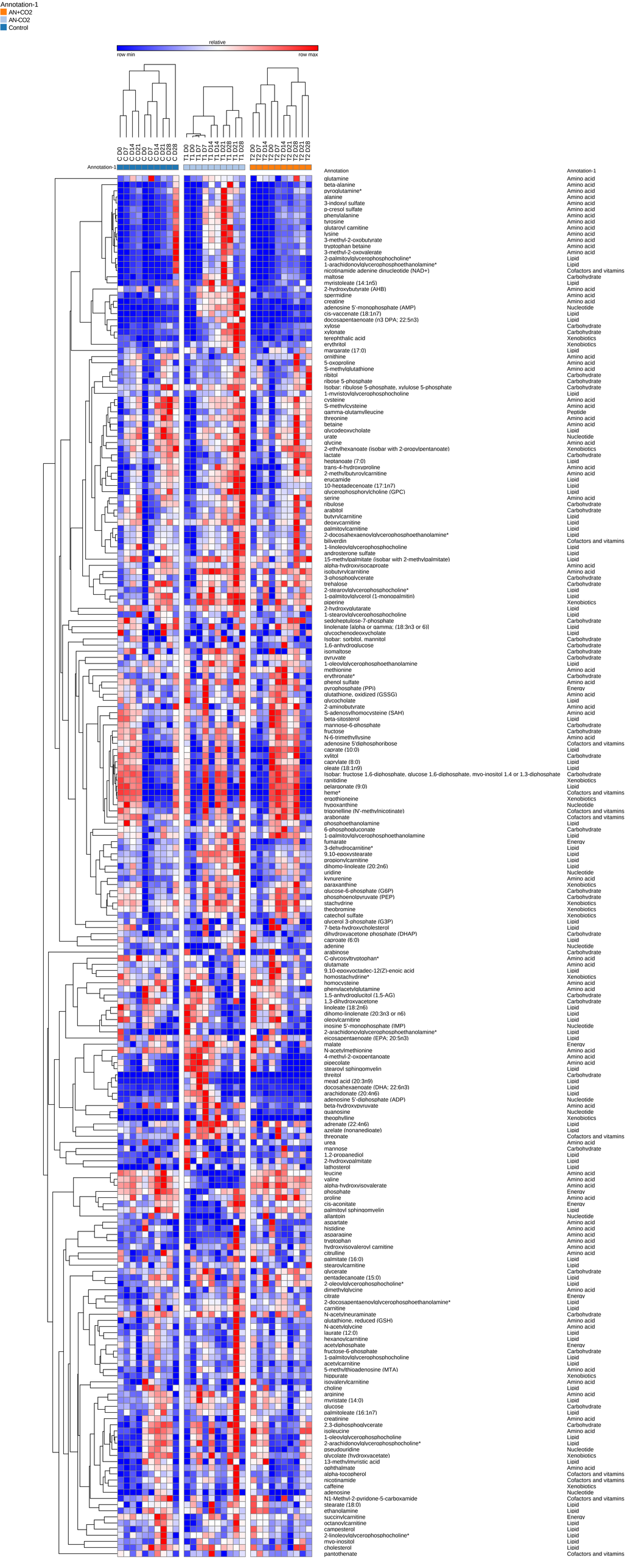
Annotation-1
AN+CO2
AN-CO2
Control
relative
row min
row max
C D0
C D7
C D14
C D21
C D0
C D7
C D14
C D21
C D28
C D28
T1 D0
T1 D0
T1 D7
T1 D7
T1 D14
T1 D14
T1 D21
T1 D21
T1 D28
T1 D28
T2 D0
T2 D7
T2 D14
T2 D21
T2 D7
T2 D14
T2 D21
T2 D28
T2 D21
T2 D28
Annotation-1
Annotation
Annotation-1
glutamine
Amino acid
beta-alanine
Amino acid
pyroglutamine*
Amino acid
alanine
Amino acid
3-indoxyl sulfate
Amino acid
p-cresol sulfate
Amino acid
phenylalanine
Amino acid
tyrosine
Amino acid
glutaroyl carnitine
Amino acid
lysine
Amino acid
3-methyl-2-oxobutyrate
Amino acid
tryptophan betaine
Amino acid
3-methyl-2-oxovalerate
Amino acid
2-palmitoylglycerophosphocholine*
Lipid
1-arachidonoylglycerophosphoethanolamine*
Lipid
nicotinamide adenine dinucleotide (NAD+)
Cofactors and vitamins
maltose
Carbohydrate
myristoleate (14:1n5)
Lipid
2-hydroxybutyrate (AHB)
Amino acid
spermidine
Amino acid
creatine
Amino acid
adenosine 5'-monophosphate (AMP)
Nucleotide
cis-vaccenate (18:1n7)
Lipid
docosapentaenoate (n3 DPA; 22:5n3)
Lipid
xylose
Carbohydrate
xylonate
Carbohydrate
terephthalic acid
Xenobiotics
erythritol
Xenobiotics
margarate (17:0)
Lipid
ornithine
Amino acid
5-oxoproline
Amino acid
S-methylglutathione
Amino acid
ribitol
Carbohydrate
ribose 5-phosphate
Carbohydrate
Isobar: ribulose 5-phosphate, xylulose 5-phosphate
Carbohydrate
1-myristoylglycerophosphocholine
Lipid
cysteine
Amino acid
S-methylcysteine
Amino acid
gamma-glutamylleucine
Peptide
threonine
Amino acid
betaine
Amino acid
glycodeoxycholate
Lipid
urate
Nucleotide
glycine
Amino acid
2-ethylhexanoate (isobar with 2-propylpentanoate)
Xenobiotics
lactate
Carbohydrate
heptanoate (7:0)
Lipid
trans-4-hydroxyproline
Amino acid
2-methylbutyrylcarnitine
Amino acid
erucamide
Lipid
10-heptadecenoate (17:1n7)
Lipid
glycerophosphorylcholine (GPC)
Lipid
serine
Amino acid
ribulose
Carbohydrate
arabitol
Carbohydrate
butyrylcarnitine
Lipid
deoxycarnitine
Lipid
palmitoylcarnitine
Lipid
2-docosahexaenoylglycerophosphoethanolamine*
Lipid
biliverdin
Cofactors and vitamins
1-linoleoylglycerophosphocholine
Lipid
androsterone sulfate
Lipid
15-methylpalmitate (isobar with 2-methylpalmitate)
Lipid
alpha-hydroxyisocaproate
Amino acid
isobutyrylcarnitine
Amino acid
3-phosphoglycerate
Carbohydrate
trehalose
Carbohydrate
2-stearoylglycerophosphocholine*
Lipid
1-palmitoylglycerol (1-monopalmitin)
Lipid
piperine
Xenobiotics
2-hydroxyglutarate
Lipid
1-stearoylglycerophosphocholine
Lipid
sedoheptulose-7-phosphate
Carbohydrate
linolenate [alpha or gamma; (18:3n3 or 6)]
Lipid
glycochenodeoxycholate
Lipid
Isobar: sorbitol, mannitol
Carbohydrate
1,6-anhydroglucose
Carbohydrate
isomaltose
Carbohydrate
pyruvate
Carbohydrate
1-oleoylglycerophosphoethanolamine
Lipid
methionine
Amino acid
erythronate*
Carbohydrate
phenol sulfate
Amino acid
pyrophosphate (PPi)
Energy
glutathione, oxidized (GSSG)
Amino acid
glycocholate
Lipid
2-aminobutyrate
Amino acid
S-adenosylhomocysteine (SAH)
Amino acid
beta-sitosterol
Lipid
mannose-6-phosphate
Carbohydrate
fructose
Carbohydrate
N-6-trimethyllysine
Amino acid
adenosine 5'diphosphoribose
Cofactors and vitamins
caprate (10:0)
Lipid
xylitol
Carbohydrate
caprylate (8:0)
Lipid
oleate (18:1n9)
Lipid
Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate
Carbohydrate
ranitidine
Xenobiotics
pelargonate (9:0)
Lipid
heme*
Cofactors and vitamins
ergothioneine
Xenobiotics
hypoxanthine
Nucleotide
trigonelline (N'-methylnicotinate)
Cofactors and vitamins
arabonate
Cofactors and vitamins
phosphoethanolamine
Lipid
6-phosphogluconate
Carbohydrate
1-palmitoylglycerophosphoethanolamine
Lipid
fumarate
Energy
3-dehydrocarnitine*
Lipid
9,10-epoxystearate
Lipid
propionylcarnitine
Lipid
dihomo-linoleate (20:2n6)
Lipid
uridine
Nucleotide
kynurenine
Amino acid
paraxanthine
Xenobiotics
glucose-6-phosphate (G6P)
Carbohydrate
phosphoenolpyruvate (PEP)
Carbohydrate
stachydrine
Xenobiotics
theobromine
Xenobiotics
catechol sulfate
Xenobiotics
glycerol 3-phosphate (G3P)
Lipid
7-beta-hydroxycholesterol
Lipid
dihydroxyacetone phosphate (DHAP)
Carbohydrate
caproate (6:0)
Lipid
adenine
Nucleotide
arabinose
Carbohydrate
C-glycosyltryptophan*
Amino acid
glutamate
Amino acid
9,10-epoxyoctadec-12(Z)-enoic acid
Lipid
homostachydrine*
Xenobiotics
homocysteine
Amino acid
phenylacetylglutamine
Amino acid
1,5-anhydroglucitol (1,5-AG)
Carbohydrate
1,3-dihydroxyacetone
Carbohydrate
linoleate (18:2n6)
Lipid
dihomo-linolenate (20:3n3 or n6)
Lipid
oleoylcarnitine
Lipid
inosine 5'-monophosphate (IMP)
Nucleotide
2-arachidonoylglycerophosphoethanolamine*
Lipid
eicosapentaenoate (EPA; 20:5n3)
Lipid
malate
Energy
N-acetylmethionine
Amino acid
4-methyl-2-oxopentanoate
Amino acid
pipecolate
Amino acid
stearoyl sphingomyelin
Lipid
threitol
Carbohydrate
mead acid (20:3n9)
Lipid
docosahexaenoate (DHA; 22:6n3)
Lipid
arachidonate (20:4n6)
Lipid
adenosine 5'-diphosphate (ADP)
Nucleotide
beta-hydroxypyruvate
Amino acid
guanosine
Nucleotide
theophylline
Xenobiotics
adrenate (22:4n6)
Lipid
azelate (nonanedioate)
Lipid
threonate
Cofactors and vitamins
urea
Amino acid
mannose
Carbohydrate
1,2-propanediol
Lipid
2-hydroxypalmitate
Lipid
lathosterol
Lipid
leucine
Amino acid
valine
Amino acid
alpha-hydroxyisovalerate
Amino acid
phosphate
Energy
proline
Amino acid
cis-aconitate
Energy
palmitoyl sphingomyelin
Lipid
allantoin
Nucleotide
aspartate
Amino acid
histidine
Amino acid
asparagine
Amino acid
tryptophan
Amino acid
hydroxyisovalerovl carnitine
Amino acid
citrulline
Amino acid
palmitate (16:0)
Lipid
stearoylcarnitine
Lipid
glycerate
Carbohydrate
pentadecanoate (15:0)
Lipid
2-oleoylglycerophosphocholine*
Lipid
dimethylglycine
Amino acid
citrate
Energy
2-docosapentaenoylglycerophosphoethanolamine*
Lipid
carnitine
Lipid
N-acetylneuraminate
Carbohydrate
