophobic	29	42	4		454.3083	-	Neutral and/or hydrophobic
inones (pathway unknown)	V Ubiquinone-4	CoQ4		_	Neutral	Hydrophobic	34	50	4	\Box	522.3709		Neutral and/or hydrophobi
nones (pathway unknown)	V Ubiquinone-5	CoQ5	_	_	Neutral	Hydrophobic	39	58	4		590.4335	_	Neutral and/or hydrophob
nones (pathway unknown)	V Ubiquinone-6			_	Neutral	Hydrophobic	39	58	4	\Box	590.4335		Neutral and/or hydrophob
nones (pathway unknown)	V Ubiquinone-6	CoQ6			Neutral	Hydrophobic		66	4		658.4961		Neutral and/or hydrophob
inones (pathway unknown)	V Ubiquinone-7	CoQ7		_	Neutral	Hydrophobic			4	+++	726.5587	_	Neutral and/or hydrophob
iquinone biosynthesis	I Ubiquinone-8	CoQ8	+	_	Neutral	Hydrophobic		\rightarrow	4	+	726.5587		Neutral and/or hydrophob
inones (pathway unknown)	V Ubiquinone-9	CoQ9	C01967	+	Neutral	Hydrophobic	_		4	+++	862.6839		Neutral and/or hydrophob
mmon antigen biosynthesis	I UDP-N-acetyl-D-mannosamine	UDP-ManNAc	C01907	-	Nucleotide	Hydrophilic			17 2	+	607.0816	606.0743	
, ,	I UDP-N-acetyl-D-mannosaminouronic acid	UDP-ManNAcUA	C06240	_					18 2	+	621.0608	620.0536	
nmon antigen biosynthesis		UDP-Marinacua UDP-GlcNAc	C00240	+	Nucleotide Nucleotide	Hydrophilic			17 2	+++	607.0816	606.0743	
P-N-acetylglucosamine biosynthesis	UDP-N-acetyl-D-glucosamine					Hydrophilic				+			
otideglycan biosynthesis	I UDP-N-acetylmuramic acid	UDP-MurNaAcA	C01050	-	Nucleotide	Hydrophilic			19 2	+	679.1027	678.0954	
otideglycan biosynthesis	I UDP-N-acetylmuramoyl-L-alanine	UDP-MurNAcAla	C01212		Nucleotide	Hydrophilic			20 2	+	750.1398	749.1325	
otideglycan biosynthesis	I UDP-N-acetylmuramoyl-L-alanyl-D-glutamic acid	UDP-GlcNAcMurAlaGlu	C00692	_	Nucleotide	Hydrophilic		43 5 2		$\perp \perp \perp$	879.1824	878.1751	
A (in vitro)	VI UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-L-lysyl-D-alanyl-D-alanine		C04846	_	Nucleotide	Hydrophilic	40			Ш	1149.3516		Out of the MS range
otideglycan biosynthesis	I UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminoheptanedic acid	UDP-GlcNAcMurAlaGludAHeA	_	-	Nucleotide	Hydrophilic			26 2		1050.2594		Out of the MS range
otidoglycan turnover	II UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminoheptanedioate-D-alanine	UDP-MurNAcAlaGluDAHAla	-	-	Nucleotide	Hydrophilic	38	60 8 2	27 2		1122.3043	1121.2970	Out of the MS range
otideglycan biosynthesis	I UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminoheptanedioate-D-alanyl-D-alanine	UDP-MurNAcAlaGludAHeAlaAla	C04882	_	Nucleotide	Hydrophilic	41	65 9 2	28 2		1193.3414	1192.3342	Out of the MS range
dification of lipid A	I UDP-4-amino-4-deoxy-L-arabinose	UDP-Ara4N	C16153	-	Nucleotide	Hydrophilic	14	22 3 1	15 2		534.0526	533.0453	
O biosynthesis	I UDP-2,3-bis(3-hydroxymyristoyl)glucosamine	UDP-BHMyrGlc	C04652	-	Nucleotide	Hydrophobic	43	77 3 2	20 2		1017.4576	1016.4503	Out of the MS range
dification of lipid A	I UDP-4-(N-formylamino)-4-deoxy-L-arabinose	UDP-Ara4FN	C16156	-	Nucleotide	Hydrophilic	15	22 3 1	16 2	\Box	562.0475	561.0403	
antigen biosynthesis (not in K-12)	VI UDP-D-galacto-1,4-furanose		C03733	-	Nucleotide	Hydrophilic		\rightarrow	17 2	\Box	566.0550	565.0478	
olanic acid biosynthesis	I UDP-galactose	UDP-Gal	C00052	+	Nucleotide	Hydrophilic	_		17 2	++	566.0550	565.0478	
ptideglycan biosynthesis	I UDP-GlcNAc-pyruvateenolether	UDP-GlcNacPvrEE	C04631	-	Nucleotide	Hydrophilic			19 2	+++	677.0871	676.0798	
olanic acid biosynthesis	I UDP-D-glucose	GDP-GIC	C00029	+	Nucleotide	Hydrophilic			17 2	+++	566.0550	565.0478	
		GDP-GICA	C00029							+++	582.0499	581.0427	
olanic acid biosynthesis D biosynthesis	I UDP-D-glucuronic acid I UDP-3- O-(3-hydroxymyristoyl)glucosamine	UDP-HMyrGlc	C06022	+	Nucleotide	Hydrophilic			18 2	+	791.2643		Neutral and/or hydrophol
				_	Nucleotide	Hydrophobic			18 2	+			<u> </u>
O biosynthesis	UDP-3- <i>O</i> -(3-hydroxymyristoyl)- <i>N</i> -acetylglucosamine	UDP-HMyrGlcNAc	C04738	_	Nucleotide	Hydrophobic			19 2	$\perp \perp \perp$	833.2749		Neutral and/or hydrophol
dification of lipid A	I UDP-4-ketopyranose	UDP-Ara40	C16155	-	Nucleotide	Hydrophilic			16 2	ш	533.0210	532.0137	
dification of lipid A	I Undecaprenyl phosphate-4-amino-4-deoxy-L-arabinose	Undecaprenyl-P-Ara4N	C16157	-	Anion	Hydrophobic			7 1	ш	976.7159		Neutral and/or hydrophob
prenoid biosynthesis	I Undecaprenyldiphosphate	UPrPP	C03543	-	Nucleotide	Hydrophobic			7 2	ш	926.6318		Neutral and/or hydrophob
mmon antigen biosynthesis	$I \\ Undecaprenyl- \textit{N}-acetylglucosaminyl- \textit{N}-acetylmannosaminuronate-4-acetamido-4, 6-dideoxy-D-galactosepyrophosphate} \\ I \\ Undecaprenyl- \textit{N}-acetylmannosaminuronate-4$	UnGlcNAcManNAcAAdDGalP		-	Nucleotide	Hydrophobic	79	129 3 2	22 2	Ш	1533.8543	1532.8470	Out of the MS range
mmon antigen biosynthesis	I Undecaprenyl-N-acetylglucosaminyl-N-acetylmannosaminuronatepyrophosphate	UnPGlcNAcManNAcNPP	-	-	Nucleotide	Hydrophobic	71	116 2 1	18 2	Ш	1346.7698	1345.7626	Out of the MS range
mmon antigen biosynthesis	I Undecaprenyl-N-acetyl-α-D-glucosaminylpyrophosphate	UnPrenylGlcNAcPP	C01289	-	Nucleotide	Hydrophobic	63	105 1 1	12 2		1129.7112	1128.7039	Out of the MS range
mmon antigen biosynthesis	I Undecaprenylphosphate	UnPreP	C00348	-	Nucleotide	Hydrophobic	55	91	4 1		846.6655	845.6582	Neutral and/or hydrophob
ptideglycan biosynthesis	I Undecaprenyl-pyrophosphoryl-MurNAc-(pentapeptide)- N-acetylglucosamine	UnPPMurNAcPentaPepNAc	C05898	-	Nucleotide	Hydrophobic	95	156 8 2	28 2		1919.0504	1918.0432	Out of the MS range
lvage of pyrimidine	I Uracil		C00106	+	Cation	Hydrophilic	4	4 2	2		112.0273	113.0346	1
yamine biosynthesis	I Urea		C00086	+	Cation	Hydrophilic	1	4 2	1	\Box	60.0324	61.0396	
antoin degradation	III (S)-Ureidoglycolic acid		C00603	<u> </u>	Anion	Hydrophilic	3	6 2	4	\vdash	134.0328	133.0255	
vage of Ade, HypXan	I Uric acid		C00366	+	Cation	Hydrophilic	5	4 4	3	+++	168.0283	169.0356	
vage of pyrimidine	Uridine		C00299	+	Cation	Hydrophilic	9		6	+++	244.0695	245.0768	
rimidine biosynthesis	I Uridine-5'-diphosphate	UDP	C00277	+	Nucleotide	Hydrophilic			12 2	+	404.0022	402.9949	ļ
	I Uridine-5'-phosphate	UMP	C00015	+			9			+	324.0359	323.0286	
rimidine biosynthesis				·	Nucleotide	Hydrophilic			9 1	$\perp \perp \mid$			ļ
rimidine biosynthesis	Uridine-5'-triphosphate	UTP	C00075	+	Nucleotide	Hydrophilic			15 3	ш	483.9685	482.9613	
to- and siroheme biosynthesis	I Uroporphyrin III		C02469	-	Anion	Hydrophilic	_	\rightarrow	16	ш	828.2126	827.2054	
to- and siroheme biosynthesis	I Uroporphyrinogen-III	UroPorgen-III	C01051	_	Anion	Hydrophilic	_		16	ш	836.2752	835.2680	
ine biosynthesis	I L-Valine	Val	C00183	+	Cation	Hydrophilic			2	$\sqcup \sqcup$	117.0790	118.0863	
vage of Ade, HypXan	I Xanthine		C00385	+	Cation	Hydrophilic			2	\Box	152.0334	153.0407	
vage of Gua, Xan	I Xanthosine		C01762	+	Cation	Hydrophilic	10	12 4	6	шТ	284.0757	285.0830	
rine biosynthesis	I Xanthosine-5-phosphate	XMP	C00655	+	Anion	Hydrophilic	10	13 4	9 1		364.0420	363.0347	
, XTP dephosphorelation	IV Xanthosine-5'-triphosphate	XTP	C00700	+	Nucleotide	Hydrophilic	10	15 4 1	15 3		523.9747	522.9674	
ose degradation	III D-Xylose		C00181	+	Neutral	Hydrophilic	5		5		150.0528		Neutral and/or hydropho
ylose transport	III L-Xylose		C01510	_	Neutral	Hydrophilic			5	+++	150.0528	_	Neutral and/or hydropho
ose degradation	III D-Xylulose		C00310	+	Neutral	Hydrophilic			5	+++	150.0528		Neutral and/or hydrophol
yxose degradation	III L-XVIulose		C00312	<u> </u>	Neutral	Hydrophilic			5	+++	150.0528		Neutral and/or hydropho
entose phosphate pathway (non-oxidative)	I D-Xylulose-5-phosphate	X5P	C00312	+	Anion	Hydrophilic			8 1	+++	230.0192	229.0119	<u> </u>
ncose phosphate pathway (HOH-OXIDALIVE)	III L-Xylulose-5-phosphate	L-X5P	C03291	т	Anion	Hydrophilic	-		8 1	+++	230.0192	229.0119	
corbic acid degradation													

	Class ^a Metabolite	Addreviation	Standard Chemical	Analytical mode ^c	Molecular weight	m/z ^d	Map position	e 0 min	15 min	is shift do 30 min	60 min	Description
Alanine biosynthesis AppppA biosynthesis	I L-Alanine I P(1),P(4)-Bis(5'-adenosyl)tetraphosphate	Ala AppppA	+	Cation Nucleotide	89.0477 836.0483	90.0550 835.0410	C-3 A-1	0.1303 0.0019	0.3287 0.0016	0.3488 0.0009	0.7112 0.0008	
Arginine biosynthesis Arginine biosynthesis	I L-Arginine I L-Argininosuccinic acid	Arg ArgSuccinate	+ +	Cation Cation	174.1117 290.1226	175.1190 291.1299	B-4 B-4	0.1622 0.0057	0.2450 0.0283	0.3125 0.0229	1.0536 0.0349	
Arginine biosynthesis Arginine biosynthesis	I Carbamoylphosphate I L-Citrulline	Carbamoyl-P Citrulline	+ +	Anion Cation	140.9827 175.0957	139.9754 176.1030	C-4 B-4	0.0307	0.2098	ND 0.1315	0.0062	
Arginine biosynthesis Arginine biosynthesis	I N-Acetyl-L-glutamic acid I N-Acetylglutamylphosphate	N-AcGlu N-AcGlu-P	+	Cation Anion	189.0637 269.0301	190.0710 268.0228	C-4	0.0034 UID	0.0176 UID	0.0338 UID	0.0082 UID	
Arginine biosynthesis Arginine biosynthesis	I N-Acetylglutamatesemialdehyde I N-α-Acetylornithine	N-AcGlu-semialdehyde N-AcOrn	- +	Anion Cation	173.0688 174.1004	172.0615 175.1077	C-4	UID 0.9074	UID 2.1800		0.0091	
Arginine biosynthesis Asparagine biosynthesis	I L-Ornithine I L-Asparagine	Ornithine Asn	+	Cation Cation	132.0899 132.0535	133.0972 133.0608	C-4 B-3	0.0658	0.0373	0.0249	0.0043	
Aspartic acid biosynthesis Biotin biosynthesis	L-Aspartic acid T,8-Diaminononanoic acid	Asp 7,8DANA	+	Cation	133.0375 188.1525	134.0448 189.1598	B-3 C-2	0.1074	0.1057	0.1393	0.3255	
Biotin biosynthesis	I 8-Amino-7-oxononanoic acid	8A7ONA	-	Cation	187.1208	188.1281	C-2	UID	UID	UID	UID	
Biotin biosynthesis Biotin biosynthesis	I Biotin I Dethiobiotin	Biotin Dethiobiotin	+	Cation	244.0882	245.0954 215.1390	D-2 C-2	0.1057 0.0126	0.1339	0.1234	0.1201 ND	
Biotin biosynthesis Biotin biosynthesis	I Pimelic acid I Pimeloyl-CoA	Pimelic acid Pimeloyl-CoA	+	Anion Nucleotide	160.0736 909.1782	159.0663 908.1709	C-2 C-2	ND UID	ND	UID	UID	
Biotin biosynthesis Biotin oxidation	I S-Adenosyl-4-methylthio-2-oxobutanoic acid I d-Biotin-d-sulfoxide	SA4MT2OBA BiotinSul	-	Cation Cation	398.1134 260.0831	398.1134 261.0904	C-2 D-2	UID	UID	UID	UID	Including trinary sulfur
CAMP biosynthesis CGMP biosynthesis	I 3',5'-Cyclicadenosine-5'-phosphate I 3',5'-Cyclicguanosine-5'-phosphate	cAMP cGMP	+	Nucleotide Nucleotide	329.0525 345.0474	328.0452 344.0402	A-1 B-1	0.0336 ND	0.0449 ND	0.0446 ND	0.0468 ND	
Cholanic acid biosynthesis Cholanic acid biosynthesis	I α-D-Galactose-1-phosphate I GDP-4-dehydro-6-deoxy-D-mannose	Gal1P GDP-DDMan	+	Anion Nucleotide	260.0297 587.0666	259.0224 586.0593	C-1	0.0273 UID	0.2024 UID	0.1826 UID	0.2002 UID	
Cholanic acid biosynthesis Cholanic acid biosynthesis	I GDP-L-fucose I UDP-D-glucose	GDP-fucose GDP-Glc	+ +	Nucleotide Nucleotide	589.0822 566.0550	588.0750 565.0478	C-1 D-4	ND	ND See U	ND OP-Gal	ND	
Cholanic acid biosynthesis Cholanic acid biosynthesis	I UDP-D-glucuronic acid I GDP-mannose	GDP-GlcA GDP-Man	+	Nucleotide Nucleotide	582.0499 605.0772	581.0427 604.0699	D-4 C-1	ND ND	ND ND		ND ND	
Cholanic acid biosynthesis Cholanic acid biosynthesis	I D-Mannose-1-phosphate I D-Mannose-6-phosphate	Man1P Man6P	+	Anion Anion	260.0297 260.0297	259.0224 259.0224	C-1			Gal1P Gal1P		
Cholanic acid biosynthesis	I UDP-galactose I 3-Deoxy-D-arabinoheptulosonate-7-phosphate	UDP-Gal 3DAH7P	+	Nucleotide Anion	566.0550 288.0246	565.0478 287.0174	D-4 B-2	0.3853	1.3488 0.0155	1.2339 0.0083	2.0746 0.0060	
Chorismic acid biosynthesis	3-Dehydroquinatic acid 3-Dehydroshikimic acid	3DQA 3DSA	_	Anion Anion	190.0500 172.0372	189.0405 171.0299	B-3 B-3	UID	UID	UID	UID	
horismic acid biosynthesis	I 5-Enolpyruvylshikimate-3-phosphate	5EPS3P	-	Anion	324.0246	323.0174	B-3	0.0278	0.0293	0.0359	0.0496	
Chorismic acid biosynthesis	I Shikimate-3-phosphate	Chorismic acid S3P	+	Anion Anion	226.0477 254.0192	225.0405 253.0119	A-3 B-3	UID	0.0076	0.0051	UID	
Chorismic acid biosynthesis CoA biosynthesis	I Shikimic acid I D-4'-Phosphopantothenic acid	Shikimic acid 4'PPA	+	Anion Nucleotide	174.0528 299.0770	173.0455 298.0697	B-3 D-2	UID	UID	UID	UID	
oA biosynthesis oA biosynthesis	I 4'-Phospho- <i>N</i> -pantothenoylcysteine I Coenzyme A	4'PPC CoA	+	Nucleotide Nucleotide	402.0862 767.1152	401.0789 382.5503	D-2 D-2	0.2960	UID 0.3911	0.1867	UID 0.4736	Detected as divalent ion in MS
oA biosynthesis oA biosynthesis	I Dephospho-CoA I Pantetheine-4'-phosphate	dePCoA P4'P	+	Nucleotide Nucleotide	687.1489 358.0964	686.1416 357.0891	D-2 D-2	0.0027 0.0065	0.0024 0.0071	0.0011 0.0053	0.0025 0.0081	
Common antigen biosynthesis Common antigen biosynthesis	I dTDP-4-acetamido-4,6-dideoxy-D-galactose I dTDP-D-fucosamine	dTDP-AADDGal dTDP-FAN	_	Nucleotide Nucleotide	589.1074 547.0968	588.1001 546.0896	D-2	0.0032 UID	0.0059 UID	0.0057 UID	0.0122 UID	
Common antigen biosynthesis	UDP-N-acetyl-D-mannosamine UDP-N-acetyl-D-mannosaminouronic acid	UDP-ManNAc UDP-ManNAcUA	-	Nucleotide Nucleotide	607.0816	606.0743		UID		-GlcNAc	UID	
ysteine biosynthesis ysteine biosynthesis	1 O-Acetyl-L-serine 1 L-Cysteine	AcSer Cys	+++++++++++++++++++++++++++++++++++++++	Cation	147.0532 121.0198	148.0604 122.0270	C-3	0.0278 ND	0.0173 ND	0.0498	ND ND	
ITDP-rhamnose biosynthesis	I dTDP-4-dehydro-6-deoxy-D-glucose	dTDP-DDGlc	-	Nucleotide	546.0652 546.0652	545.0579	C-1 D-1	UID	UID	UID	UID	
ITDP-rhamnose biosynthesis ITDP-rhamnose biosynthesis	I dTDP-4-dehydro-6-deoxy-L-mannose I dTDP-D-glucose	dTDP-DDMan dTDP-Glc	+	Nucleotide Nucleotide	564.0758	545.0579 563.0685	C-1	0.0034	0.0063	0.0051	0.0050	
ITDP-rhamnose biosynthesis Intner-Doudoroff pathway	I dTDP-α-L-rhamnose I 2-Keto-3-deoxy-6-phosphogluconic acid	dTDP-Rhm KDPGlcA	_	Nucleotide Anion	548.0808 258.0141	547.0736 257.0068	D-1 C-2	0.3977 UID	0.5828 UID		0.5994 UID	
atty acid biosynthesis ormyltetrahydrofolic acid biosynthesis	I Malonyl-CoA I 5,10-Methylene-THF	Malonyl-CoA 5,10MeL-THF	+	Nucleotide Cation	853.1156 457.1710	403.5556 458.1783	B-3 D-1	ND UID	ND UID	UID	UID	Detected as acetyl-CoA in MS