glutathione, reduced (GSH)
Amino acid
N-acetylglycine
Amino acid
laurate (12:0)
Lipid
hexanoylcarnitine
Lipid
acetylphosphate
Energy
fructose-6-phosphate
Carbohydrate
1-palmitoylglycerophosphocholine
Lipid
acetylcarnitine
Lipid
5-methylthioadenosine (MTA)
Amino acid
hippurate
Xenobiotics
isovalerylcarnitine
Amino acid
choline
Lipid
arginine
Amino acid
myristate (14:0)
Lipid
glucose
Carbohydrate
palmitoleate (16:1n7)
Lipid
creatinine
Amino acid
2,3-diphosphoglycerate
Carbohydrate
isoleucine
Amino acid
1-oleoylglycerophosphocholine
Lipid
2-arachidonoylglycerophosphocholine*
Lipid
pseudouridine
Nucleotide
glycolate (hydroxyacetate)
Xenobiotics
13-methylmyristic acid
Lipid
ophthalmate
Amino acid
alpha-tocopherol
Cofactors and vitamins
nicotinamide
Cofactors and vitamins
caffeine
Xenobiotics
adenosine
Nucleotide
N1-Methyl-2-pyridone-5-carboxamide
Cofactors and vitamins
stearate (18:0)
Lipid
ethanolamine
Lipid
succinylcarnitine
Energy
octanoylcarnitine
Lipid
campesterol
Lipid
2-linoleoylglycerophosphocholine*
Lipid
myo-inositol
Lipid
cholesterol
Lipid
pantothenate
Cofactors and vitamins

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 905 | 1,2-propanediol | Lipid | Ketone bodies | 57-55-6; | C00717,C02912,C00583,C01506,C02917 |
| 532 | 1,3-dihydroxyacetone | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 62147-49-3; | C00184 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 154-58-5; | C07326 |
| 523 | 1,6-anhydroglucose | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 498-07-7; | |
| 636 | 10-heptadecenoate (17:1n7) | Lipid | Long chain fatty acid | 29743-97-3; | |
| 742 | 13-methylmyristic acid | Lipid | Fatty acid, branched | 2485-71-4; | |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | Lipid | Fatty acid, branched | | |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | Lipid | Lysolipid | | |
| 938 | 1-linoleoylglycerophosphocholine | Lipid | Lysolipid | | C04100 |
| 926 | 1-myristoylglycerophosphocholine | Lipid | Lysolipid | 20559-16-4; | |
| 936 | 1-oleoylglycerophosphocholine | Lipid | Lysolipid | 19420-56-5; | |
| 915 | 1-oleoylglycerophosphoethanolamine | Lipid | Lysolipid | | |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | Lipid | Monoacylglycerol | 542-44-9; | |
| 929 | 1-palmitoylglycerophosphocholine | Lipid | Lysolipid | 17364-16-8; | |
| 909 | 1-palmitoylglycerophosphoethanolamine | Lipid | Lysolipid | | |
| 934 | 1-stearoylglycerophosphocholine | Lipid | Lysolipid | 19420-57-6; | |
| 533 | 2,3-diphosphoglycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 102783-53-9; | C01159 |
| 263 | 2-aminobutyrate | Amino acid | Butanoate metabolism | 1492-24-6; | C02261 |
| 945 | 2-arachidonoylglycerophosphocholine* | Lipid | Lysolipid | | |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | Lipid | Lysolipid | | |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | Lipid | Lysolipid | | |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | Lipid | Lysolipid | | |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | Xenobiotics | Chemical | | |
| 229 | 2-hydroxybutyrate (AHB) | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 3347-90-8; | C05984 |
| 714 | 2-hydroxyglutarate | Lipid | Fatty acid, dicarboxylate | 40951-21-1; | C02630 |
| 706 | 2-hydroxypalmitate | Lipid | Fatty acid, monohydroxy | 764-67-0; | |
| 939 | 2-linoleoylglycerophosphocholine* | Lipid | Lysolipid | | |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 202 | 2-methylbutyroylcarnitine | Amino acid | Valine, leucine and isoleucine metabolism | 31023-25-3; | |
| 937 | 2-oleoylglycerophosphocholine* | Lipid | Lysolipid | | |
| 930 | 2-palmitoylglycerophosphocholine* | Lipid | Lysolipid | | |
| 935 | 2-stearoylglycerophosphocholine* | Lipid | Lysolipid | | |
| 821 | 3-dehydrocarnitine* | Lipid | Carnitine metabolism | 10457-99-5; | C02636 |
| 170 | 3-indoxyl sulfate | Amino acid | Tryptophan metabolism | 2642-37-7; | |
| 172 | 3-methyl-2-oxobutyrate | Amino acid | Valine, leucine and isoleucine metabolism | 3715-29-5; | C00141 |
| 173 | 3-methyl-2-oxovalerate | Amino acid | Valine, leucine and isoleucine metabolism | 51829-07-3; | C00671 |
| 529 | 3-phosphoglycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 80731-10-8; | C00597 |
| 193 | 4-methyl-2-oxopentanoate | Amino acid | Valine, leucine and isoleucine metabolism | 816-66-0; | C00233 |
| 266 | 5-methylthioadenosine (MTA) | Amino acid | Polyamine metabolism | 2457-80-9; | C00170 |
| 282 | 5-oxoproline | Amino acid | Glutathione metabolism | 98-79-3; | C01879 |
| 545 | 6-phosphogluconate | Carbohydrate | Nucleotide sugars, pentose metabolism | 921-62-0;53411-70-4; | C00345 |
| 1024 | 7-beta-hydroxycholesterol | Lipid | Sterol/Steroid | 566-27-8; | C03594 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | Lipid | Long chain fatty acid | | C14825 |
| 672 | 9,10-epoxystearate | Lipid | Fatty acid, oxidized | | |
| 822 | acetylcarnitine | Lipid | Carnitine metabolism | 5080-50-2; | C02571 |
| 601 | acetylphosphate | Energy | Oxidative phosphorylation | 94249-01-1; | C00227 |
| 1105 | adenine | Nucleotide | Purine metabolism, adenine containing | 73-24-5; | C00147 |
| 1106 | adenosine | Nucleotide | Purine metabolism, adenine containing | 58-61-7; | C00212 |
| 1116 | adenosine 5'-diphosphate (ADP) | Nucleotide | Purine metabolism, adenine containing | 20398-34-9; | C00008 |
| 1232 | adenosine 5'diphosphoribose | Cofactors and vitamins | Nicotinate and nicotinamide metabolism | 68414-18-6; | C00301 |
| 1114 | adenosine 5'-monophosphate (AMP) | Nucleotide | Purine metabolism, adenine containing | 149022-20-8; | C00020 |
| 665 | adrenate (22:4n6) | Lipid | Long chain fatty acid | 2091-25-0; | C16527 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 27 | alanine | Amino acid | Alanine and aspartate metabolism | 56-41-7; | C00041 |
| 1150 | allantoin | Nucleotide | Purine metabolism, urate metabolism | 97-59-6; | C02350 |
| 179 | alpha-hydroxyisocaproate | Amino acid | Valine, leucine and isoleucine metabolism | 10303-64-7; | C03264 |
| 198 | alpha-hydroxyisovalerate | Amino acid | Valine, leucine and isoleucine metabolism | 600-37-3; | |
| 1266 | alpha-tocopherol | Cofactors and vitamins | Tocopherol metabolism | 59-02-9;10191-41-0; | C02477 |
| 1034 | androsterone sulfate | Lipid | Sterol/Steroid | 2479-86-9 ; | C00523 |
| 566 | arabinose | Carbohydrate | Nucleotide sugars, pentose metabolism | 28697-53-2; | C00181 |
| 546 | arabitol | Carbohydrate | Nucleotide sugars, pentose metabolism | 488-82-4; | C00474 |
| 1202 | arabonate | Cofactors and vitamins | Ascorbate and aldarate metabolism | 7643-75-7; | |
| 659 | arachidonate (20:4n6) | Lipid | Long chain fatty acid | 506-32-1; | C00219 |
| 241 | arginine | Amino acid | Urea cycle; arginine-, proline-, metabolism | 1119-34-2; | C00062 |
| 25 | asparagine | Amino acid | Alanine and aspartate metabolism | 70-47-3; | C00152 |
| 24 | aspartate | Amino acid | Alanine and aspartate metabolism | 56-84-8; | C00049 |
| 721 | azelate (nonanedioate) | Lipid | Fatty acid, dicarboxylate | 123-99-9; | C08261 |
| 26 | beta-alanine | Amino acid | Alanine and aspartate metabolism | 56-41-7;107-95-9; | C00099 |
| 7 | beta-hydroxypyruvate | Amino acid | Glycine, serine and threonine metabolism | 3369-79-7; | C00168 |
| 22 | betaine | Amino acid | Glycine, serine and threonine metabolism | 107-43-7; | |
| 1057 | beta-sitosterol | Lipid | Sterol/Steroid | 83-46-5; | C01753 |
| 1216 | biliverdin | Cofactors and vitamins | Hemoglobin and porphyrin metabolism | 55482-27-4;55482-27-4 ; | C00500 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 811 | butyrylcarnitine | Lipid | Fatty acid metabolism (also BCAA metabolism) | 25576-40-3; | |
| 1612 | caffeine | Xenobiotics | Xanthine metabolism | 58-08-2; | C07481 |
| 1059 | campesterol | Lipid | Sterol/Steroid | 474-62-4; | C01789 |
| 622 | caprate (10:0) | Lipid | Medium chain fatty acid | 112-37-8; | C01571 |
| 618 | caproate (6:0) | Lipid | Medium chain fatty acid | 142-62-1; | C01585 |
| 620 | caprylate (8:0) | Lipid | Medium chain fatty acid | 124-07-2; | C06423 |
| 820 | carnitine | Lipid | Carnitine metabolism | 461-05-2; | |
| 1300 | catechol sulfate | Xenobiotics | Benzoate metabolism | | C00090 |
| 164 | C-glycosyltryptophan* | Amino acid | Tryptophan metabolism | | |
| 1020 | cholesterol | Lipid | Sterol/Steroid | 57-88-5; | C00187 |
| 881 | choline | Lipid | Glycerolipid metabolism | 67-48-1; | |
| 582 | cis-aconitate | Energy | Krebs cycle | 585-84-2; | C00417 |
| 641 | cis-vaccenate (18:1n7) | Lipid | Long chain fatty acid | 693-72-1; | C08367 |
| 579 | citrate | Energy | Krebs cycle | 77-92-9; | C00158 |
| 248 | citrulline | Amino acid | Urea cycle; arginine-, proline-, metabolism | 372-75-8; | C00327 |
| 259 | creatine | Amino acid | Creatine metabolism | 57-00-1; | C00300 |
| 260 | creatinine | Amino acid | Creatine metabolism | 60-27-5; | C00791 |
| 213 | cysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 52-90-4;56-89-3; | C00097 |
| 819 | deoxycarnitine | Lipid | Carnitine metabolism | 6249-56-5; | C01181 |
| 655 | dihomo-linoleate (20:2n6) | Lipid | Long chain fatty acid | 2091-39-6; | C16525 |
| 609 | dihomo-linolenate (20:3n3 or n6) | Lipid | Essential fatty acid | | C03242 |
| 531 | dihydroxyacetone phosphate (DHAP) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 102783-56-2; | C00111 |
| 3 | dimethylglycine | Amino acid | Glycine, serine and threonine metabolism | 1118-68-9; | C01026 |
| 613 | docosahexaenoate (DHA; 22:6n3) | Lipid | Essential fatty acid | 6217-54-5; | C06429 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | Lipid | Essential fatty acid | 2234-74-4 ; | C16513 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | Lipid | Essential fatty acid | 10-2005-9;10417-94-4; | C06428 |
| 1565 | ergothioneine | Xenobiotics | Food component/Plant | 58511-63-0; | C05570 |
| 735 | erucamide | Lipid | Fatty acid, amide | 112-84-5; | |
| 1632 | erythritol | Xenobiotics | Sugar, sugar substitute, starch | 149-32-6; | C00503 |
| 453 | erythronate* | Carbohydrate | Aminosugars metabolism | 13752-84-6; | |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 876 | ethanolamine | Lipid | Glycerolipid metabolism | 141-43-5; | C00189 |
| 472 | fructose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 57-48-7; | C00095 |
| 524 | fructose-6-phosphate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 103213-47-4; | C05345 |
| 594 | fumarate | Energy | Krebs cycle | 100-17-8; | C00122 |
| 404 | gamma-glutamylleucine | Peptide | gamma-glutamyl | 2566-39-4; | |
| 521 | glucose | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 50-99-7; | C00293 |
| 519 | glucose-6-phosphate (G6P) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 103192-55-8; | C00668 |
| 39 | glutamate | Amino acid | Glutamate metabolism | 56-86-0; | C00025 |
| 44 | glutamine | Amino acid | Glutamate metabolism | 56-85-9; | C00064 |
| 80 | glutaroyl carnitine | Amino acid | Lysine metabolism | 102636-82-8; | |
| 283 | glutathione, oxidized (GSSG) | Amino acid | Glutathione metabolism | 103239-24-3; | C00127 |
| 280 | glutathione, reduced (GSH) | Amino acid | Glutathione metabolism | 70-18-8; | C00051 |
| 517 | glycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 600-19-1; | C00258 |
| 882 | glycerol 3-phosphate (G3P) | Lipid | Glycerolipid metabolism | 29849-82-9; | C00093 |
| 883 | glycerophosphorylcholine (GPC) | Lipid | Glycerolipid metabolism | 28319-77-9; | C00670 |
| 1 | glycine | Amino acid | Glycine, serine and threonine metabolism | 56-40-6; | C00037 |