formyltetrahydrofolic acid biosynthesis formyltetrahydrofolic acid biosynthesis	I 5,10-Methenyl-THF I 5-Methyl-THF	5,10Me-THF Me-THF	+	Cation Cation	457.1704 459.1866	457.1704 460.1939	D-1 D-1	UID ND	UID		UID	Including quarternary amine
ravin biosynthesis ravin biosynthesis	I 2,5-Diamino-6-(ribosylamino)-4-(3H)-pyrimidinone-5'-phosphate I 3,4-Dihydroxy-2-butanone-4-phosphate	2,5DA6RA4P5P 3,4D2B4P	-	Anion Anion	353.0737 184.0137	352.0664 183.0064	B-2 A-2	UID	UID		UID	
ravin biosynthesis ravin biosynthesis	I 5-Amino-6-(5'-phosphoribosylamino)uracil I 5-Amino-6-(5'-phosphoribitylamino)uracil	5A6-5'PRAU 5A6-5'PRbAU	_	Anion Anion	354.0577 356.0733	353.0504 355.0660	B-2 B-2	UID	UID		UID	
ravin biosynthesis	I 5-Amino-6-ribitylamino-2,4(1H,3H)-pyrimidinedione I 6,7-Dimethyl-8-(1-D-ribityl)lumazine	5A6RbA2,4PD 6,7D81RbL	-	Cation Anion	276.1070 326.1226	277.1143 325.1154	A-2 B-2	UID	0.0019 UID	0.0014 UID	0.0027 UID	
ravin biosynthesis	I Flavinadeninedinucleotide (oxidized form) I Flavinadeninedinucleotide (reduced form)	FAD FADH ₂	+	Nucleotide Nucleotide	785.1571 787.1728	391.5713 786.1655	B-2 A-2	0.0011 UID	0.0013 UID	0.0007 UID	0.0007 UID	Detected as divalent ion in MS
ravin biosynthesis	Flavinmononucleotide (voidized form)	FMN FMNH ₂	+	Nucleotide Nucleotide	456.1046 458.1203	455.0973 457.1130	B-2 B-2	0.0062 UID	0.0088 UID	0.0030	0.0056 UID	
ravin biosynthesis	I Riboflavin	Riboflavin	+	Cation	376.1383 147.0532	377.1456	B-2 C-4	ND	ND	ND	ND	
Glutamic acid biosynthesis Glutamine biosynthesis	I L-glutamic acid I L-Glutamine	Glu Gln	+	Cation	146.0691	148.0604	C-4	3.2033 0.2763	8.8863 0.1228	7.8141 0.3678	9.3902 0.5476	
Glutathione biosynthesis Glutathione biosynthesis	I L-γ-Glutamylcysteine I Glutathione (reduced form)	GluCys GSH	+	Cation	250.0623 307.0838	251.0696 308.0911	C-3	0.0096 5.6358	0.0210 2.9306	0.0147 1.5100	7.3357	
Glutathione biosynthesis Glutathionylspermidine metabolism	I Glutathione (oxidized form) I Glutathionylspermidine	GSSG GSH-spermidine	+	Cation Cation	612.1520 434.2311	307.0833 435.2384	D-3 D-3	0.0236 0.0007	0.0187 UID	0.0196 UID	UID	Detected as divalent ion in MS
Glycine biosynthesis Glycogen biosynthesis	I Glycine I ADP-D-glucose	Gly ADP-Glc	+	Cation Nucleotide	75.0320 589.0822	76.0393 588.0750	C-2	0.1901 ND	0.2894 ND	0.2619 ND	0.4944 ND	
Glycogen biosynthesis Glycolysis (Embden-Meyerhof-Parnas)	I α-D-Glucose-1-phosphate I 1,3-Diphosphateglyceric acid	G1P 1,3-DPG	+ +	Anion Anion	260.0297 265.9593	259.0224 264.9520	C-2	ND ND	ND ND		ND ND	
Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas)	2-Phosphoglyceric acid 3-Phosphoglyceric acid	2-PG 3-PG	+	Anion Anion	185.9929 185.9929	184.9857 184.9857	C-3	0.1180	See 0.1270	3PG 0.0759	0.0764	
Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas)	I Dihydroxyacetonephosphate I D-Fructose-1,6-diphosphate	DHAP F1,6P	+	Anion Anion	169.9980 339.9961	168.9908 338.9888	C-2	ND 0.0129	0.0150	0.0136	0.0012	
Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas)	D-Fructose-6-phosphate D-glyceraldehyde-3-phosphate	F6P G3P	+ +	Anion Anion	260.0297 169.9980	259.0224 168.9908	C-2	ND ND	0.0142	ND 0.0136	0.0016	
Glycolysis (Embden-Meyerhof-Parnas)	I α-D-Glucose-6-phosphate	G6P	+	Anion	260.0297	259.0224	C-2	0.0273	0.2024	0.1826	0.2002	
Glycolysis (Embden-Meyerhof-Parnas) Glycolysis (Embden-Meyerhof-Parnas)	I Phosphoenolpyruvic acid I Pyruvic acid	PEP Pyruvic acid	+	Anion Anion	167.9824 88.0160	166.9751 87.0088	C-3	0.0314	0.0418 ND		0.0279 ND	
Glyoxylic acid pathway Histidine biosynthesis	I Glyoxylic acid I D-Erythroimidazoleglycerolphosphate	Glyoxylic acid EIGP	+	Anion Nucleotide	74.0004 238.0355	72.9931 237.0282	C-3 A-2	ND UID	ND	0.0371	0.1594	
Histidine biosynthesis Histidine biosynthesis	I L-Histidine I L-Histidinol	His Histidinol	+	Cation Cation	155.0695 141.0902	156.0768 142.0975	B-1 B-1	3.5663 ND	0.4468 0.0165	0.0197 0.1116	0.0095 1.4940	
Histidine biosynthesis Histidine biosynthesis	I L-Histidinolphosphate I Imidazoleacetolphosphate	Histidinol-P IAP	_	Nucleotide Nucleotide	221.0565 220.0249	220.0493 219.0176	B-2 B-2	UID	UID		0.0122 0.0456	
listidine biosynthesis listidine biosynthesis	I Phosphoribosyl-AMP I Phosphoribosyl-ATP	PR-AMP PR-ATP	_	Nucleotide Nucleotide	559.0717 719.0043	558.0644 717.9971	A-2 B-2	UID	UID		0.0009 UID	
listidine biosynthesis listidine biosynthesis	I Phosphoribosylformimino-AlCAR-phosphate I Phosphoribulosylformimino-AlCAR-phosphate	PRFAP PRuFAP	_	Nucleotide Nucleotide	577.0822 577.0822	576.0750 576.0750	A-2 A-2	UID	0.0006	0.0051 RFAP	0.0039	
Homoserine biosynthesis	I L-Aspartyl-4-phosphate I L-Aspartatesemialdehyde	Asp-P AspSA	_	Anion Cation	213.0038 117.0426	211.9966 118.0499	B-3 B-3	UID	UID	UID	UID	
lomoserine biosynthesis	I L-Homoserine	HomoSer	+	Cation	119.0582	120.0655	A-3	0.0714	0.0461	0.0342	0.0173	
norganic metabolite norganic metabolite	I Orthophosphate I Pyrophosphate	PPi	+	Anion Anion	177.9432	96.9696 176.9360	D-1 D-1	0.0219	0.0602	1.1999 0.0416	0.0309	
soleucine biosynthesis	I 2,3-Dihydroxy-3-methylvaleric acid I 2-Aceto-2-hydroxybutyric acid	2,3DH3MVA 2A2HBA	-	Anion Anion	148.0736 146.0579	147.0663 145.0506	A-4 A-4	0.0150	0.0134	0.0150	0.0109	
oleucine biosynthesis oleucine biosynthesis	I 2-Keto-3-methylvaleric acid I 2-Oxobutanoic acid	2K3MVA 2-OBA	+	Anion Anion	130.0630 102.0317	129.0557 101.0244	A-4 A-4	ND ND	ND ND	ND	ND ND	
oleucine biosynthesis opentenyldiphosphate biosynthesis	I L-Isoleucine I Dimethylallylpyrophosphate	Ile DMAProP	+	Cation Anion	131.0946 246.0058	132.1019 244.9986	A-4	0.0952 ND	0.0210 ND	ND	0.1233 ND	
opentenyldiphosphate biosynthesis opentenyldiphosphate biosynthesis	I 1-Hydroxy-2-methyl-2-(<i>E</i>)-butenyl-4-diphosphate I Δ3-lsopentenyldiphosphate	HMeBuPP IPPP	-	Anion Anion	262.0007 246.0058	260.9935 244.9986	C-3	UID	0.0094 UID	0.0107 UID	0.0129 UID	
opentenyldiphosphate biosynthesis opentenyldiphosphate biosynthesis	1 2-C-Methyl-D-erythritol-2,4-cyclodiphosphate 1 2-C-Methyl-D-erythritol-4-phosphate	MeEry2,4CP MeEry4P	-	Anion Anion	277.9957 216.0399	276.9884 215.0326	C-2	0.0093 UID	0.0240 UID	0.0255 UID	0.0387 UID	
opentenyldiphosphate biosynthesis opentenyldiphosphate biosynthesis	I 4-Diphosphocytidyl-2- C -methylerythritol I 4-Diphosphocytidyl-2- C -methylerythritol-2-phosphate	PPCytMeEry PPCytMeEryP	-	Nucleotide Nucleotide	521.0812 601.0475	520.0739 600.0402		UID	UID		UID	
DO biosynthesis DO biosynthesis	D-Arabinose-5-phosphate CMP-3-deoxy-D-mannooctulosonic acid	Ara5P CMP-DManOA	+	Anion Nucleotide	230.0192 543.1102	229.0119 542.1029	B-2	0.0274 UID	0.0080 UID	0.0089	ND	
DO biosynthesis DO biosynthesis DO biosynthesis	CMP-3-deoxy-D-mannooctulosonic acid 3-Deoxy-D-mannooctulosonic acid 3-Deoxy-D-mannooctulosonate-8-phosphate	DManOA DManOP	_	Anion	238.0689 318.0352	237.0616 317.0279		UID	UID	UID	UID	
actic acid fermentation	I L-Lactic acid	Lactic acid	-	Anion	90.0317	89.0244	C-3	0.7079	0.9533	0.6650	0.5742	
eucine biosynthesis eucine biosynthesis	2-Isopropyl-3-oxosuccinic acid 2-Isopropylmalic acid	2IP3OSA 2IPMA	+	Anion Anion	174.0528 176.0685	173.0455 175.0612	C-4 C-3	0.3659	0.0331	0.0221	ND	
eucine biosynthesis eucine biosynthesis	I 2-Ketoisocaproic acid I 3-Isopropylmalic acid	2KICA 3IPMA	+	Anion Anion	130.0630 176.0685	129.0557 175.0612	C-4 C-3	0.0222 UID	0.0546	0.0225	0.0165 UID	
eucine biosynthesis ysine biosynthesis	I L-Leucine I L-2,3,4,5-Tetrahydrodipicolinic acid	Leu 2,3,4,5-THDPA	+	Cation Anion	131.0946 171.0532	132.1019 170.0459	C-4 B-3	0.0705 UID	0.9572 UID	0.6944 UID	0.9460 UID	
ysine biosynthesis ysine biosynthesis	I L-2,3-Dihydrodipicolinic acid I L,L-Diaminopimelatic acid	2,3-DPA DPA	- +	Anion Anion	169.0375 190.0954	168.0302 189.0881	B-3 A-3	UID 0.0882	UID 0.2606	UID 0.1490	UID 0.0661	
ysine biosynthesis ysine biosynthesis	L-Lysine I meso-Diaminopimelic acid	Lys meso-DPA	+	Cation	146.1055 190.0954	147.1128	A-3 A-3	0.5240	10.5664 See	9.0975	8.9085	
			_	Anion					200			

Menaquinone biosynthesis	I	1,4-Dihydroxy-2-naphthoic acid	1,4DHNaphA	+	Anion	204.0423	203.0350	A-4	ND	ND	ND	ND	
Menaquinone biosynthesis Menaquinone biosynthesis	l I	Isochorismic acid O-Succinylbenzoic acid	Isochorismic acid OSucBA	- 1	Anion Anion	226.0477 222.0528	225.0405 221.0455	A-3 A-3	UID UID	UID UID	UID	UID	
Menaquinone biosynthesis Menaquinone biosynthesis	- I - I	O-Succinylbenzoyl-CoA 2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylic acid	OSucB-CoA SucCycHexCA		Nucleotide Anion	971.1575 240.0634	970.1502 239.0561	A-4 A-3	UID UID	UID UID	UID	UID	
Methionine biosynthesis Methionine biosynthesis	I 	5-Methyltetrahydropteroyltri-L-glutamic acid Cystathionine	5MTHTGlu Cystathionine	_	Cation Cation	640.2453 222.0674	641.2525 223.0747	A-3 A-3	UID 0.0091	UID 0.0120	0.0060	UID	
Methionine biosynthesis Methionine biosynthesis	 	Homocysteine L-Methionine	HomoCys Met	+	Cation Cation	135.0354 149.0511	136.0427 150.0583	A-3 A-4	0.0054 0.0371	0.0066 0.0724	0.0080 0.0654	0.0048 0.0605	
Methionine biosynthesis Methionine biosynthesis	I	O-Succinyl-L-homoserine Tetrahydropteroyltri-L-glutamic acid	SucHomoSer THPTGlu	+	Cation Cation	219.0743 626.2296	220.0816 627.2369	A-3 A-3	0.0379 UID	0.0714 UID	0.0613 UID	0.0079 UID	
Methylglyoxal pathway	1	L-Methionine sulfoxide D-Lactic acid	MetSFX D-Lactic acid	+	Cation	165.0460 90.0317	166.0532 89.0244	A-4	0.0017	0.0032 See Lac		0.0031	
Methylglyoxal pathway Modification of lipid A	1	S-Lactoylglutathione 4-Amino-4-deoxy-L-arabinose	SL-GSH Ara4N	+	Cation	379.1049 149.0688	380.1122 150.0761	D-2	0.0076 UID UID	0.0092 UID	0.0075 UID	0.0144 UID UID	
Modification of lipid A Modification of lipid A Modification of lipid A	I	UDP-4-(<i>N</i> -formylamino)-4-deoxy-L-arabinose UDP-4-amino-4-deoxy-L-arabinose UDP-4-ketopyranose	UDP-Ara4FN UDP-Ara4N UDP-Ara4O	-	Nucleotide Nucleotide Nucleotide	562.0475 534.0526 533.0210	561.0403 533.0453 532.0137		UID	UID UID UID	UID UID UID	UID	
Molybdopterin biosynthesis Molybdopterin biosynthesis	1	Molybdopterin formA Molybdopterin formA-GMP	Mol-form A Mol-form A-GMP		Anion Nucleotide	326.0290 671.0765	325.0218 670.0692		UID	UID	UID	UID	
Molybdopterin biosynthesis Molybdopterin biosynthesis	1 1	Molybdopteringuaninedinucleotide Molybdopterin	MolGDN Molybdopterin	_	Nucleotide Anion	738.0441 395.0123	737.0368 394.0050		UID	UID	UID	UID	
Molybdopterin biosynthesis NAD biosynthesis	 	Precursor-Z Deamido-NAD	Precousor-Z Deamido-NAD	-+	Cation Nucleotide	345.0474 665.1004	346.0547 663.0859	B-4	UID ND	UID 0.0008	UID 0.0007	UID 0.0008	Including quarternary amine
NAD biosynthesis NAD biosynthesis	1 	Iminoaspartic acid Nicotinamideadeninedinucleotide (reduced form)	Iminoaspartic acid NAD*	+	Cation Nucleotide	131.0219 664.1164	132.0291 662.1019	B-3 B-4	UID 0.4564	UID 0.6664	UID 0.5548	UID 0.6989	Including quarternary amine
NAD biosynthesis NAD biosynthesis	I 	Nicotinamideadeninedinucleotide (oxidized form) Nicotinamideadeninedinucleotidephosphate (reduced form)	NADH NADP⁺	+	Nucleotide Nucleotide	665.1248 744.0827	664.1175 742.0682	B-4 B-4	0.0032 0.1046	0.0038 0.1730	0.0027 0.1382	0.0023 0.1543	Including quarternary amine
NAD biosynthesis NAD biosynthesis	I	Nicotinamideadeninedinucleotidephosphate (oxidized form) Nicotinatenucleotide	NADPH Nicotinatenucleotide	+	Nucleotide Nucleotide	745.0911 336.0484	371.5383 334.0339	B-4 B-4	0.0086 ND	0.0151 ND	0.0113 ND	ND	Detected as divalent ion in MS Including quarternary amine
NAD biosynthesis Pantothenic acid biosynthesis	1	Quinolinic acid 2-Dehydropantoic acid	Quinolinic acid 2DHPA	+	Anion Anion	167.0219 146.0579	166.0146 145.0506	B-3 D-3	0.0150	0.0090	0.0150	0.0072	
Pantothenic acid biosynthesis Pantothenic acid biosynthesis	1	B-Alanine L-Pantoic acid	β-Ala Pantoic acid	+	Cation Anion	89.0477 148.0736	90.0550	D-3	UID	UID	UID	UID	
Pantothenic acid biosynthesis Pentose phosphate pathway (non-oxidative) Pentose phosphate pathway (non-oxidative)	I	Pantothenic acid D-Erythrose-4-phosphate D-Ribose-5-phosphate	Pantothenic acid E4P R5P	+ + +	Anion Anion Anion	219.1107 200.0086 230.0192	218.1034 199.0013 229.0119	D-2 B-2 B-2	0.0207 0.0014 ND	0.0134 0.0058 0.0061	0.0139 0.0057 0.0089	0.0216 0.0024 0.0069	
Pentose phosphate pathway (non-oxidative)	L	D-Sedoheptulose-7-phosphate	S7P X5P	- +	Anion	290.0403	289.0330	B-2 B-2	0.0100 ND	0.0308 ND	0.0089 0.0293 ND	0.0069 0.0299 ND	
Pentose phosphate pathway (non-oxidative) Pentose phosphate pathway (oxidative) Pentose phosphate pathway (oxidative)	1	D-Xylulose-5-phosphate 6-Phospho-D-gluconic acid D-Glucono-\(\text{-lactone-6-phosphate}\)	6-PG GlcnL6P	+	Anion Anion Anion	230.0192 276.0246 258.0141	229.0119 275.0174 257.0068	B-2 B-2	0.0014 UID	0.0159 UID	0.0157 UID	0.0122 UID	
Pentose phosphate pathway (oxidative) Pentose phosphate pathway (oxidative) Peptideglycan biosynthesis	 	D-Ribulose-5-phosphate D-Alanyl-D-alanine	Ru5P AlaAla	+	Anion	230.0192 160.0848	229.0119 161.0921	B-2 B-2 D-2	0.0214 0.2194	0.0080 0.1643	0.0116 0.1755	0.0145 0.5799	
Peptideglycan biosynthesis Peptideglycan biosynthesis Peptideglycan biosynthesis	1 1	D-Ataniye-D-atanine L-alanyl-D-glutamyl- <i>meso</i> -A2pm D-Atanine	AlaGluA2pm D-Ala	- +	Cation	390.1751 89.0477	391.1823 90.0550	D-2 D-2	UID	UID See	0.0035	0.0065	
Peptideglycan biosynthesis Peptideglycan biosynthesis	I	D-Glutamic acid UDP-N-acetylmuramoyl-L-alanyl-D-glutamic acid	D-Glu UDP-GlcNAcMurAlaGlu	+	Cation Nucleotide	147.0532 879.1824	148.0604 878.1751		UID	See UID		UID	
Peptideglycan biosynthesis Peptideglycan biosynthesis	I	UDP-GlcNAc-pyruvateenolether UDP-N-acetylmuramic acid	UDP-GlcNacPyrEE UDP-MurNaAcA	_	Nucleotide Nucleotide	677.0871 679.1027	676.0798 678.0954	D-2	UID 0.0682	UID 0.0912	UID 0.0630	UID 0.0548	
Peptideglycan biosynthesis Phenylalanine biosynthesis	I I	UDP- <i>N</i> -acetylmuramoyl-L-alanine L-Phenylalanine	UDP-MurNAcAla Phe	+	Nucleotide Cation	750.1398 165.0790	749.1325 166.0863	A-3	UID 0.1028	UID 0.4073	UID 0.3727	UID 0.7846	