| 851 | glycochenodeoxycholate | Lipid | Bile acid metabolism | 16564-43-5; | C05466 |
| 840 | glycocholate | Lipid | Bile acid metabolism | 475-31-0;863-57-0; | C01921 |
| 849 | glycodeoxycholate | Lipid | Bile acid metabolism | 360-65-6; | C05464 |
| 1318 | glycolate (hydroxyacetate) | Xenobiotics | Chemical | 79-14-1; | C00160 |
| 1128 | guanosine | Nucleotide | Purine metabolism, guanine containing | 118-00-3; | C00387 |
| 1212 | heme* | Cofactors and vitamins | Hemoglobin and porphyrin metabolism | 14875-96-8; | |
| 619 | heptanoate (7:0) | Lipid | Medium chain fatty acid | 111-14-8; | C17714 |
| 823 | hexanoylcarnitine | Lipid | Carnitine metabolism | 6920-35-0; | C01585 |
| 1288 | hippurate | Xenobiotics | Benzoate metabolism | 495-69-2; | C01586 |
| 50 | histidine | Amino acid | Histidine metabolism | 5934-29-2; | C00135 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 231 | homocysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 454-29-5; | C00155 |
| 1585 | homostachydrine* | Xenobiotics | Food component/Plant | 1195-94-4; | C08283 |
| 206 | hydroxyisovaleroyl carnitine | Amino acid | Valine, leucine and isoleucine metabolism | 99159-87-2; | |
| 1098 | hypoxanthine | Nucleotide | Purine metabolism, (hypo)xanthine/inosine containing | 68-94-0; | C00262 |
| 1101 | inosine 5'-monophosphate (IMP) | Nucleotide | Purine metabolism, (hypo)xanthine/inosine containing | 4691-65-0; | C00130 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | | |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | Carbohydrate | Nucleotide sugars, pentose metabolism | | |
| 496 | Isobar: sorbitol, mannitol | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | | C00392,C01722,C01697,C01489,C00794,C01507 |
| 200 | isobutyrylcarnitine | Amino acid | Valine, leucine and isoleucine metabolism | 25518-49-4; | |
| 180 | isoleucine | Amino acid | Valine, leucine and isoleucine metabolism | 73-32-5; | C00407 |
| 478 | isomaltose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 499-40-1; | C00252 |
| 205 | isovalerylcarnitine | Amino acid | Valine, leucine and isoleucine metabolism | | |
| 144 | kynurenine | Amino acid | Tryptophan metabolism | 2922-83-0; | C00328 |
| 536 | lactate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 79-33-4; | C00186 |
| 1018 | lathosterol | Lipid | Sterol/Steroid | 80-99-9 ; | C01189 |
| 625 | laurate (12:0) | Lipid | Medium chain fatty acid | 143-07-7; | C02679 |
| 181 | leucine | Amino acid | Valine, leucine and isoleucine metabolism | 61-90-5; | C00123 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 604 | linoleate (18:2n6) | Lipid | Essential fatty acid | 60-33-3; | C01595 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | Lipid | Essential fatty acid | | C06427 |
| 69 | lysine | Amino acid | Lysine metabolism | 56-87-1; | C00047 |
| 598 | malate | Energy | Krebs cycle | 6915-15-7; | C00149 |
| 482 | maltose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 6363-53-7; | C00208 |
| 487 | mannose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 3458-28-4; | C00159 |
| 489 | mannose-6-phosphate | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 70442-25-0;104872-94-8; | C00275 |
| 635 | margarate (17:0) | Lipid | Long chain fatty acid | 506-12-7; | |
| 658 | mead acid (20:3n9) | Lipid | Long chain fatty acid | 20590-32-3; | |
| 225 | methionine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 63-68-3; | C00073 |
| 890 | myo-inositol | Lipid | Inositol metabolism | 87-89-8; | C00137 |
| 629 | myristate (14:0) | Lipid | Long chain fatty acid | 544-63-8; | C06424 |
| 630 | myristoleate (14:1n5) | Lipid | Long chain fatty acid | 544-64-9 ; | C08322 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | Cofactors and vitamins | Nicotinate and nicotinamide metabolism | 701-44-0; | C05842 |
| 75 | N-6-trimethyllysine | Amino acid | Lysine metabolism | 23284-33-5; | |
| 4 | N-acetylglycine | Amino acid | Glycine, serine and threonine metabolism | 543-24-8; | |
| 227 | N-acetylmethionine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 65-82-7; | C02712 |
| 455 | N-acetylneuraminate | Carbohydrate | Aminosugars metabolism | 131-48-6; | C00270 |
| 1221 | nicotinamide | Cofactors and vitamins | Nicotinate and nicotinamide metabolism | 98-92-0; | C00153 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | Cofactors and vitamins | Nicotinate and nicotinamide metabolism | 53-84-9; | C00003 |
| 825 | octanoylcarnitine | Lipid | Carnitine metabolism | 3671-77-0; | |
| 639 | oleate (18:1n9) | Lipid | Long chain fatty acid | 112-80-1; | C00712 |
| 835 | oleoylcarnitine | Lipid | Carnitine metabolism | | |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 285 | ophthalmate | Amino acid | Glutathione metabolism | 495-27-2; | |
| 244 | ornithine | Amino acid | Urea cycle; arginine-, proline-, metabolism | 3184-13-2; | C00077 |
| 632 | palmitate (16:0) | Lipid | Long chain fatty acid | 57-10-3; | C00249 |
| 633 | palmitoleate (16:1n7) | Lipid | Long chain fatty acid | 373-49-9; | C08362 |
| 1004 | palmitoyl sphingomyelin | Lipid | Sphingolipid | | |
| 833 | palmitoylcarnitine | Lipid | Carnitine metabolism | 6865-14-1; | |
| 1243 | pantothenate | Cofactors and vitamins | Pantothenate and CoA metabolism | 137-08-6; | C00864 |
| 1613 | paraxanthine | Xenobiotics | Xanthine metabolism | 611-59-6; | C13747 |
| 88 | p-cresol sulfate | Amino acid | Phenylalanine & tyrosine metabolism | 3233-57-7; | C01468 |
| 621 | pelargonate (9:0) | Lipid | Medium chain fatty acid | 112-05-0; | C01601 |
| 631 | pentadecanoate (15:0) | Lipid | Long chain fatty acid | 1002-84-2; | C16537 |
| 135 | phenol sulfate | Amino acid | Phenylalanine & tyrosine metabolism | 937-34-8; | C02180 |
| 128 | phenylacetylglutamine | Amino acid | Phenylalanine & tyrosine metabolism | 28047-15-6; | C05597 |
| 83 | phenylalanine | Amino acid | Phenylalanine & tyrosine metabolism | 63-91-2; | C00079 |
| 602 | phosphate | Energy | Oxidative phosphorylation | 7664-38-2 ; | C00009 |
| 534 | phosphoenolpyruvate (PEP) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 10526-80-4; | C00074 |
| 877 | phosphoethanolamine | Lipid | Glycerolipid metabolism | 1071-23-4; | C00346 |
| 74 | pipecolate | Amino acid | Lysine metabolism | 4043-87-2; | C00408 |
| 1531 | piperine | Xenobiotics | Food component/Plant | 94-62-2; | C03882 |
| 246 | proline | Amino acid | Urea cycle; arginine-, proline-, metabolism | 147-85-3; | C00148 |
| 809 | propionylcarnitine | Lipid | Fatty acid metabolism (also BCAA metabolism) | 17298-37-2 ; | C03017 |
| 1181 | pseudouridine | Nucleotide | Pyrimidine metabolism, uracil containing | 1445-07-4; | C02067 |
| 45 | pyroglutamine* | Amino acid | Glutamate metabolism | | |
| 603 | pyrophosphate (PPi) | Energy | Oxidative phosphorylation | 1466-09-3; | C00013 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 535 | pyruvate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 127-17-3; | C00022 |
| 1469 | ranitidine | Xenobiotics | Drug | 66357-59-3; | D00422 |
| 548 | ribitol | Carbohydrate | Nucleotide sugars, pentose metabolism | 488-81-3; | C00474 |
| 557 | ribose 5-phosphate | Carbohydrate | Nucleotide sugars, pentose metabolism | 18265-46-8;108321-05-7; | C00117 |
| 559 | ribulose | Carbohydrate | Nucleotide sugars, pentose metabolism | 488-84-6; | C00309 |
| 224 | S-adenosylhomocysteine (SAH) | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 979-92-0; | C00021 |
| 551 | sedoheptulose-7-phosphate | Carbohydrate | Nucleotide sugars, pentose metabolism | 2646-35-7; | C05382 |
| 8 | serine | Amino acid | Glycine, serine and threonine metabolism | 56-45-1; | C00065 |
| 216 | S-methylcysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 1187-84-4; | |
| 281 | S-methylglutathione | Amino acid | Glutathione metabolism | 2922-56-7; | C11347 |
| 270 | spermidine | Amino acid | Polyamine metabolism | 124-20-9; | C00315 |
| 1584 | stachydrine | Xenobiotics | Food component/Plant | 4136-37-2; | C10172 |
| 637 | stearate (18:0) | Lipid | Long chain fatty acid | 57-11-4; | C01530 |
| 1005 | stearoyl sphingomyelin | Lipid | Sphingolipid | 85187-10-6;85187-10-6; | C00550 |
| 834 | stearoylcarnitine | Lipid | Carnitine metabolism | 18822-91-8; | |
| 591 | succinylcarnitine | Energy | Krebs cycle | | |
| 1662 | terephthalic acid | Xenobiotics | Phthalate | 100-21-0; | C06337 |
| 1614 | theobromine | Xenobiotics | Xanthine metabolism | 83-67-0; | C07480 |
| 1615 | theophylline | Xenobiotics | Xanthine metabolism | 58-55-9; | C07130 |
| 549 | threitol | Carbohydrate | Nucleotide sugars, pentose metabolism | 2418-52-2; | C16884 |
| 1199 | threonate | Cofactors and vitamins | Ascorbate and aldarate metabolism | 70753-61-6; | C01620 |
| 17 | threonine | Amino acid | Glycine, serine and threonine metabolism | 72-19-5; | C00188 |
| 252 | trans-4-hydroxyproline | Amino acid | Urea cycle; arginine-, proline-, metabolism | 51-35-4; | C01157 |

| PATHWAY SORT ORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | CAS | KEGG |
|---|---|---|---|---|---|
| 501 | trehalose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 6138-23-4; | C01083 |
| 1242 | trigonelline (N'-methylnicotinate) | Cofactors and vitamins | Nicotinate and nicotinamide metabolism | 6138-41-6 ; | |
| 145 | tryptophan | Amino acid | Tryptophan metabolism | 73-22-3; | C00078 |
| 151 | tryptophan betaine | Amino acid | Tryptophan metabolism | 20671-76-5; | C09213 |
| 99 | tyrosine | Amino acid | Phenylalanine & tyrosine metabolism | 60-18-4; | C00082 |
| 1149 | urate | Nucleotide | Purine metabolism, urate metabolism | 69-93-2;120K5305; | C00366 |
| 245 | urea | Amino acid | Urea cycle; arginine-, proline-, metabolism | 57-13-6; | C00086 |
| 1180 | uridine | Nucleotide | Pyrimidine metabolism, uracil containing | 58-96-8; | C00299 |
| 190 | valine | Amino acid | Valine, leucine and isoleucine metabolism | 72-18-4; | C00183 |
| 565 | xylitol | Carbohydrate | Nucleotide sugars, pentose metabolism | 87-99-0; | C00379 |
| 570 | xylonate | Carbohydrate | Nucleotide sugars, pentose metabolism | 73686-31-7; | C00502,C05411 |
| 569 | xylose | Carbohydrate | Nucleotide sugars, pentose metabolism | 609-06-3; | C00181 |

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|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 905 | 1,2-propanediol | HMDB01881 | 848,843 | 3,867,385 |
| 532 | 1,3-dihydroxyacetone | HMDB01882 | 72,358 | 86,588 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | HMDB02712 | 9,119,645 | 7,888,787 |
| 523 | 1,6-anhydroglucose | HMDB00640 | 383,268 | 291,235 |
| 636 | 10-heptadecenoate (17:1n7) | | 62,398 | 92,393 |
| 742 | 13-methylmyristic acid | | 62,907 | 119,838 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | | 113,326 | 278,457 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | HMDB11517 | 34,842 | 42,908 |
| 938 | 1-linoleoylglycerophosphocholine | | 272,671 | 354,976 |
| 926 | 1-myristoylglycerophosphocholine | HMDB10379 | | |
| 936 | 1-oleoylglycerophosphocholine | | 83,831 | 44,483 |
| 915 | 1-oleoylglycerophosphoethanolamine | HMDB11506 | 20,885 | 24,750 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | | 15,799 | 43,332 |
| 929 | 1-palmitoylglycerophosphocholine | | 339,238 | 368,197 |
| 909 | 1-palmitoylglycerophosphoethanolamine | HMDB11503 | 20,300 | 27,592 |
| 934 | 1-stearoylglycerophosphocholine | | 234,253 | 155,235 |
| 533 | 2,3-diphosphoglycerate | HMDB01294 | 439,404 | 176,181 |
| 263 | 2-aminobutyrate | HMDB00650 | 1,286,677 | 1,365,578 |