Phenylalanine biosynthesis Polyamine acetylation	I	Phenylpyruvic acid N^1 -Acetylspermidine	Phenylpyruvic acid N1AcSpermidine	+	Anion Cation	164.0473 187.1685	163.0401 188.1757	A-3 A-4	ND 0.0354	0.0161 0.0276	0.0098 0.0172	0.0069 0.0352	
Polyamine acetylation Polyamine acetylation	- I - I	<i>N</i> ¹ -Acetylspermine Spermine	N1AcSpermine Spermine	+	Cation Cation	244.2263 202.2157	245.2336 203.2230	A-4 A-4	ND ND	ND ND	ND ND		
Polyamine biosynthesis Polyamine biosynthesis	- I	Agmatine S-Adenosylmethioninamine	Agmatine dAdoMet	+	Cation Cation	130.1218 355.1552	131.1291 355.1552	B-4 A-4	0.0014 UID	0.0126 0.0111	0.0125 UID		Including trinary sulfur
Polyamine biosynthesis Polyamine biosynthesis	I	5'-Methylthioadenosine Putrescine	MTA Putrescine	+	Cation Cation	297.0896 88.1000	298.0968 89.1073	A-4 B-4	0.1223 1.5761	0.2122 1.2554	0.2002 1.2431	0.3119 1.2192	
Polyamine biosynthesis Polyamine biosynthesis	 	Spermidine Urea	Spermidine Urea	+	Cation	145.1579 60.0324	146.1652 61.0396	A-4 B-4	0.0229	0.0334	0.0351	0.0482	
ppGpp biosynthesis ppGpp biosynthesis	1	Guanosine-5'-diphosphate, 3'-diphosphate Guanosine-3'-diphosphate-5'-triphosphate	ppGpp pppGpp	+	Nucleotide Nucleotide	602.9570 682.9233	601.9497 681.9161	B-1 B-1	UID	0.0163 UID	0.0047 UID	0.0116 UID	
Prephenic acid biosynthesis Proline biosynthesis	I	Prephenic acid L-Glutamate-5-phosphate L-Glutamate-γ-semialdehyde	Prephenic acid Glu-5-P	-	Anion Anion Cation	226.0477 227.0195 131.0582	225.0405 226.0122 132.0655	A-3 C-4 C-4	UID UID	ND UID UID	UID UID	UID UID	
Proline biosynthesis Proline biosynthesis Proline biosynthesis	1	L-Proline L-A1-pyroline-5-carboxylic acid	Glu-semialdehyde Pro Pyrroline-5-carboxylate	+	Cation	115.0633 113.0477	116.0706 112.0404	B-4 C-4	0.0245 ND	0.1245 ND	0.0520 ND	0.0531 ND	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	1	5-Aminolevulinic acid Coproporphyrinogen III	5-Aminolevulinic acid CoPorgen III	+	Cation Anion	131.0582	132.0655 659.3086	C-4	ND UID	ND UID	ND UID	ND UID	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	I I	Glutamate-1-semialdehyde Hydroxymethylbilane	GluSA HMB	_	Cation Anion	131.0582 854.2858	132.0655 853.2785	C-4	UID	UID	UID	UID	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	 	Protoporphyrin IX Porphobilinogen	Por IX Porphobilinogen	+	Anion Cation	562.2580 226.0954	561.2507 227.1026	C-4	ND 0.0077	ND 0.0084	ND 0.0104	ND 0.0084	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	I I	Precorrin-1 Precorrin-2	Precorrin-1 Precorrin-2	_	Anion Anion	850.2909 864.3065	849.2836 863.2993		UID UID	UID UID	UID	UID	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	- I	Protoheme IX Protoporphyrinogen IX	Protoheme IX Protoporphyrinogen IX		Anion Anion	614.1616 564.2737	613.1544 563.2664	C-4	0.8815 UID	0.4759 UID	0.2597 UID	UID	Detected as divalent ion in MS
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	1	S-Adenosylhomocysteine Siroheme	SAHC Siroheme	+	Cation Anion	384.1216 916.2102	385.1289 915.2029	C-4 C-4	UID	ND UID	UID	UID	
Proto- and siroheme biosynthesis Proto- and siroheme biosynthesis	I	Sirohydrochlorin Uroporphyrinogen-III	Sirohydrochlorin UroPorgen-III	_	Anion Anion	862.2909 836.2752	861.2836 835.2680		UID	UID	UID	UID	
Proto- and siroheme biosynthesis PRPP biosynthesis PRPP biosynthesis	I	Uroporphyrin III 5-Phosphoribosyldiphosphate D-Ribose-1,5-diphosphate	Uroporphyrin III PRPP R1,5P	+	Anion Nucleotide Nucleotide	828.2126 389.9518 309.9855	827.2054 388.9445 308.9782	B-2 B-2	UID ND 0.0157	0.0252 0.0295	0.0121 0.0203	0.0137 0.0089	
Purine biosynthesis Purine biosynthesis	1	Adenosine-5'-diphosphate Aminoimidazole carboxamide ribonucleotide	ADP AICAR	+	Nucleotide Nucleotide	427.0294 338.0628	426.0221 337.0555	A-1 A-1	0.2736 ND	0.0293 0.4401 0.0013	0.0203 0.3575 0.0080	0.2055 0.0100	
Purine biosynthesis Purine biosynthesis	1	5-Aminoimidazoleribonucleotide Adenine-5'-phosphate	AIR AMP	-+	Nucleotide Nucleotide	295.0569 347.0631	294.0497 346.0558	A-2 A-1	UID 0.0769	UID 0.0643	UID 0.0607	UID 0.0523	
Purine biosynthesis Purine biosynthesis	1	Adenylosuccinic acid Adenosine-5'-triphosphate	ASA ATP	+	Nucleotide Nucleotide	449.0584 506.9958	448.0511 505.9885	A-1 A-1	ND 0.5021	ND 2.2443	ND 1.5756	ND 0.7624	
Purine biosynthesis Purine biosynthesis	- I - I	5-Phosphoribosyl-4-carboxy-5-aminoimidazole Deoxyadenosine-5-diphosphate	CAIR dADP	+	Nucleotide Nucleotide	339.0468 411.0345	338.0395 410.0272	A-1 A-1	UID 0.0313	UID 0.0293	UID 0.0316	UID 0.0236	
Purine biosynthesis Purine biosynthesis	I	Deoxyadenine-5'-triphosphate Phosphoribosylformamidocarboxamide	dATP FAICAR	+	Nucleotide Nucleotide	491.0008 366.0577	489.9936 365.0504	A-1 A-1	0.0519 UID	0.1308 UID	0.1210 UID	0.0844 UID	
Purine biosynthesis Purine biosynthesis	I	5-Phosphoribosyl- <i>N</i> -formylglycineamidine 5-Phosphoribosyl- <i>N</i> -formylglycineamide	FGAM FGAR	-	Nucleotide Nucleotide	313.0675 314.0515	312.0602 313.0442	A-2 A-2	0.0028 UID	0.0044 0.0019	0.0017 0.0036	UID 0.0015	
Purine biosynthesis Purine biosynthesis	1 1	5-Phosphoribosylglycineamide Guanosine-5'-diphosphate	GAR GDP	-+	Nucleotide Nucleotide	286.0566 443.0243	285.0493 442.0171	A-2 B-1	0.0630	UID 0.0938	0.1106	0.0921	
	İ	and the same of th	C::-		** *	2.00	143 0507	B-1	0.0055	0.0058	0.0078	0.0064 0.2215	
Purine biosynthesis Purine biosynthesis	1	Guanine-5'-phosphate Guanosine-5'-triphosphate	GMP GTP	+	Nucleotide Nucleotide	363.0580 521.9828	362.0507 520.9756	B-1	0.0682		0.3277		ĺ
Purine biosynthesis Purine biosynthesis Purine biosynthesis Purine biosynthesis	1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate N°-Carboxyaminoimidazoleribonucleotide	GTP IMP N5-CAIR	+ + + -	Nucleotide Nucleotide Nucleotide	521.9828 348.0471 338.0389	520.9756 347.0398 337.0317	A-1 A-2	ND UID	ND UID	ND UID	UID	
Purine biosynthesis Purine biosynthesis Purine biosynthesis Purine biosynthesis Purine biosynthesis Purine biosynthesis	ı	Guanosine-5'-triphosphate Inosine-5'-phosphate N*3-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosylamine 5'-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole	GTP IMP N5-CAIR PRA SAICAR	+ + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737	520.9756 347.0398 337.0317 228.0279 453.0664	A-1 A-2 A-2 A-1	ND UID UID UID	ND UID UID UID	UID UID UID	UID UID UID	
Purine biosynthesis	ı	Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosylamine 5'-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide	+ + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553	A-1 A-2 A-2 A-1 B-1 B-4	UID UID UID 0.0026 0.1195	ND UID UID UID 0.0053 0.1726	UID UID UID 0.0044 0.1313	UID UID UID 0.0038 0.1825	
Purine biosynthesis	1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate N ⁵ -Carboxyaminoimidazoleribonucleotide 5-Phosphoribosylamine 5'-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate	GTP IMP N5-CAIR PRA SAICAR XMP	+ + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347	A-1 A-2 A-2 A-1 B-1	UID UID UID 0.0026	ND UID UID UID 0.0053	UID UID UID 0.0044 0.1313	UID UID UID 0.0038 0.1825 ND	Including quarternary amine
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling	1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-triphosphate N5-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN	+ + + - - - + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3	ND UID UID UID 0.0026 0.1195 ND	ND UID UID UID 0.0053 0.1726 ND	ND UID UID UID 0.0044 0.1313 ND	UID UID UID 0.0038 0.1825 ND	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10°-phosphate biosynthesis Pyridoxal-11'-phosphate biosynthesis	1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate N³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5*P Pyn5*P	+ + + + + + + -	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Anion Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3 C-1 D-1	ND UID UID UID 0.0026 0.1195 ND ND ND	ND UID UID 0.0053 0.1726 ND ND 0.0129	ND UID UID 0.0044 0.1313 ND ND 0.0074	UID UID 0.0038 0.1825 ND ND 0.0161	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10°-phosphate biosynthesis Pyridoxal-11°-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis	1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinic acid Nicotinic acid Nicotiniamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5'P Pyn5'P 1AP203P 3H4PHKBA	+ + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Anion Anion Anion Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728	A-1 A-2 A-2 A-1 B-1 B-4 B-3 C-1 D-1 C-1	ND UID UID 0.0026 0.1195 ND ND UID UID	ND UID UID 0.0053 0.1726 ND ND 0.0129 UID UID	ND UID UID UID 0.0044 0.1313 ND ND 0.0074 UID UID UID UID UID UID	UID UID 0.0038 0.1825 ND 0.0161 UID UID	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridone nucleotide cycling Pyridoxal-10°-phosphate biosynthesis Pyridoxal-5°-phosphate biosynthesis Pyridoxal-6°-phosphate biosynthesis Pyridoxal-6°-phosphate biosynthesis Pyridoxal-8°-phosphate biosynthesis Pyridoxal-9°-phosphate biosynthesis Pyridoxal-9°-phosphate biosynthesis Pyridoxal-9°-phosphate biosynthesis Pyridinie biosynthesis	1 1 1 1 1 1 1 1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinic acid Nicotinamide D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate 1-Aminopropane-2-one-3-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-1-aspartic acid Cytidine-5'-diphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5'P Pyn5'P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP	+ + + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.0242 214.0243 214.0243 214.0243 214.0343 403.0182	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3 C-1 D-1 C-1 C-1 C-1 C-1 C-4 D-4	ND UID UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID 0.0044 0.1313 ND ND UID UID UID UID UID UID UID UID UID 0.2897	UID UID UID UID UID UID 0.0038 0.1825 ND ND 0.0161 UID UID UID UID UID UID UID 0.1006 0.0819	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-11'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-8'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis	1 1 1 1 1 1 1 1 1 1 1	Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Cytidine-5'-triphosphate Cytidine-5'-triphosphate Cytidine-5'-triphosphate Deoxycitidine-5'-diphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5-P Pyn5-P 1AP2O3P 3H4PHKBA 1DX5-P Ery4-P PHThr Carbamoyl-Asp CDP CTP dCDP	+ + + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9929 386.0160	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3 C-1	ND UID UID UID O.0026 0.1195 ND ND UID UID UID UID UID UID UID UID 0.01110 0.0822 0.1321	ND UID UID UID UID 0.0053 0.1726 ND ND UID UID UID UID UID UID UID UID 0.1128 0.0435 0.1656 0.0080	ND UID UID 0.0044 0.1313 ND ND UID UID UID UID UID UID UID UID 0.2897 0.0512 0.1694 0.0088	UID UID UID UID 0.0038 0.1825 ND ND UID UID UID UID UID UID 0.1006 0.0819 0.2889 0.0081	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-7'-phosphate biosynthesis Pyridoxal-8'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate Pyridoxine-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-a-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Cytidine-5'-diphosphate Deoxycytidine-5'-triphosphate Deoxycytidine-5'-triphosphate Deoxycytidine-5'-triphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydroorotic acid	+ + + - - - + + + + - - - - - - - - - -	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.929 487.9980 157.0255	A-1 A-2 A-2 A-1 B-4 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-4	ND UID UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0195 ND	ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID 0.0044 0.1313 ND ND 0.0074 UID UID UID UID UID UID 0.2897 0.0512 0.1694 0.0088 0.0313 0.0595	UID	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10°-phosphate biosynthesis Pyridoxal-11°-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-8'-phosphate biosynthesis Pyridoxal-9-phosphate biosynthesis Pyridoxal-9-phosphate biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4'-(N-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid -phidoxy-5-phosphate 1-Aminopropane-2-one-3-phosphate 1-Aminopropane-2-one-3-phosphate 1-Aminopropane-2-one-3-phosphate 1-Phosphophydroxythreonine 1-Phosphophydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5'P Pyn5'P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydroorotic acid dTDP dTMP	+ + + - - - + + + + - - - - - - + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Anion Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9929 386.0160 467.980 467.980 157.0255 401.0157 321.0493	A-1 A-2 A-2 A-1 B-1 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-4 D-3 D-3	ND UID UID UID UID UID O.0026 0.1195 ND ND UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0155 ND	ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID 0.0044 0.1313 ND ND 0.0074 UID UID UID UID UID UID UID 0.0512 0.1694 0.0088 0.0313 0.0595 0.0279 0.0149	UID UID UID 0.0038 0.1825 ND ND 0.0161 UID UID UID UID UID 0.0819 0.2889 0.0081 0.0328 0.0274 0.0218	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-7'-phosphate biosynthesis Pyridoxal-8'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinamide Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxine-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Deoxyctidine-5'-triphosphate Deoxyctidine-5'-triphosphate Deoxyctidine-5'-triphosphate Deoxythymidine-5'-diphosphate Deoxythymidine-5'-diphosphate Deoxythymidine-5'-diphosphate Deoxythymidine-5'-triphosphate Deoxythymidine-5'-triphosphate Deoxythymidine-5'-triphosphate Deoxythymidine-5'-triphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydroorotic acid dTDP dTMP dTTP dUDP	+ + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566 481.9893 388.0073	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9929 386.0160 467.9980 157.0255 401.0157 321.0493 480.9820 387.0000	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-4 D-4 D-3 D-3 D-3	ND UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0195 ND 0.0439 0.0439 0.0768	ND UID UID 0.0053 0.1726 ND ND UID UID UID UID UID UID UID UID UID 0.1128 0.0435 0.1656 0.0080 0.0312 0.0315 0.0315 0.0914	ND UID UID 0.0044 0.1313 ND ND UID UID UID UID UID UID UID UID UID UI	UID UID UID UID 0.0038 0.1825 ND ND 0.0161 UID UID UID UID UID 0.1006 0.0819 0.2889 0.0081 0.0328 0.0274 0.0218	