| 945 | 2-arachidonoylglycerophosphocholine* | | 30,785 | 33,968 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | | 106,856 | 90,289 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | | 50,987 | |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | | 32,223 | 51,932 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | | 34,165 | 41,323 |
| 229 | 2-hydroxybutyrate (AHB) | HMDB00008 | 1,395,042 | 1,168,788 |
| 714 | 2-hydroxyglutarate | HMDB00606 | 67,436 | 55,569 |
| 706 | 2-hydroxypalmitate | | 44,836 | 57,604 |
| 939 | 2-linoleoylglycerophosphocholine* | | | 88,889 |

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|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 202 | 2-methylbutyroylcarnitine | HMDB00378 | 47,519 | 54,219 |
| 937 | 2-oleoylglycerophosphocholine* | | | |
| 930 | 2-palmitoylglycerophosphocholine* | | | |
| 935 | 2-stearoylglycerophosphocholine* | | 65,500 | |
| 821 | 3-dehydrocarnitine* | HMDB12154 | 1,065,773 | 977,149 |
| 170 | 3-indoxyl sulfate | HMDB00682 | 11,032 | 8,631 |
| 172 | 3-methyl-2-oxobutyrate | HMDB00019 | 38,821 | 44,517 |
| 173 | 3-methyl-2-oxovalerate | HMDB03736 | 53,292 | 53,366 |
| 529 | 3-phosphoglycerate | HMDB00807 | 2,151,451 | 1,081,048 |
| 193 | 4-methyl-2-oxopentanoate | HMDB00695 | 116,549 | 122,839 |
| 266 | 5-methylthioadenosine (MTA) | HMDB01173 | 46,891 | 84,011 |
| 282 | 5-oxoproline | HMDB00267 | 46,823 | 170,475 |
| 545 | 6-phosphogluconate | HMDB01316 | 188,497 | 90,500 |
| 1024 | 7-beta-hydroxycholesterol | HMDB06119 | 37,063 | 32,538 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | HMDB04701 | 15,263 | 86,068 |
| 672 | 9,10-epoxystearate | | 292,557 | 5,466,700 |
| 822 | acetylcarnitine | HMDB00201 | 3,688,832 | 3,081,463 |
| 601 | acetylphosphate | HMDB01494 | 3,238,971 | 3,234,994 |
| 1105 | adenine | HMDB00034 | 46,158,980 | 36,248,408 |
| 1106 | adenosine | HMDB00050 | | 15,757 |
| 1116 | adenosine 5'-diphosphate (ADP) | HMDB01341 | 251,985 | 267,661 |
| 1232 | adenosine 5'diphosphoribose | HMDB01178 | 131,568 | 117,241 |
| 1114 | adenosine 5'-monophosphate (AMP) | HMDB00045 | 2,991,014 | 4,314,713 |
| 665 | adrenate (22:4n6) | HMDB02226 | 34,852 | 145,403 |

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|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 27 | alanine | HMDB00161 | 49,301,460 | 46,689,744 |
| 1150 | allantoin | HMDB00462 | 39,195 | 27,663 |
| 179 | alpha-hydroxyisocaproate | HMDB00746 | | |
| 198 | alpha-hydroxyisovalerate | HMDB00407 | 406,667 | 337,453 |
| 1266 | alpha-tocopherol | HMDB01893 | 259,705 | 236,793 |
| 1034 | androsterone sulfate | HMDB02759 | 6,335 | 4,875 |
| 566 | arabinose | HMDB00646 | 359,692 | 285,425 |
| 546 | arabitol | HMDB01851 | 608,598 | 484,073 |
| 1202 | arabonate | HMDB00539 | 109,163 | 89,223 |
| 659 | arachidonate (20:4n6) | HMDB01043 | 850,050 | 1,218,465 |
| 241 | arginine | HMDB00517 | 1,044,174 | 521,652 |
| 25 | asparagine | HMDB00168 | 1,333,427 | 1,139,404 |
| 24 | aspartate | HMDB00191 | 5,837,734 | 5,138,599 |
| 721 | azelate (nonanedioate) | HMDB00784 | 7,020 | 18,214 |
| 26 | beta-alanine | HMDB00056 | 84,654 | 94,481 |
| 7 | beta-hydroxypyruvate | HMDB01352 | 341,291 | 239,597 |
| 22 | betaine | HMDB00043 | 1,105,156 | 991,686 |
| 1057 | beta-sitosterol | HMDB00852 | 24,409 | |
| 1216 | biliverdin | HMDB01008 | | |

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|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 811 | butyrylcarnitine | | 16,911 | 14,330 |
| 1612 | caffeine | HMDB01847 | 2,855,568 | 2,509,127 |
| 1059 | campesterol | HMDB02869 | 237,124 | 110,634 |
| 622 | caprate (10:0) | HMDB00511 | 15,587 | 28,666 |
| 618 | caproate (6:0) | HMDB00535 | 77,173 | 55,538 |
| 620 | caprylate (8:0) | HMDB00482 | 13,339 | 30,641 |
| 820 | carnitine | | 834,820 | 718,340 |
| 1300 | catechol sulfate | | 91,756 | 83,703 |
| 164 | C-glycosyltryptophan* | | 28,900 | 25,554 |
| 1020 | cholesterol | HMDB00067 | 34,703,420 | 32,446,710 |
| 881 | choline | | 645,180 | 780,927 |
| 582 | cis-aconitate | HMDB00072 | 560,918 | 929,571 |
| 641 | cis-vaccenate (18:1n7) | | 292,696 | 194,918 |
| 579 | citrate | HMDB00094 | 394,077,408 | 320,473,280 |
| 248 | citrulline | HMDB00904 | 148,972 | 145,526 |
| 259 | creatine | HMDB00064 | 3,278,860 | 3,139,046 |
| 260 | creatinine | HMDB00562 | 324,911 | 388,210 |
| 213 | cysteine | HMDB00574 | 634,807 | 652,845 |
| 819 | deoxycarnitine | HMDB01161 | 548,836 | 478,623 |
| 655 | dihomo-linoleate (20:2n6) | | 35,591 | 56,119 |
| 609 | dihomo-linolenate (20:3n3 or n6) | HMDB02925 | 81,689 | 109,604 |
| 531 | dihydroxyacetone phosphate (DHAP) | HMDB01473 | 23,885 | 69,834 |
| 3 | dimethylglycine | HMDB00092 | 267,234 | 277,681 |
| 613 | docosahexaenoate (DHA; 22:6n3) | HMDB02183 | 127,566 | 212,381 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | HMDB01976 | 51,249 | 73,295 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | HMDB01999 | 178,046 | 249,841 |
| 1565 | ergothioneine | HMDB03045 | 535,149 | 531,221 |
| 735 | erucamide | | 139,553 | 198,771 |
| 1632 | erythritol | HMDB02994 | 918,980 | 1,080,344 |
| 453 | erythronate* | HMDB00613 | 313,920 | 376,749 |

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|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 876 | ethanolamine | HMDB00149 | 321,089 | 658,117 |
| 472 | fructose | HMDB00660 | 65,757,520 | 63,837,628 |
| 524 | fructose-6-phosphate | HMDB00124 | 496,403 | 512,296 |
| 594 | fumarate | HMDB00134 | 275,184 | 296,538 |
| 404 | gamma-glutamylleucine | HMDB11171 | 29,809 | 24,092 |
| 521 | glucose | HMDB00122 | 1,100,230,656 | 954,082,560 |
| 519 | glucose-6-phosphate (G6P) | HMDB01401 | 1,454,115 | 1,323,591 |
| 39 | glutamate | HMDB03339 | 5,532,164 | 4,146,794 |
| 44 | glutamine | HMDB00641 | 1,830,972 | 1,718,438 |