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-7'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyrindine biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Cytidine-5'-diphosphate Deoxyctidine-5'-triphosphate Deoxyctidine-5'-triphosphate Deoxytythymidine-5'-triphosphate Deoxythymidine-5'-triphosphate Deoxythymidine-5'-friphosphate Deoxythymidine-5'-friphosphate Deoxythymidine-5'-friphosphate Deoxytytymidine-5'-diphosphate Deoxyuridine-5'-diphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5P 1AP203P 3H4PHKBA 1DX5P Ery4P PHTTr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydroorotic acid dTDP dTMP dTTP dUDP dUMP dUTP	+ + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Anion Cation Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566 481.9893 388.0073 388.0073 308.0410 467.9736	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9929 386.0160 467.9980 157.0255 401.0157 321.0493 480.9820 387.0000 307.0337 466.9663	A-1 A-2 A-2 A-1 B-1 B-4 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-4 D-3 D-3 D-3 D-3 D-3 D-3	ND UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0195 ND 0.0439 0.0186 0.0768 0.0768 ND	ND UID UID UID 0.0053 0.1726 ND ND 0.0129 UID UID UID UID UID 0.1128 0.0435 0.1656 0.0080 0.0312 0.0315 0.0175 0.0914 0.0021 ND	ND UID UID UID 0.0044 0.1313 ND ND 0.0074 UID UID UID UID UID UID 0.2897 0.0512 0.1694 0.0088 0.0313 0.0595 0.0279 0.0149 0.0868 0.0023 ND	UID	Including quarternary amine
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-11'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-7-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyridoxal-9'-phosphate biosynthesis Pyrindine biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxine-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxyctidine-5'-triphosphate Deoxytyhmidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxyuridine-5'-diphosphate Deoxyuridine-5'-fiphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5'P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydrorotic acid dTDP dTMP dTP dUDP dUMP dUMP dUTP Orotic acid Orotidine5'P	+ + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Auton Anion Anion Anion Anion Anion Auton Anion Auton Anion Auton Anion Auton Auton Auton Auton Auton Auton Auton Auton Nucleotide Anion Anion	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0422 169.0140 214.0246 249.0402 169.0140 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566 481.9893 388.0073 308.0410 407.9736 407.9736 415.0171 368.0257	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 248.0330 168.0067 211.9728 213.070 213.9884 213.0170 213.9884 213.0170 213.9884 213.0170 210.0199 386.0160 467.9980 157.0255 401.0157 321.0493 480.9820 387.0000 307.0337 466.9663 155.0098 367.0184	A-1 A-2 A-2 A-1 B-4 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-5 D-3 D-3 D-3 D-3 D-3 D-3 D-3 D-3 D-4 D-4 D-4	ND UID UID UID UID OOZOE 0.1195 ND ND UID UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0195 ND 0.0439 0.0439 0.0186 0.0768 0.0018 ND ND	ND UID UID UID 0.0053 0.1726 ND ND 0.0129 UID UID UID UID UID UID UID 0.1128 0.0435 0.1656 0.0080 0.0311 0.0175 0.0914 0.0021 ND ND	ND UID UID UID UID UID UID UID UID UID UI	UID	Including quarternary amine
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridone nucleotide cycling Pyridoxal-10°-phosphate biosynthesis Pyridoxal-5°-phosphate biosynthesis Pyridoxal-5°-phosphate biosynthesis Pyridoxal-7°-phosphate biosynthesis Pyridoxal-8°-phosphate biosynthesis Pyridoxal-9°-phosphate biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinic acid Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxal-5'-phosphate Pyridoxine-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-a-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Cytidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxythymidine-5'-diphosphate Deoxythymidine-5'-diphosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxythymidine-5'-phosphate Deoxyuridine-5'-diphosphate Deoxyuridine-5'-diphosphate Deoxyuridine-5'-phosphate Deoxyuridine-5'-phosphate Deoxyuridine-5'-phosphate Deoxyuridine-5'-triphosphate Deoxyuridine-5'-triphosphate Deoxyuridine-5'-triphosphate Deoxyuridine-5'-triphosphate Deoxyuridine-5'-triphosphate Deoxyuridine-5'-triphosphate Uridine-5'-diphosphate Uridine-5'-diphosphate Uridine-5'-diphosphate Uridine-5'-phosphate Uridine-5'-phosphate Uridine-5'-phosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5P 1AP203P 3H4PHKBA 1DX5P Ery4P PHTTr Carbamoyl-Asp COP CTP dCDP dCTP Dihydroorotic acid dTDP dTMP dTTP dUDP dUMP dUTP Orotic acid Orotidine5'P UDP UMP	+ + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Anion Anion Anion Anion Anion Anion Anion Cation Anion Cation Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566 481.9893 388.0073 308.0410 467.9736 156.0171 368.0257 404.0002 324.0359	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 334.0572 246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9229 386.0160 467.9980 157.0255 401.0157 321.0493 480.9820 387.0000 307.0337 466.9663 155.0098 367.0184 402.9949 323.0286	A-1 A-2 A-2 A-2 A-1 B-4 B-4 B-3 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-3 D-3 D-3 D-3 D-3 D-3 D-3 D-3 D-3 D-4 D-4 D-4 D-4	ND UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID UID UID 0.0110 0.0822 0.1321 0.0113 0.0195 ND 0.0439 0.0186 0.0768 ND	ND UID UID UID 0.0053 0.1726 ND ND 0.0129 UID UID UID UID UID UID 0.1128 0.0435 0.1656 0.0080 0.0312 0.0315 0.0311 0.0175 0.0914 ND ND ND ND ND ND 0.1517	ND UID UID UID UID UID UID UID UID UID UI	UID	Including quarternary amine
Purine biosynthesis Pyridine nucleotide cycling Pyridine nucleotide cycling Pyridoxal-10'-phosphate biosynthesis Pyridoxal-11'-phosphate biosynthesis Pyridoxal-5'-phosphate biosynthesis Pyridoxal-6'-phosphate biosynthesis Pyridoxal-8'-phosphate biosynthesis Pyridoxal-9-phosphate biosynthesis Pyridoxal-9-phosphate biosynthesis Pyridoxal-9-phosphate biosynthesis Pyrimidine biosynthesis		Guanosine-5'-triphosphate Inosine-5'-phosphate M³-Carboxyaminoimidazoleribonucleotide 5-Phosphoribosyl-4-(M-succinocarboxamide)-5-aminoimidazole Xanthosine-5-phosphate Nicotinamide Nicotinamide Nicotinamide Nicotinamide-D-ribonucleotide Pyridoxal-5'-phosphate Pyridoxine-5'-phosphate 1-Aminopropane-2-one-3-phosphate 3-Hydroxy-4-phospho-hydroxy-α-ketobutyric acid 1-Deoxy-D-xylulose-5-phosphate Erythronate-4-phosphate Phosphohydroxythreonine Carbamoyl-L-aspartic acid Cytidine-5'-diphosphate Deoxyctidine-5'-diphosphate Deoxyctidine-5'-triphosphate Deoxytymidine-5'-triphosphate Deoxytymidine-5'-triphosphate Deoxytymidine-5'-triphosphate Deoxytymidine-5'-phosphate Deoxytymidine-5'-phosphate Deoxytymidine-5'-phosphate Deoxyuridine-5'-phosphate Uridine-5'-diphosphate Uridine-5'-diphosphate	GTP IMP N5-CAIR PRA SAICAR XMP Nicotinamide Nicotinic acid NicRN Pyr5P Pyn5P 1AP203P 3H4PHKBA 1DX5P Ery4P PHThr Carbamoyl-Asp CDP CTP dCDP dCTP Dihydroorotic acid dTDP dTMP dTTP dUDP dUMP dUTP Orotic acid Orotidine5P UDP	+ + + + + + + + + + + + + + + + + + +	Nucleotide Nucleotide Nucleotide Nucleotide Nucleotide Anion Cation Cation Anion Anion Anion Anion Anion Anion Anion Anion Anion Cation Cation Cation Mucleotide Nucleotide	521.9828 348.0471 338.0389 229.0351 454.0737 364.0420 122.0480 122.0242 335.0644 247.0246 249.0402 169.0140 212.9800 214.0242 214.9957 214.0117 176.0433 403.0182 485.0002 387.0233 469.0053 158.0328 402.0229 322.0566 481.9893 388.0073 308.0410 467.9736 6.0171 368.0257 404.0022	520.9756 347.0398 337.0317 228.0279 453.0664 363.0347 123.0553 123.0315 2246.0173 248.0330 168.0067 211.9728 213.0170 213.9884 213.0044 177.0506 402.0109 483.9929 386.0160 467.9980 157.0255 401.0157 321.0493 480.9820 387.0000 307.0337 466.9663 155.0098 367.0184 402.9949	A-1 A-2 A-2 A-1 B-4 B-4 B-4 B-7 C-1 C-1 C-1 C-1 C-1 C-4 D-4 D-4 D-4 D-4 D-3 D-3 D-3 D-3 D-3 D-3 D-4 D-4 D-4 D-4	ND UID UID 0.0026 0.1195 ND ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID UID UID UID UID UID UID UI	ND UID UID UID UID UID UID UID UID UID UI	UID	Including quarternary amine

Salvage of Ade, HypXan	1	Adenine	Adenine	+	Cation	135.0545	136.0618	A-1	0.0056	0.0073	0.0094	0.0053	
Salvage of Ade, HypXan	- 1	Adenosine	Adenosine	+	Cation	267.0968	268.1040	A-1	0.0077	0.0243	0.0221	0.0046	
Salvage of Ade, HypXan	- 1	Deoxyadenosine	dAdenosine	+	Cation	251.1018	252.1091	A-1	ND	ND	ND	ND	
Salvage of Ade, HypXan	- 1	Deoxyinosine	dInosine	+	Cation	252.0859	253.0931	A-1	ND	ND	ND		
Salvage of Ade, HypXan	- 1	Hypoxanthine	Hypoxanthine	+	Cation	136.0385	137.0458	A-1	0.0844	0.0368	0.0387	0.0517	
Salvage of Ade, HypXan	I	Inosine	Inosine	+	Cation	268.0808	269.0880	A-1	0.0290	0.0072	0.0129	0.0157	
Salvage of Ade, HypXan	1	Uric acid	Uric acid	+	Cation	168.0283	169.0356	B-1	ND	ND	ND		
Salvage of Ade, HypXan	I	Xanthine	Xanthine	+	Cation	152.0334	153.0407	B-1	0.0189	ND	ND		
Salvage of Gua, Xan		Deoxyguanosine	dGuanosine	+	Cation	267.0968	268.1040	B-1	0.0077	0.0243	0.0234	0.0046	
Salvage of Gua, Xan Salvage of Gua, Xan	+ +	Deoxyribose-1-phosphate Guanine	dR1P Guanine	+	Anion Cation	214.0242 151.0494	213.0170 152.0567	D-3 B-1	ND 0.0316	ND 0.0037	ND 0.0074	0.0154	
Salvage of Gua, Xan	+ †	Guanosine	Guanosine	+	Cation	283.0917	284.0989	B-1	0.0310	0.0037	0.0074	0.0134	
Salvage of Gua, Xan	i i	D-Ribose-1-phosphate	R1P	-	Anion	230.0192	229.0119	B-2	UID	UID	UID		
Salvage of Gua, Xan	i	Xanthosine	Xanthosine	+	Cation	284.0757	285.0830	B-1	ND	ND	ND		
Salvage of pyridoxal-5'-phosphate	T i	Pyridoxal	Pyridoxal	+	Cation	167.0582	168.0655		ND	ND	ND		
Salvage of pyridoxal-6'-phosphate	Ť	Pyridoxamine	Pyridoxamine	+	Cation	168.0899	169.0972		0.0016	0.0231	0.0221	0.0239	
Salvage of pyridoxal-7'-phosphate	1	Pyridoxamine-5'-phosphate	PX5'P	+	Anion	248.0562	247.0489		0.0174	0.0117	0.0193	0.0220	
Salvage of pyridoxal-8'-phosphate	- 1	Pyridoxine	Pyridoxine	+	Cation	169.0739	170.0812		ND	ND	ND	ND	
Salvage of pyrimidine	- 1	Cytidine-5'-phosphate	CMP	+	Nucleotide	323.0519	322.0446	D-4	0.0254	0.0239	0.0222	0.0456	
Salvage of pyrimidine	- 1	Cytidine	Cytidine	+	Cation	243.0855	244.0928	D-4	ND	ND	ND	ND	
Salvage of pyrimidine	- 1	Cytosine	Cytosine	+	Cation	111.0433	112.0505	D-4	0.0090	0.0029	0.0026	0.0044	
Salvage of pyrimidine	- 1	Deoxycytidine	dCyt	+	Cation	227.0906	228.0979	D-3	ND	ND	ND		
Salvage of pyrimidine	- 1	Deoxyuridine	dUri	+	Cation	228.0746	229.0819	D-3	ND	ND	ND		
Salvage of pyrimidine	- 1	Thymidine	Thymidine	+	Cation	242.0903	243.0975	D-3	ND	ND	ND		
Salvage of pyrimidine	- 1	Thymine	Thymine	+	Cation	126.0429	127.0502	D-3	0.0027	ND	ND		
Salvage of pyrimidine	I	Uracil	Uracil	+	Cation	112.0273	113.0346	D-4	ND	ND	ND		
Salvage of pyrimidine	I	Uridine	Uridine	+	Cation	244.0695	245.0768	D-4	ND	ND	ND		
SAM biosynthesis		S-Adenosyl-L-methionine	SAM	+	Cation	399.1451	399.1451	A-4	0.0420	0.0693	0.0671	0.1181	Including trinary sulfur
Serine biosynthesis	1	3-Phosphoserine	3PHPA 3PSer	+	Anion Anion	183.9773 185.0089	182.9700 184.0017	C-3	UID	UID ND	0.0017	UID	
Serine biosynthesis Serine biosynthesis	+	3-Phosphoserine L-Serine	Ser	+	Cation	185.0089	184.0017	C-3	0.1112	0.2028	0.0017	0.1815	
Sulfuric acid assimilation	H	Adenosine-5'-phosphosulfate	APS	+	Nucleotide	427.0199	426.0126	C-3	0.1112	0.2028	0.1328	0.1813	
Sulfuric acid assimilation	H	Adenosine-3-priospriosurate Adenosine-3',5'-diphosphate	pAp	+	Nucleotide	427.0199	426.0126	D-2	0.0182	0.0675	0.0526	0.0233	
Sulfuric acid assimilation	Ė	3'-Phosphoadenosine-5'-phosphosulfate	PAPS	-	Nucleotide	506.9862	505.9790	C-2	UID	UID	UID		
TCA cycle	Ιİ	2-Oxoglutaric acid	2-OG	+	Anion	146.0215	145.0142	C-4	ND	0.0911	0.0423	0.0303	
TCA cycle	Ť	cis-Aconitic acid	cis-Aconitic acid	+	Anion	174.0164	173.0092	C-3	ND	0.0057	0.0064	0.0006	
TCA cycle	- 1	Citric acid	Citric acid	+	Nucleotide	192.0270	191.0197	C-3	0.0763	0.6989	0.5342	0.2005	
TCA cycle	1	Fumaric acid	Fumaric acid	+	Anion	116.0110	115.0037	B-4	0.0128	0.0872	0.0481	0.0368	
TCA cycle	l i	Isocitric acid	Isocitric acid	+	Nucleotide	192.0270	191.0197	C-4	ND	ND	ND		
TCA cycle	_ I	Malic acid	Malic acid	-	Anion	134.0215	133.0142	B-3	0.0197	0.2072	0.1314	0.1180	
TCA cycle	- 1	Succinic acid	Succinic acid	+	Anion	118.0266	117.0193	B-4	0.0720	0.6073	0.3211	0.2371	
TCA cycle	I	Succinyl-CoA	SucCoA	+	Nucleotide	867.1313	432.5584	C-4	0.0009	0.0076	0.0021	0.0021	Detected as divalent ion in MS
Tetrahydrofolic acid biosynthesis	- 1	4-Amino-4-deoxychorismic acid	ADCA	-	Cation	225.0637	226.0710	C-1	UID	UID	UID	UID	
Tetrahydrofolic acid biosynthesis	- 1	2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridinediphosphate	AHHMeDHPDP	-	Nucleotide	355.0083	354.0010	C-1	0.0011	0.0012	0.0007	UID	
Tetrahydrofolic acid biosynthesis	- 1	7,8-Dihydrofolic acid	DHFA	+	Cation	443.1553	444.1626	D-1	ND	ND	ND		
Tetrahydrofolic acid biosynthesis	- 1	Dihydromonapterin-3'-triphosphate	DHMPTP	-	Nucleotide	494.9958	493.9885	B-1	UID	UID	UID		
Tetrahydrofolic acid biosynthesis	1	7,8-Dihydroneopterin	DHN	+	Cation	255.0968	256.1040	C-1	ND	ND	ND		
Tetrahydrofolic acid biosynthesis	- 1	Dihydroneopterinphosphate	DHNPMP	-	Nucleotide	335.0631	334.0558	C-1	UID	UID	UID		
Tetrahydrofolic acid biosynthesis		7,8-Dihydroneopterin-3'-triphosphate	DHNPTP	_	Nucleotide	494.9958	493.9885	B-1	UID	UID	UID		
Tetrahydrofolic acid biosynthesis		7,8-Dihydropteroic acid	DHPA	_	Cation	314.1127	315.1200	C-1	UID	UID	UID		
Tetrahydrofolic acid biosynthesis	+ +	6-Hydroxymethyldehydropterin	HMeDHP N10F-THF	_	Cation	195.0756 473.1659	196.0829 474.1732	C-1 D-1	UID	UID	UID		
Tetrahydrofolic acid biosynthesis	- 1	N¹¹-Formyl-THF	NIUF-IHF	_		4/3.1039		D-1	עוט	עוט	UID	UID	
(Totrahydrofolic acid biocynthosic	1	n Aminohonzoic acid	DARA					C 1	ND	ND	ND	ND	
Tetrahydrofolic acid biosynthesis	1	p-Aminobenzoic acid	PABA 4A5HMe2MeDvrDD	+	Cation	137.0477	138.0550	C-1	ND 0.0014	ND 0.0021	ND 0.0021		
Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate	4A5HMe2MePyrPP	_	Cation Nucleotide	137.0477 299.0072	138.0550 298.0000	C-1 D-1	0.0014	0.0021	0.0021	0.0019	
Thiamine biosynthesis Thiamine biosynthesis	1 1 1		4A5HMe2MePyrPP 4Me5BHEthThiazole		Cation Nucleotide Cation	137.0477 299.0072 143.0405	138.0550 298.0000 144.0478		0.0014 ND	0.0021 ND	0.0021 ND	0.0019 ND	
Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-{β-hydroxyethyl)thiazole 4-Methyl-5-{β-hydroxyethyl)thiazolephosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP	- +	Cation Nucleotide	137.0477 299.0072 143.0405 223.0068	138.0550 298.0000		0.0014	0.0021	0.0021	0.0019 ND UID	
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr	- + -	Cation Nucleotide Cation Anion	137.0477 299.0072 143.0405	138.0550 298.0000 144.0478 221.9995 140.0818		0.0014 ND UID	0.0021 ND UID	0.0021 ND UID	0.0019 ND UID UID	
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-{β-hydroxyethyl)thiazole 4-Methyl-5-{β-hydroxyethyl)thiazolephosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP	- + - -	Cation Nucleotide Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746	138.0550 298.0000 144.0478 221.9995		0.0014 ND UID UID	0.0021 ND UID UID	0.0021 ND UID UID	0.0019 ND UID UID	
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP	- + - -	Cation Nucleotide Cation Anion Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336	D-1	0.0014 ND UID UID UID	0.0021 ND UID UID UID	0.0021 ND UID UID	0.0019 ND UID UID	Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis	1 1 1 1 1 1	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyr Thiamine	- + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123	D-1	0.0014 ND UID UID UID 0.2570	0.0021 ND UID UID UID 0.2594	0.0021 ND UID UID UID 0.2030	0.0019 ND UID UID UID 0.2280	Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis	1	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP	- + - - - + +	Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Nucleotide	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304	D-1 D-1 D-1	0.0014 ND UID UID UID 0.2570 0.3180	0.0021 ND UID UID UID 0.2594 0.4812	0.0021 ND UID UID UID 0.2030 0.4164	0.0019 ND UID UID UID 0.2280 0.4198	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP	- + - - - + +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786	D-1 D-1 D-1 D-1	0.0014 ND UID UID UID 0.2570 0.3180 0.3903	0.0021 ND UID UID UID 0.2594 0.4812 0.6529	0.0021 ND UID UID 0.2030 0.4164 0.5103	0.0019 ND UID UID 0.2280 0.4198 0.5588	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis	1 1 1 1 1 1 1 1 1	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate O-Phospho-L-homoserine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer	- + - - - + + +	Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753	D-1 D-1 D-1 A-3 A-4 C-1	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trendine biosynthesis Trendine biosynthesis Trendine biosynthesis Treptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid	- + - - + + + + + + +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Cation Anion Cation Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550	D-1 D-1 D-1 A-3 A-4 C-1 A-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Trehalose biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP	- + - - + + + + + + +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Trehalose biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P	- + - - + + + + + + - -	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Nucleotide	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND UID	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Trehalose biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate U-Threonine Trehalose-6-phosphate Trehalose-6-phosphate Anthranilic acid 1-(σ-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Nucleotide Nucleotide Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 149.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate U-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5'-Phosphoribosyl)anthranilic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth	- + - - + + + + + + + + - - + + + + -	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Nucleotide Cation Nucleotide Nucleotide Cation Nucleotide	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND UID UID ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.091 0.2374 ND ND UID UID UID UID UID UID	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminephosphate - O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(σ-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole - N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp	- + - - + + + + + + - - - - - - - - + + + + + - - - - - - - - - - - - - - - + - - - - + - - - + - - - + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND UID UID UID UID UID UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND UID UID UID UID UID OOD UID UI	0.0019 ND UID UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND UID UID UID UID UID 0.0761	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminephosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(o-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan p-Hydroxyphenylpyruvic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP	- + - - + + + + + + - - + + + + + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Nucleotide Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0665 421.0753 138.0550 348.0490 286.0486 118.0651 138.0550 348.0490 205.0972 179.0350	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID ND UID ND UID ND UID ND UID ND UID ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND UID UID UID O.0519	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID UID UID ND UID UID	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID UID 0.0761	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Trytosine biosynthesis Tyrosine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate - Thiaminephosphate Thiaminephosphate Thiaminephosphate - Thenophosphosphate - Thenophosphosphate - Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Cation Cation Cation Cation Cation Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 435.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID UID UID O.2976	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0519 0.0167	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID ND ND ND 0.0521 ND 0.0521	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Typtosine biosynthesis Ubiquinone biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate - Thiaminephosphate - Thiaminephosphate - Thiaminephosphate - Thiaminephosphate - Thiaminephosphate - The alose - 6-phosphate - Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole - 3-glycerolphosphate Indole - N-(5'-Phosphoribosyl)anthranilic acid - Tryptophan - P-Hydroxyphenylpyruvic acid - Tryrosine - Hydroxybenzoic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA	- + - - + + + + + + - - + + + + + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-3 A-3	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID ND UID ND UID ND UID ND UID ND UID ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID UID 0.0519 0.0519 0.05519 0.05519	0.0021 ND UID UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID ND UID 0.0521 ND 0.6505 0.0130	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID UID 0.0761	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Tyrosine biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryosine ρ-Hydroxyphenylosphate ρ-Hydroxyphenylosphate ρ-Hydroxyphenylosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P	- + - - + + + + + + - - - + + + + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Anion Anion Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3 C-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.0338 ND 0.2976 0.0072	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID UID O.05521 ND 0.6505 0.0130 lc-66P	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID ND ND 1.00761 0.0085 1.2055 0.0184	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Trytophan biosynthesis Tyrosine biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5-Phosphor-bosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr HMePyrP Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID UID UID O.2976	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID UID 0.0519 0.0519 0.05519 0.05519	0.0021 ND UID UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID ND UID 0.0521 ND 0.6505 0.0130	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID UID UID 0.3449 1.000 ND ND ND ND ND ND ND ND ND ND ND ND ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Tyrosine biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryosine ρ-Hydroxyphenylosphate ρ-Hydroxyphenylosphate ρ-Hydroxyphenylosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P	- + - - + + + + + + - - - + + + + - - - +	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Anion Anion Anion Anion Anion Anion Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3 C-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID 0.0338 ND 0.0338 ND 0.2976 0.0072	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.6505 0.0130 0.6569 0.0359	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID UID UID 0.3449 1.000 ND ND ND ND ND ND ND ND ND ND ND ND ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Tryosine biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminephosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxybenylpyruvic acid L-Tryptosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA GIC-1P GIC-6P GICNAC-P	- + - - + + + + + - - - + + + + + -	Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Nucleotide Cation Nucleotide Cation Anion Cation Anion Anion Anion Anion Anion Anion Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID 0.0338 ND 0.0398 ND 0.0398 0.0072	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.05505 0.0130 Ic-6P 0.0359	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID UID 0.0761 0.0085 1.2055 0.0184 0.0326	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Upohan biosynthesis Upohan biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole 3-glycerolphosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Nucleotide	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 300.0490 606.0743	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 0.0061 0.0070 0.0070 0.0070 0.0070 0.0070	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND UID UID 0.0521 ND 0.6505 0.0130 lc-6P 0.0359 ND 0.2426	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND ND ND ND ND ND ND ND ND ND ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Uppehan biosynthesis Upophan biosynthesis Upophan biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole W-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Trystophan ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Anion Anion Anion Anion Anion Nucleotide Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 349.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 307.0816 134.0579	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 133.0506	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-3	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.9061 2.4406 ND ND UID UID UID 0.0338 ND 0.0338 ND 0.0338 ND 0.0338 ND 0.0338 ND 0.0338 ND 0.037	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.2364 ND ND UID UID UID 0.05519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.3081	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID ND UID ND 0.05521 ND 0.6505 0.0130 Ic-6P 0.0359 ND 0.2426 0.0536	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID NE UID UID 0.3449 NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.01477 0.0139	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Uppenson biosynthesis Uppenson biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Nucleotide Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 606.0743 133.0506 131.0350	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.00321 0.00331 0.00333 UID	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 ND UID UID UID UID 0.2564 ND UID UID UID 0.0519 0.0167 0.6528 ND 0.0102 See G 0.0263 ND 0.3081 0.0555	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID UID O.0521 ND 0.6505 0.0130 lc-6P 0.0359 ND 0.2426 0.0536 0.0050	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.01477 0.0139 0.0111	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryotonine biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan p-Hydroxyphenylpyruvic acid L-Tryptophan p-Hydroxyphenylpyruvic acid L-Trytosine p-Hydroxybenzoic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-6-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid L-Vatine N-Acetyl-D-mannosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 149.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 111.0790 301.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 133.0506 131.0350 115.0401 118.0863 300.0490	D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3 C-3	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.1931 0.0233 UID ND UID 0.0233 UID ND UID 0.0233	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0255 0.02426 UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND UID 0.0521 ND 0.6505 0.0130 lc-6P 0.0359 ND 0.2426 0.0536 0.0050 ND 0.3240 UID	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND ND ND ND ND ND ND ND ND ND ND	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Uppehan biosynthesis Uprosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryrosine ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid L-Valine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 259.0457 131.