| 80 | glutaroyl carnitine | HMDB13130 | 19,378 | 14,312 |
| 283 | glutathione, oxidized (GSSG) | HMDB03337 | 1,549,227 | 1,150,501 |
| 280 | glutathione, reduced (GSH) | HMDB00125 | 26,491,108 | 17,362,302 |
| 517 | glycerate | HMDB00139 | 264,687 | 360,365 |
| 882 | glycerol 3-phosphate (G3P) | HMDB00126 | 322,127 | 285,538 |
| 883 | glycerophosphorylcholine (GPC) | HMDB00086 | 184,227 | 155,277 |
| 1 | glycine | HMDB00123 | 31,483,824 | 30,068,884 |
| 851 | glycochenodeoxycholate | HMDB00637 | 16,931 | 16,697 |
| 840 | glycocholate | HMDB00138 | 6,120 | 4,136 |
| 849 | glycodeoxycholate | HMDB00631 | 6,487 | |
| 1318 | glycolate (hydroxyacetate) | HMDB00115 | 425,658 | 396,184 |
| 1128 | guanosine | HMDB00133 | 40,847 | 33,118 |
| 1212 | heme* | | 1,775,876 | 524,329 |
| 619 | heptanoate (7:0) | HMDB00666 | 10,987 | 17,158 |
| 823 | hexanoylcarnitine | HMDB00705 | 70,206 | 34,266 |
| 1288 | hippurate | HMDB00714 | 58,525 | 52,699 |
| 50 | histidine | HMDB00177 | 36,496 | 39,560 |

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|---|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 | |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 | |
| | | **SAMPLE ID** | 997731 | 997714 | |
| | | **PARENT SAMPLE ID** | 991346 | 991347 | |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 | |
| | | **COND DAY** | T2 D0 | T2 D7 | |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 | |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 | |
| 231 | homocysteine | HMDB00742 | 16,193 | 24,733 | |
| 1585 | homostachydrine* | | 49,015 | 41,677 | |
| 206 | hydroxyisovaleroyl carnitine | | 193,039 | 159,446 | |
| 1098 | hypoxanthine | HMDB00157 | 255,963 | 315,974 | |
| 1101 | inosine 5'-monophosphate (IMP) | HMDB00175 | 104,400 | 190,719 | |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | | 73,077 | 72,990 | |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | | 87,743 | 122,479 | |
| 496 | Isobar: sorbitol, mannitol | HMDB00247 | 18,878,152 | 16,521,461 | |
| 200 | isobutyrylcarnitine | | 155,407 | 137,258 | |
| 180 | isoleucine | HMDB00172 | 4,247,789 | 3,651,103 | |
| 478 | isomaltose | HMDB02923 | 2,211,305 | 1,527,311 | |
| 205 | isovalerylcarnitine | HMDB00688 | 90,170 | 74,684 | |
| 144 | kynurenine | HMDB00684 | 115,490 | 109,456 | |
| 536 | lactate | HMDB00190 | 226,508,752 | 661,456,640 | |
| 1018 | lathosterol | HMDB01170 | 75,256 | 82,920 | |
| 625 | laurate (12:0) | HMDB00638 | 110,171 | 127,732 | |
| 181 | leucine | HMDB00687 | 7,866,940 | 7,253,589 | |

| | | | | |
|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 604 | linoleate (18:2n6) | HMDB00673 | 1,811,663 | 2,917,321 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | HMDB01388 | 446,144 | 662,587 |
| 69 | lysine | HMDB00182 | 2,060,373 | 2,375,808 |
| 598 | malate | HMDB00156 | 802,391 | 1,133,712 |
| 482 | maltose | HMDB00163 | 1,213,462 | 1,061,234 |
| 487 | mannose | HMDB00169 | 15,465,050 | 13,156,129 |
| 489 | mannose-6-phosphate | HMDB01078 | 223,451 | 283,027 |
| 635 | margarate (17:0) | HMDB02259 | 281,578 | 453,773 |
| 658 | mead acid (20:3n9) | HMDB10378 | 16,233 | 21,473 |
| 225 | methionine | HMDB00696 | 846,151 | 600,002 |
| 890 | myo-inositol | HMDB00211 | 1,625,582 | 1,678,786 |
| 629 | myristate (14:0) | HMDB00806 | 391,047 | 759,814 |
| 630 | myristoleate (14:1n5) | HMDB02000 | 15,905 | 17,880 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | HMDB04193 | 296,358 | 288,787 |
| 75 | N-6-trimethyllysine | | 95,814 | 90,583 |
| 4 | N-acetylglycine | HMDB00532 | 97,087 | 71,552 |
| 227 | N-acetylmethionine | HMDB11745 | | 4,377 |
| 455 | N-acetylneuraminate | HMDB00230 | 28,716 | 46,233 |
| 1221 | nicotinamide | HMDB01406 | 2,316,366 | 2,552,832 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | HMDB00902 | 3,710 | 3,123 |
| 825 | octanoylcarnitine | | 56,396 | 54,946 |
| 639 | oleate (18:1n9) | HMDB00207 | 504,038 | 723,002 |
| 835 | oleoylcarnitine | HMDB05065 | 75,050 | 74,734 |

| | | | | |
|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 285 | ophthalmate | HMDB05765 | 116,806 | 21,847 |
| 244 | ornithine | HMDB03374 | 12,248,723 | 12,194,642 |
| 632 | palmitate (16:0) | HMDB00220 | 5,527,414 | 8,850,880 |
| 633 | palmitoleate (16:1n7) | HMDB03229 | 349,886 | 541,673 |
| 1004 | palmitoyl sphingomyelin | | 14,824,070 | 13,545,406 |
| 833 | palmitoylcarnitine | | 64,191 | 29,147 |
| 1243 | pantothenate | HMDB00210 | 97,336 | 91,691 |
| 1613 | paraxanthine | HMDB01860 | 520,139 | 445,282 |
| 88 | p-cresol sulfate | | 81,049 | 73,182 |
| 621 | pelargonate (9:0) | HMDB00847 | 170,061 | 292,268 |
| 631 | pentadecanoate (15:0) | HMDB00826 | 164,538 | 256,296 |
| 135 | phenol sulfate | | 22,748 | 21,602 |
| 128 | phenylacetylglutamine | HMDB06344 | 83,959 | 75,806 |
| 83 | phenylalanine | HMDB00159 | 8,846,152 | 8,204,792 |
| 602 | phosphate | HMDB01429 | 1,032,504,064 | 1,055,862,016 |
| 534 | phosphoenolpyruvate (PEP) | HMDB00263 | 464,449 | 166,197 |
| 877 | phosphoethanolamine | HMDB00224 | 82,493 | 71,777 |
| 74 | pipecolate | HMDB00070 | 107,952 | 92,948 |
| 1531 | piperine | | 97,887 | 107,407 |
| 246 | proline | HMDB00162 | 1,868,739 | 2,240,127 |
| 809 | propionylcarnitine | HMDB00824 | 824,474 | 702,798 |
| 1181 | pseudouridine | HMDB00767 | 14,590 | 12,637 |
| 45 | pyroglutamine* | | 81,527 | 64,527 |
| 603 | pyrophosphate (PPi) | HMDB00250 | 171,761 | 114,179 |

| | | | | |
|---|---|---|---|---|
| | | **SAMPLE NAME** | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | 991346 | 991347 |
| | | **ACTUAL** | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | T2 D0 | T2 D7 |
| 535 | pyruvate | HMDB00243 | 1,815,000 | 3,412,879 |
| 1469 | ranitidine | HMDB01930 | 366,122 | 357,222 |
| 548 | ribitol | HMDB00508 | 190,964 | 165,369 |