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 133.0506 131.0350 1115.0401 118.0863 300.0490 308.0997	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-3 C-3 C-3 C-3 D-2	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.9031 0.0061 2.4406 ND ND UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0072	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 ND UID UID UID UID UID 0.2561 ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID 0.0521 ND 0.05505 0.0130 Ic-6P 0.0359 0.02426 0.0536 ND 0.2426 0.0536 ND 0.3240 UID 0.0165	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.01477 0.0139 0.0111 0.0011 0.00290	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Upp-Nacetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis	II II	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate 0-Glucosamine-1-phosphate N-Acetylglucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucArg		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Cation Anion Cation Anion Anion Anion Anion Cation Anion Anion Anion Anion Anion Cation Anion	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 308.0596 115.0401 118.0863 300.0490 308.0987 275.1350	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 D-2 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.00331 0.1931	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 ND UID UID UID 0.2564 ND UID UID 0.0519 0.0167 0.6528 ND 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0245 0.4426 UID 0.0198	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.0505 0.0130 0.0496 0.0506 ND 0.2426 0.0536 0.0050 ND 0.2426 0.0536 0.0050 ND 0.3240 0.0150 0.0150	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID 0.3749 NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.01477 0.0139 0.0111 0.0011 0.0001 0.0089 UID	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Tyrosine biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation	II II	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminediphosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Trysosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2-3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid L-Valine N-Acetylneuraminic acid N²-Succinyl-L-arginine N²-Succinyl-L-arginine N²-Succinylglutamic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc NZSucArg N2SucGlu		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Anion Cation Anion Cation Anion Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 180.0423 181.0739 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 248.0765	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 0.4006 ND UID UID 0.0338 ND 0.0976 0.0072 0.0071 0.1031	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.0019	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.0521 ND 0.6505 0.0130 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0165 0.0015	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.1477 0.0139 0.0111 0.0011 0.5089 UID 0.0220 0.0222	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryotophan biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine degradation Arginine degradation Arginine degradation	II II II	4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryrosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid 1-Valine N-Acetyl-D-mannosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc NZSucArg NZSucGlu NZSucGluSA		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Cation Cation Cation Cation Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 135.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 248.0765 234.0972	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 D-2 B-4 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 0.0010 ND UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.1931 0.0233 UID ND 0.1214 UID ND 0.0035 0.00015	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.0011	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.05505 0.0130 0.2426 0.0556 0.0050 ND 0.3240 UID 0.0165 0.0015 0.0015	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND UID 0.0761 0.0085 1.2055 0.0184 0.0326 ND 0.1477 0.0139 0.0111 0.0011 0.5089 UID 0.0229 0.0026	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Arginine degradation Arginine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid L-Vatine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-L-arginine N-Succinyl-L-arginine N-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAC-P UDP-GlcNAC 2,3-DIV 2-Ac 2-KIV Val ManNAC6P NeuNAC N2SucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGra		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Anion Cation Anion Anion Anion Anion Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Cation Cation Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 19.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 258.0384 130.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 233.1132	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.1931 0.0233 UID ND UID UID UID UID UID UID UID 0.0035 0.0014 UID UID UID UID UID 0.00373	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0255 0.02426 UID 0.0198 0.0119	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND ND UID 0.0521 ND 0.6505 0.0130 1c-6P 0.0359 ND 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0165 0.0015	0.0019 ND UID UID 0.2280 0.4198 0.5588 UID 0.3449 ND ND ND ND 0.0761 0.0085 1.2055 0.0184 0.1477 0.0139 0.0111 0.5089 UID 0.0290 0.0222 0.0026 UID 0.0116	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Uppenance biosynthesis Upophan biosynthesis Uppenacetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Glucosamine degradation Glucosamine degradation Glucosamine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate - Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole - N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan - P-Hydroxyphenylpyruvic acid L-Tryptophan - P-Hydroxyphenylpyruvic acid L-Tyrosine - P-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate - O-Glucosamine-6-phosphate - N-Acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketolsovaleric acid - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-glucosamine - N-Succinylglutamate-5-semialdehyde - N-Succinylglutamate-5-semialdehyde - N-Succinylglutamate-5-semialdehyde - N-Acetyl-D-glucosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNac-P UDP-GlcNac 2,3-DIV 2-Ac 2-KIV Val ManNac6P NeuNac NZSucArg NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlr NAcGlcNP		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Cation Cation Cation Cation Cation Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0380 115.0401 131.0350 115.0401 131.0350 115.0401 130.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0072 0.01214 UID ND 0.1214 UID 0.0035 0.0014 UID 0.0337 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.0562 0.0265 0.0245 0.4426 UID 0.0198 0.0011 0.0030 UID 0.0030 UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID 0.0521 ND 0.05505 0.0130 0.2404 0.0505 ND 0.3240 UID 0.0165 0.0015 0.0019 UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.01407 0.0110 0.0011 0.00290 0.0222 0.0026 UID 0.0116 NE	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenalose biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-Nacetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Acetylglucosamine dissimilation Arginine degradation Arginine degradation Glucosamine degradation Histidine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminedphosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N'-Succinyl-L-arginine N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylglutamic acid N'-Succinylornithine N'-Acetyl-D-glucosamine-6-phosphate Imidazole lactic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlr NAcGlcNP Im-lactate		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Cation Anion Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Cation Cation Anion Anion Anion Anion Cation Anion Cation Anion Cation Anion Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 118.0865 111.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.3903 0.0061 2.4406 ND UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.0013 ND 0.1214 UID 0.0035 0.0014 UID 0.0035 0.0014 UID 0.0037 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 ND 0.3081 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.0426 UID 0.0198 0.0110 0.0198	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.05521 ND 0.0505 0.0130 0.6505 0.0130 0.2426 0.0536 0.0050 ND 0.3240 0.0155 0.0165 0.0165 0.0165 0.0165 0.0161 ND 0.0161 ND	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID 0.0761 0.0085 1.2055 0.0184 0.0349 0.0111 0.0011 0.0001 0.0222 0.0026 UID 0.0101 NE	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-Nacetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Trysosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2-3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid L-Valine N-Acetylneuraminic acid N²-Succinyl-L-arginine N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamic acid Imidazolepyruvic acid Imidazolepyruvic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucArg N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu Im-pyruvic acid		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Anion Anion Anion Anion Anion Cation Anion Cation Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 118.0863 300.0490 205.0972 233.1132 248.0765 234.0972 233.1132 2330.0490 157.0608 155.0451	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 ND UID UID 0.0338 ND 0.2976 0.0072 0.0072 0.0011 0.1931 0.0233 UID ND 0.1214 UID 0.0373 ND UID UID 0.0373 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0030 UID 0.0030 UID 0.0038 UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.6505 0.0130 0.2426 0.0536 0.0536 0.0050 ND 0.3240 UID 0.0165 0.0165 0.0019 UID UID UID UID UID UID UID UID UID UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID UID UID 0.0761 0.0085 1.2055 0.0184 0.01477 0.0139 0.0111 0.00011 0.5089 UID 0.0220 0.0220 0.0226 UID 0.0116 UID	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryntophan biosynthesis Tryptophan biosynthesis Tryotophan biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Lysine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminephosphate - O-Phospho-L-homoserine - Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole - M-(5-Phosphoribosyl)anthranilic acid - Tryptophan - Hydroxyphenylpyruvic acid - Tryrosine - P-Hydroxybenzoic acid - O-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP- M-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid - V-Acetyl-D-mannosamine-6-phosphate - M-Acetyl-D-mannosamine-6-phosphate - M-Acetyl-D-mannosamine-6-phosphate - M-Succinyl-L-arginine - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Succinylglutamic acid - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate - M-Acetyl-D-glucosamine-6-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC NZSucArg NZSucGlu NZSucGluSA NZSucGluN NZSucGlcNP Im-lactate Im-pyruvic acid Cadaverine		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Anion Anion Anion Anion Anion Cation Anion Cation Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 287.0559 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0335	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 224.0972 233.1132 300.0490 157.0608 155.0451 103.1230	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.05519 0.0167 0.6528 0.0167 0.6528 0.00263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.00198 0.00198 0.0036 ND 0.0036 ND 0.0036 ND 0.0036 ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.6505 0.0130 0.4560 0.03240 UID 0.0165 0.0050 ND 0.0161 ND UID UID 0.0161 ND UID 0.0161 ND	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0117 0.0011 0.5089 UID 0.0292 0.0026 UID 0.0116 NE	Including quarternary amine Including quarternary amine Including quarternary amine
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Lysine degradation Methylmalonyl pathway		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxybenylpyruvic acid L-Tryrosine ρ-Hydroxybenzoic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Succinyl-L-arginine N-Succinyl-L-arginine N-Succinyl-L-arginine N-Succinyl-glutamate-5-semialdehyde N-Succinyl-glutamate-5-semialdehyde N-Succinyl-glutamate-5-semialdehyde N-Succinyl-glutamic-6-phosphate Imidazole lactic acid Imidazole lactic acid Imidazole pyruvic acid Cadaverine D-Methylmalonyl-CoA	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA GIC-1P GIC-6P GICNAC-P UDP-GICNAC 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucArg N2SucGlu N2SucGluSA N2SucGrn NAcGICNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-CoA		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Cation Anion Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 156.0535 156.0535	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 421.0753 138.0550 421.0753 138.0550 421.0753 138.0550 138.0490 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 ND UID UID 0.0338 ND 0.2976 0.0072 0.0072 0.0011 0.1931 0.0233 UID ND 0.1214 UID 0.0373 ND UID UID 0.0373 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0245 0.4426 UID 0.0198 0.0011 0.0030 UID 0.0033 UID 0.0038 ND 0.0035	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.0521 ND 0.6505 0.0130 1c-6P 0.0359 ND 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0165 0.00167 ND UID 0.00161 ND UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0117 0.0011 0.5089 UID 0.0292 0.0026 UID 0.0116 NE	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Uppenancia biosynthesis Uppenancia biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Glucosamine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Methylmalonyl pathway		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate Thiaminephosphate - Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole - W-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan - p-Hydroxyphenylpyruvic acid L-Trystophan - p-Hydroxyphenylpyruvic acid L-Tyrosine - p-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate W-Acetylglucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid 2-Acetolactic acid - V-Acityl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine N-Succinylglutamic acid N²-Succinylglutamic acid N²-Succinylglutamic acid N²-Succinylglutamate-5-semialdehyde	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P Glc-6P Glc-6P Glc-AC-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu NACGlcNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-CoA		Cation Nucleotide Cation Anion Cation Anion Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Anion Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 156.0535 156.0535 156.0535	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 300.0490 313.0506 131.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND ND UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.0011 0.0023 UID ND 0.1214 UID 0.0035 0.0014 UID 0.0035 0.0014 UID 0.0036 ND 0.0044 UID	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 ND UID UID UID 0.0519 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.0562 0.0245 0.0245 0.0446 UID 0.0198 0.0011 0.0030 UID 0.0030 ND 0.0008 UID 0.0008 UID 0.0008 UID 0.0053 ND	0.0021 ND UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID 0.05521 ND 0.05521 ND 0.0550 0.0130 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0165 0.0016 0.0016 0.0016 0.0016 ND 0.0161 ND 0.00081 0.0081	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.00761 0.0085 1.2055 0.0184 0.0346 NE 0.0110 0.0011 0.0011 0.0011 0.0011 0.0010 0.00290 0.0222 0.0026 NE UID 0.0016 NE 0.00172 0.0012	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-Nacetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Va		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminedphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan μ-Hydroxyphenylpyruvic acid L-Tryosine μ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate Indiazole lactic acid Imidazole lactic acid Imidazole lactic acid Imidazolepyruvic acid Cadaverine D-Methylmalonyl-CoA Anhydro-N-acetylmuramic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu Im-pyruvic acid Cadaverine D-MeMal-CoA L-MeMal-CoA AHMurNAc		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Cation Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Cation Anion Cation Anion Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 308.0987 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.3903 0.0061 0.0061 ND UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.0033 UID ND UID UID ND 0.1214 UID 0.0033 UID ND 0.1214 UID 0.0033 ND 0.0044 UID 0.0076 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.0110 0.0030 UID 0.0036 ND 0.0036 ND 0.0036 UID 0.0038 UID 0.0053 0.0055 See D-Me	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.0505 0.0130 0.6505 0.0130 0.2426 0.0536 0.0015 0.0015 0.00161 ND UID 0.0161 ND UID 0.0081 0.0009 Mal-CoA UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID 0.0761 0.0085 1.2055 0.0184 0.0349 0.0111 0.0011 0.0011 0.0022 0.0026 UID 0.0290 0.0222 0.0026 UID 0.0116 UID 0.0176	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trendiose biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Peptidoglycan turnover		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Trysosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2-3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid L-Valine N-Acetylneuraminic acid N²-Succinyl-L-arginine N²-Succinyl-L-arginine N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamic acid Imidazolepyruvic acid Cadaverine D-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-Po-glutamyl-meso-diaminopimelyl-D-alanine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu N2SucGlu Im-pyruvic acid Cadaverine D-MeMal-CoA L-MeMal-CoA AHMurNAc AlaGluDAPAla		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Anion Anion Anion Anion Anion Anion Cation Anion Anion Cation Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation 137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 154.0378 102.1157 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 275.1005 433.1809	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0385	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 ND UID 0.0338 ND 0.2976 0.0072 0.0072 0.0071 0.1214 UID ND 0.1214 UID 0.0373 0.0033 0.00373 0.00373 0.0034 UID 0.0026 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0030 UID 0.0030 UID 0.0030 UID 0.0036 ND 0.0085 0.0085 See D.0085 0.0085 UID 0.0085 UID 0.0085 0.0055	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID 0.0521 ND 0.0521 ND 0.6505 0.0130 0.2374 ND 0.2426 0.0536 0.0050 0.0165 0.0155 0.0019 UID UID UID UID 0.0161 ND UID UID UID UID UID UID UID UID UID UI	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0117 0.0011 0.5089 UID 0.0761 0.0011 0.5089 UID 0.0116 NE UID 0.0011 0.0011 0.5089 UID 0.0010 0.0116 UID UID UID UID UID UID UID UID UID UID	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS	
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryntonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryotonine biosynthesis Tryotone biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine degradation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Hyphimalonyl pathway Methylmalonyl pathway Methylmalonyl pathway Peptidoglycan turnover Peptidoglycan turnover		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminephosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-1-phosphosphate Indole-3-glycerolphosphate D-Glucosamine-1-phosphate μ-1-Tyrosine μ-Hydroxyphenylpyruvic acid L-Trysoine μ-Hydroxybenzoic acid D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine N²-Succinylglutamic acid N²-Succinylglutamic acid N²-Succinylglutamic acid N²-Succinylglutamic acid Indazole lactic acid Imidazole pyruvic acid Cadaverine D-Methylmalonyl-CoA Anhydro-N-acetylmuramic acid L-Mathylmalonyl-CoA Anhydro-N-acetylmuramic acid L-Alaninyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyrP Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc NZSucArg NZSucGlu NZSucGluSA NZSucGluNA NZSucGluNA NZSucGluNA NZSucGluNA Importate Impyruvic acid Cadaverine D-MeMal-CoA L-MeMal-CoA L-MeMal-CoA L-MeMal-CoA AlaGluDAPAla L-Ala-D-Glu-Dap		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Cation Anion Anion Anion Anion Anion Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 287.0559 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 867.1313	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 205.0972 233.1132 300.0490 157.0608 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584 432.5584 434.1882 310.1510	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.1931 0.0233 UID ND 0.1214 UID 0.0037 ND 0.1214 UID 0.0037 ND 0.0015 0.0016 UID UID 0.0037 ND 0.0016 UID UID 0.0005 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.02055 0.0245 0.0255 0.0245 0.0256 0.0236 ND 0.00236 ND 0.0030 UID 0.0030 UID 0.0030 UID 0.0035 ND 0.00055 VID 0.0055	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID 0.0521 ND 0.6505 0.0130 0.2426 0.0359 ND 0.2426 0.0050 ND 0.3240 UID 0.0165 0.0016 ND UID 0.0161 ND UID UID UID UID UID UID UID UID UID UI	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.3449 NE UID 0.0761 0.0085 1.2055 0.0184 0.0117 0.0011 0.5089 UID 0.0216 NE 0.0222 0.0026 UID 0.0116 NE UID 0.0011 0.0011 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Methylmalonyl pathway Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole Hydroxymethylpyrimidine Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole W-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan μ-Hydroxyphenylpyruvic acid L-Tryptophan μ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid W-Succinyl-L-arginine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate Imidazole lactic acid Imidazole lactic acid Imidazole lactic acid Imidazole pyruvic acid L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiaminePP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNac-P UDP-GlcNac 2,3-DIV 2-Ac 2-KIV Val ManNac6P NeuNac N2SucArg N2SucArg N2SucGlu N2SucGlu N2SucGlu N2SucGlu NACGlcNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-Coa L-MeMal-Coa L-MeJournap 4ABA		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 867.1313 867.1313 87.10584	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 258.0384 258.0384 278.0380 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584 432.5584 276.1078 88.0757	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.9031 0.0061 2.4406 ND ND UID UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0072 0.0321 0.0014 UID UID UID UID 0.0333 UID ND 0.0044 UID UID UID UID UID UID 0.00373 ND 0.0044 UID UID UID UID 0.0026 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID UID 0.05519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.0364 UID 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.0011 0.0030 UID 0.0038 UID 0.0038 UID 0.0038 UID 0.0055 See D-Me UID UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID 0.0521 ND 0.0550 0.0130 0.4164 0.5133 0.0091 ND 0.0550 ND 0.100091 ND 0.0161 ND 0.0161 ND UID 0.00091 ND UID 0.00091 Mal-COA	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0110 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 UID 0.0011 UID 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upphan biosynthesis Upphan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Ribosephosphate degradation Ribosephosphate degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminedphosphate Thiaminephosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole 3-glycerolphosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tyrosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate 0-Glucosamine-6-phosphate N-Acetylglucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid 2-Acetolactic acid 2-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate N-Acetyl-D-glutamylamea-5-semialdehyde N-2-Succinylglutamic acid N²-Succinylglutamic acid M²-Succinylglutamic acid Imidazole lactic acid Imidazole pyruvic acid Cadaverine D-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA Anhydro-N-acetylmuramic acid L-Alaninyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-γ-D-glutamyl-diaminopimelic acid 4-Aminobutyraldehyde Deoxyribose-5-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucGlu ANSucGloNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-Coa L-MeMal-Coa AHMurNAc AlaGluDAPAla L-Ala-D-Glu-Dap 4ABA dR5P		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Anion Cation Anion Anion Anion Anion Anion Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 287.0559 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 867.1313	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 313.0506 131.0350 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584 432.5584 432.5584 276.1078 434.1882 310.1510 88.0757 213.0170	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.3903 0.0061 2.4406 ND UID UID UID 0.0338 ND 0.0338 ND 0.0338 ND 0.2976 0.0072 0.0321 0.0011 0.1931 0.0014 UID 0.0035 0.0014 UID 0.00373 ND 0.0014 UID 0.00373 ND 0.0044 UID 0.0026 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.0562 0.0263 ND 0.00562 0.0245 0.0426 UID 0.0198 0.0011 0.0030 UID 0.0030 UID 0.0030 UID 0.0055 See D-Me UID 0.0055 See D-Me	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.05505 0.0130 0.6505 0.0130 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0165 0.0016 0.0016 0.0016 0.0016 ND UID UID UID UID UID UID UID UID UID UI	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0110 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 UID 0.0011 UID 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Trenoline biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Methylmalonyl pathway Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole Hydroxymethylpyrimidine Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole W-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan μ-Hydroxyphenylpyruvic acid L-Tryptophan μ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-6-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid W-Succinyl-L-arginine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-glucosamine-6-phosphate Imidazole lactic acid Imidazole lactic acid Imidazole lactic acid Imidazole pyruvic acid L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiaminePP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNac-P UDP-GlcNac 2,3-DIV 2-Ac 2-KIV Val ManNac6P NeuNac N2SucArg N2SucArg N2SucGlu N2SucGlu N2SucGlu N2SucGlu NACGlcNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-Coa L-MeMal-Coa L-MeJournap 4ABA		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Anion Anion Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 275.1005 433.1809 437.140842	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 198.0173 120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 258.0384 258.0384 258.0384 278.0380 115.0401 118.0863 300.0490 308.0987 275.1350 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584 432.5584 276.1078 88.0757	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3 C-2 C-2 C-2 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.9031 0.0061 2.4406 ND ND UID UID UID UID 0.0338 ND 0.2976 0.0072 0.0321 0.0072 0.0321 0.0014 UID UID UID UID 0.0333 UID ND 0.0044 UID UID UID UID UID UID 0.00373 ND 0.0044 UID UID UID UID 0.0026 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID UID 0.05519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.0364 UID 0.0562 0.0255 0.0245 0.4426 UID 0.0198 0.0011 0.0030 UID 0.0038 UID 0.0038 UID 0.0038 UID 0.0055 See D-Me UID UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID 0.0521 ND 0.0550 0.0130 0.4164 0.5133 0.0091 ND 0.0550 ND 0.100091 ND 0.0161 ND 0.0161 ND UID 0.00091 ND UID 0.00091 Mal-COA	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID 0.0761 0.0085 1.2055 0.0184 0.03496 NE 0.0117 0.0119 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Treptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiamine Thiaminephosphate 0-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole 3-glycerolphosphate Indole N-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Tryosine ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate N-Acetylglucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Acetolactic acid 2-Acetolactic acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N'-Succinylglutamic acid N'-Succinylglutamate-5-semialdehyde N'-Succinylglutamic acid Imidazole lactic acid Imidazole pyruvic acid Cadaverine D-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA Anhydro-N-acetylmuramic acid L-Alaninyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaniyl-γ-D-glutamyl-meso-diaminopimelyl-D-alanine	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineDP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc N2SucGlu N2SucGlu N2SucGusA	Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Anion Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 232.092 233.0899 232.1059 301.0563 309.1060 274.1277 247.0692 233.0899 100.10563 156.0535 154.0378 102.1157 867.1313 867.1313 275.1005 433.1809 309.1437 887.16313	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 300.0490 308.0987 213.0150 248.0765 234.0972 233.1132 300.0490 157.0608 155.0451 103.1230 157.0608 155.0451 103.1230 157.0608 155.0451 103.1230 157.0608 155.0451 103.1230 155.0451 103.1230 157.0608 155.0451 103.1230 157.0608 155.0451 103.1230 157.0608 155.0451 103.1230 157.0608	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3 C-2 C-2 C-2 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-1 B-1 A-4 A-4	0.0014 ND UID UID UID 0.2570 0.3180 0.3903 0.3903 0.0061 PORTOR OF CONTROL OT CONTROL OF	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0102 See G 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.0245 0.0363 ND 0.0088 UID 0.0008 UID 0.0008 UID 0.0053 0.0053 0.0055 See D-Me UID UID UID UID UID	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID UID 0.0521 ND 0.0505 0.0130 0.6505 0.0130 0.0426 0.0536 0.0015 0.0150 0.0161 ND UID UID UID UID UID UID UID UID UID UI	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE UID UID UID UID UID UID UID UID UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.01477 0.0139 0.0111 0.0011 0.5089 UID UID UID UID UID UID UID UID UID UID	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS	
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tyrosine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Methylmalonyl pathway Methylmalonyl pathway Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Potrescine degradation Short fatty acid degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazolephosphate Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate - O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(α-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole-3-glycerolphosphate Indole - N-(5-Phosphoribosyl)anthranilic acid L-Tryptophan - p-Hydroxyphenylpyruvic acid L-Trysosine - p-Hydroxyphenzoic acid D-Glucosamine-1-phosphate - N-Acetylglucosamine-1-phosphate - N-Acetylglucosamine-1-phosphate - N-Acetyl-D-glucosamine 2-3-Dihydroxyisovaleric acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid L-Valine - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-mannosamine-6-phosphate - N-Acetyl-D-glucosamine-1-s-semialdehyde - N²-Succinyl-L-arginine - N²-Succinylglutamate-5-semialdehyde - N²-Succinylglutamate-5-semialdehyde - N²-Succinylglutamate-5-semialdehyde - N²-Succinylglutamic acid - N²-Succinylglutamic acid - Imidazolepyruvic acid - Cadaverine - D-Methylmalonyl-CoA - L-Methylmalonyl-CoA - Manydro- N-acetylmuramic acid - Alaninobutyraldehyde - Deoxyribose-5-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAC N2SucArg N2SucGlu N4SucGlo Im-pyruvic acid Cadaverine D-MeMal-CoA L-MeMal-CoA AHMurNAc AlaGluDAPAla L-Ala-D-Glu-Dap 4ABA dR5P RibHomoCys Acetoacetyl-CoA		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 345.0786 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 180.0423 181.0739 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 275.1005 433.1809 309.1437 87.0684 214.0242 267.0777 851.1363	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 345.0786 198.0173 120.0655 421.0753 138.0550 348.0490 205.0972 179.0350 182.0812 137.0244 258.0385 248.0765 234.0972 233.1132 248.0765	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 C-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 C-3 C-3 C-3 C-3 C-4 C-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID 0.2570 0.3180 0.3903 0.0061 ND UID UID 0.0338 ND 0.2976 0.0072 0.0072 0.0072 0.0011 0.1931 0.0233 UID ND 0.1214 UID UID UID UID UID ND 0.1214 UID UID 0.0373 ND 0.0036 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.0263 ND 0.3081 0.0562 0.0255 0.0245 0.4426 UID 0.0030 UID 0.0030 UID 0.0033 UID 0.0033 UID 0.0085 0.0055 See D-M 0.0088 UID 0.0083 UID 0.0083 UID 0.0083 0.0055 See D-M UID 0.0081 UID 0.0081 UID 0.0083 UID 0.0083 UID 0.0083 UID 0.0083 UID 0.0083 UID 0.0084 UID 0.0085 ND 0.0085 ND 0.0095 ND 0.0096 ND 0.0096 ND 0.0096 ND 0.0097 ND 0.0097 ND	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 ND UID 0.0521 ND 0.0521 ND 0.6505 0.0130 0.0456 0.0156 0.0156 0.0156 0.0165 0.0165 0.0161 UID UID UID UID UID UID UID UID UID UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0110 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryntonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryotophan biosynthesis Tryotophan biosynthesis Tryotophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Rephidoglycan turnover Peptidoglycan turnover		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole 4-Methyl-5- (β-hydroxyethyl)thiazole Hydroxymethylpyrimidine Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(ο-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole-3-glycerolphosphate Indole M-(5-Phosphoribosyl)anthranilic acid L-Tryptophan ρ-Hydroxyphenylpyruvic acid L-Trystophan ρ-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketoisovaleric acid L-Valine N-Acetyl-D-mannosamine-6-phosphate N-Acetyl-D-mannosamine acid N²-Succinyl-L-arginine N²-Succinyl-L-arginine N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-5-semialdehyde N²-Succinylglutamate-6-phosphate Imidazole lactic acid Imidazole lactic acid Imidazole pyruvic acid Cadaverine D-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-CoA L-Methylmalonyl-Y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alaninobutyraldehyde Deoxyribose-5-phosphate	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazoleP HMePyr Thiamine ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA Glc-1P Glc-6P GlcNAc-P UDP-GlcNAc 2,3-DIV 2-Ac 2-KIV Val ManNAc6P NeuNAc NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NZSucGlu NACSICNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-CoA L-MeMal-CoA L-MeMal-CoA AHMurNAc AlaGluDAPAla L-Ala-D-Glu-Dap 4ABA dR5P RibHomoCys Acetoacetyl-CoA Aminoacetone		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Anion Cation Anion Cation Anion Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 287.0559 138.0317 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 275.1005 433.1809 309.1437 87.0684 214.0242 2267.0777 851.1363 73.0528	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 423.0304 1120.0655 421.0753 138.0550 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 258.0384 258.0384 300.0490 606.0743 133.0506 131.0350 115.0401 118.0863 300.0490 205.0972 233.1132 300.0490 157.0608 150.0451 103.1230 432.5584 432.5584 432.5584 432.5584 434.1882 310.1510 88.0757 213.0170 268.0849 850.1291 74.0600	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-2 C-2 C-2 C-2 C-3 C-3 C-3 C-3 C-3 B-4 B-4 B-4 B-4 B-4 C-4 A-4 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.0061 2.4406 ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID 0.0519 0.0167 0.6528 0.0167 0.6528 0.0025 0.0263 ND 0.3081 0.0565 0.0255 0.0245 0.0255 0.0245 0.0255 0.0008	0.0021 ND UID UID 0.2030 0.4164 0.5103 0.0091 0.2374 ND UID 0.0521 ND 0.6505 0.0130 0.2426 0.0536 0.0050 ND 0.3240 UID 0.0161 ND UID UID 0.0161 ND UID UID UID UID UID 0.0161 ND UID UID UID UID UID UID UID UID O.0081 0.0009 Mal-CoA UID UID UID UID UID UID UID UID UID UID	0.0019 NE UID UID 0.2280 0.4198 0.5588 UID 0.3449 NE NE UID 0.0761 0.0085 1.2055 0.0184 0.0326 NE 0.0110 0.0011	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS
Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Thiamine biosynthesis Threonine biosynthesis Threonine biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Tryptophan biosynthesis Upp-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis UDP-N-acetylglucosamine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Valine biosynthesis Acetylglucosamine dissimilation Arginine degradation Arginine degradation Arginine degradation Arginine degradation Histidine degradation Histidine degradation Histidine degradation Methylmalonyl pathway Methylmalonyl pathway Methylmalonyl pathway Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Peptidoglycan turnover Putrescine degradation Ribosephosphate degradation Threonine degradation Threonine degradation Threonine degradation		4-Amino-5-hydroxymethyl-2-methylpyrimidinepyrophosphate 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole 4-Methyl-5-(β-hydroxyethyl)thiazole Hydroxymethylpyrimidine Hydroxymethylpyrimidine Hydroxymethylpyrimidinephosphate Thiamine Thiaminediphosphate Thiaminephosphate O-Phospho-L-homoserine L-Threonine Trehalose-6-phosphate Anthranilic acid 1-(o-Carboxyphenylamino)-1'-deoxyribulose-5'-phosphate Indole 3-glycerolphosphate Indole W-(5'-Phosphoribosyl)anthranilic acid L-Tryptophan p-Hydroxyphenylpyruvic acid L-Tryptophan p-Hydroxyphenylpyruvic acid D-Glucosamine-1-phosphate D-Glucosamine-1-phosphate UDP-N-acetyl-D-glucosamine 2,3-Dihydroxyisovaleric acid 2-Acetolactic acid 2-Ketoisovaleric acid 2-Ketoisovaleric acid W-Succinylglutamic acid N-Succinylglutamic acid N-Succinylglutamic acid N-Succinylglutamic acid N-Succinylglutamic acid Imidazole lactic acid Imidazole lactic acid Imidazole lactic acid Imidazole lactic acid Imidazole pyruvic acid L-Alaniyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelyl-D-alanine L-Alanyl-y-D-glutamyl-meso-diaminopimelic acid 4-Aminobutyraldehyde Deoxyribose-5-phosphate 5-D-Ribosyl-L-homocysteine Acetoacetyl-CoA Aminoacetone 2-Amino-3-oxobutanoic acid	4A5HMe2MePyrPP 4Me5BHEthThiazole 4Me5BHEthThiazole 4Me5BHEthThiazole HMePyr Thiamine ThiamineP ThiamineP P-HomoSer Thr Tre6P Anthranilic acid CPADRP IG-P Indole PRAnth Trp HPP Tyr PHBA GIC-1P GIC-6P GICNAC-P UDP-GICNAC 2,3-DIV 2-Ac 2-KIV Val ManNAC6P NeuNAC NZSucArg NZSucGlu NZSucGlu NZSucGlu NZSucGlu NACGICNP Im-lactate Im-pyruvic acid Cadaverine D-MeMal-CoA AHMurNAC AlaGluDAPAla L-Ala-D-Glu-Dap 4ABA dRSP RibHomoCys Acetoacetyl-CoA Aminoacetone AOBA		Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Anion Cation Nucleotide Cation Nucleotide Cation Anion Cation Anion Cation Anion Cation Anion Anion Anion Cation Anion Anion Cation Anion Anion Anion Cation Anion Anion Cation Anion Anion Cation Anion Cation Anion Cation	137.0477 299.0072 143.0405 223.0068 139.0746 219.0409 265.1123 425.0450 199.0246 119.0582 422.0825 137.0477 349.0563 287.0559 117.0578 349.0563 204.0899 180.0423 181.0739 138.0317 259.0457 259.0457 301.0563 607.0816 134.0579 132.0423 116.0473 117.0790 301.0563 309.1060 274.1277 247.0692 233.0899 232.1059 301.0563 156.0535 154.0378 102.1157 867.1313 867.1313 867.1313 87.1052 433.1809 309.1437 87.0684 214.0242 267.0777 851.1363 73.0528 117.0426	138.0550 298.0000 144.0478 221.9995 140.0818 218.0336 265.1123 423.0304 438.0479 286.0486 118.0651 348.0490 205.0972 179.0350 182.0812 137.0244 258.0384 268.0384 278.0386 238.0972 233.1132 300.0490 157.0608 155.0451 103.1230 432.5584 432.5584 276.1078 88.0757 213.0170 268.0849 74.0600 118.0499	D-1 D-1 D-1 D-1 A-3 A-4 C-1 A-2 A-2 A-2 A-2 A-2 A-3 A-3 C-2 C-2 C-3 C-3 C-3 C-3 C-3 C-3 C-3 C-3 C-4 B-4 B-4 B-1 B-1 C-4 A-4 A-4	0.0014 ND UID UID 0.2570 0.3180 0.3903 0.9031 0.0061 2.4406 ND ND UID UID UID 0.338 ND 0.3938 0.0072 0.0321 0.0321 0.0072 0.0321 0.0011 0.1931 0.0014 UID UID UID UID UID UID UID UID UID ND 0.0337 ND 0.0044 UID UID UID UID 0.00373 ND 0.0044 UID UID UID 0.00373 ND 0.0044 UID UID UID 0.00373 ND 0.0044 UID UID UID 0.00378 ND	0.0021 ND UID UID 0.2594 0.4812 0.6529 0.0138 0.2364 ND UID UID UID UID UID UID UID UID UID UI	0.0021 ND UID 0.2030 0.4164 0.5103 0.0091 ND UID ND UID 0.0521 ND 0.0550 0.0130 0.4166 0.0091 ND 0.0550 0.0130 0.0091 ND 0.0161 ND UID 0.0172 ND UID 0.0172 ND UID UID 0.0172 ND UID UID 0.0172 ND UID UID UID 0.0172	0.0019	Including quarternary amine Including quarternary amine Including quarternary amine Including quarternary amine Detected as divalent ion in MS Detected as divalent ion in MS

Threonine degradation | II | Propionic acid | Propionic acid | Propionic acid | Propionic acid | Propionyl-CoA | Propionyl-CoA | Nucleotide | 823.1414 | 822.1342 | A-4 | 0.0176 | 0.0160 | 0.0139 | 0.0021 |
Threonine degradation | II | Propionyl-CoA | Propionyl-CoA | Nucleotide | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registration | Registratio