| 557 | ribose 5-phosphate | HMDB00618 | 174,472 | 170,644 |
| 559 | ribulose | HMDB00621,HMDB03371 | 19,113 | |
| 224 | S-adenosylhomocysteine (SAH) | HMDB00939 | 138,810 | 191,407 |
| 551 | sedoheptulose-7-phosphate | HMDB01068 | 67,916 | 22,290 |
| 8 | serine | HMDB03406 | 6,312,563 | 6,207,909 |
| 216 | S-methylcysteine | HMDB02108 | 188,357 | 196,891 |
| 281 | S-methylglutathione | | 39,472 | 24,727 |
| 270 | spermidine | HMDB01257 | 1,003,105 | 942,647 |
| 1584 | stachydrine | HMDB04827 | 187,777 | 130,368 |
| 637 | stearate (18:0) | HMDB00827 | 5,386,088 | 9,103,771 |
| 1005 | stearoyl sphingomyelin | HMDB01348 | 1,530,340 | 1,164,523 |
| 834 | stearoylcarnitine | HMDB00848 | 19,274 | |
| 591 | succinylcarnitine | | 328,477 | 332,975 |
| 1662 | terephthalic acid | HMDB02428 | 284,825 | 189,503 |
| 1614 | theobromine | HMDB02825 | 317,888 | 279,210 |
| 1615 | theophylline | HMDB01889 | 123,980 | 186,516 |
| 549 | threitol | HMDB04136 | 1,015,173 | 1,097,957 |
| 1199 | threonate | HMDB00943 | 553,578 | 487,811 |
| 17 | threonine | HMDB00167 | 166,448 | 163,121 |
| 252 | trans-4-hydroxyproline | HMDB00725 | 39,682 | 36,742 |

| | | | | | |
|---|---|---|---|---|---|
| | | **SAMPLE NAME** | | DARM-00001 | DARM-00002 |
| | | **CLIENT IDENTIFIER** | | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **SAMPLE ID** | | 997731 | 997714 |
| | | **PARENT SAMPLE ID** | | 991346 | 991347 |
| | | **ACTUAL** | | NHSCi 2003 T2 D0 | NHSCi 2003 T2 D7 |
| | | **COND DAY** | | T2 D0 | T2 D7 |
| | | **BRADFORD PROTEIN** | | 168.571 | 179.95 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | **Group HMDB** | | T2 D0 | T2 D7 |
| 501 | trehalose | HMDB00975 | | 80,991 | 488,438 |
| 1242 | trigonelline (N'-methylnicotinate) | HMDB00875 | | 262,040 | 245,429 |
| 145 | tryptophan | HMDB00929 | | 4,334,128 | 3,534,535 |
| 151 | tryptophan betaine | | | 1,527,459 | 1,476,027 |
| 99 | tyrosine | HMDB00158 | | 2,068,021 | 1,810,748 |
| 1149 | urate | HMDB00289 | | 180,006 | 175,475 |
| 245 | urea | HMDB00294 | | 32,700,246 | 27,281,750 |
| 1180 | uridine | HMDB00296 | | 13,411 | 21,360 |
| 190 | valine | HMDB00883 | | 8,529,817 | 8,012,101 |
| 565 | xylitol | HMDB00568 | | | |
| 570 | xylonate | | | 53,934 | 53,665 |
| 569 | xylose | HMDB00098 | | 108,343 | |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 905 | 1,2-propanediol | 8,051,589 | 7,677,646 | 9,385,429 | 597,231 |
| 532 | 1,3-dihydroxyacetone | 116,949 | 78,807 | 64,825 | 76,373 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 9,382,562 | 7,753,035 | 7,340,280 | 8,019,994 |
| 523 | 1,6-anhydroglucose | 270,657 | 368,639 | 345,543 | 301,535 |
| 636 | 10-heptadecenoate (17:1n7) | 66,109 | 68,237 | 110,751 | 66,773 |
| 742 | 13-methylmyristic acid | 133,631 | 124,948 | 169,573 | 48,932 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 262,782 | 235,729 | 364,262 | 136,907 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 26,206 | 25,676 | 30,731 | 26,039 |
| 938 | 1-linoleoylglycerophosphocholine | 221,573 | 229,916 | 307,841 | 260,253 |
| 926 | 1-myristoylglycerophosphocholine | 30,969 | 152,570 | 51,715 | |
| 936 | 1-oleoylglycerophosphocholine | 92,141 | 1,158,769 | 588,839 | |
| 915 | 1-oleoylglycerophosphoethanolamine | 13,225 | 14,470 | 12,040 | 17,656 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 40,748 | 41,028 | 35,678 | 33,251 |
| 929 | 1-palmitoylglycerophosphocholine | 523,311 | 6,332,508 | 4,069,074 | 281,646 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 20,110 | 23,692 | 23,426 | 16,617 |
| 934 | 1-stearoylglycerophosphocholine | 241,127 | 2,352,217 | 1,270,107 | 136,578 |
| 533 | 2,3-diphosphoglycerate | 34,908 | 8,377 | 7,875 | 570,388 |
| 263 | 2-aminobutyrate | 1,657,761 | 1,601,627 | 1,277,481 | 1,167,143 |
| 945 | 2-arachidonoylglycerophosphocholine* | | 294,864 | | |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 253,359 | 2,075,197 | 747,720 | 92,488 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 77,956 | 388,022 | 235,282 | 32,009 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 125,217 | 377,775 | 252,566 | |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 40,014 | | | 59,440 |
| 229 | 2-hydroxybutyrate (AHB) | 1,335,219 | 1,444,275 | 1,148,063 | 1,377,727 |
| 714 | 2-hydroxyglutarate | 123,980 | 98,129 | 136,377 | 69,535 |
| 706 | 2-hydroxypalmitate | 49,809 | 39,241 | 61,456 | 27,626 |
| 939 | 2-linoleoylglycerophosphocholine* | | 522,782 | 299,920 | |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 202 | 2-methylbutyroylcarnitine | 52,946 | 42,758 | 60,727 | 65,388 |
| 937 | 2-oleoylglycerophosphocholine* | 35,455 | 241,064 | 125,842 | |
| 930 | 2-palmitoylglycerophosphocholine* | 45,335 | 651,755 | 268,904 | 29,782 |
| 935 | 2-stearoylglycerophosphocholine* | | 235,000 | 115,914 | |
| 821 | 3-dehydrocarnitine* | 1,019,450 | 1,082,581 | 1,080,486 | 1,035,201 |
| 170 | 3-indoxyl sulfate | 9,820 | 10,439 | 10,683 | 9,098 |
| 172 | 3-methyl-2-oxobutyrate | 49,853 | 37,613 | 33,197 | 16,717 |
| 173 | 3-methyl-2-oxovalerate | 67,151 | 65,721 | 56,937 | 34,771 |
| 529 | 3-phosphoglycerate | 806,390 | 412,047 | 502,682 | 3,678,014 |
| 193 | 4-methyl-2-oxopentanoate | 148,392 | 116,731 | 109,200 | 68,101 |
| 266 | 5-methylthioadenosine (MTA) | 135,496 | 140,410 | 120,676 | 37,812 |
| 282 | 5-oxoproline | 288,258 | 395,101 | 514,532 | 51,196 |
| 545 | 6-phosphogluconate | 75,132 | 72,614 | 55,320 | 48,049 |
| 1024 | 7-beta-hydroxycholesterol | 31,754 | 44,742 | 30,148 | 11,625 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 136,205 | 137,891 | 156,214 | 6,467 |
| 672 | 9,10-epoxystearate | 6,637,511 | 6,963,358 | 8,534,965 | 228,260 |
| 822 | acetylcarnitine | 3,131,799 | 2,845,848 | 3,060,649 | 3,595,378 |
| 601 | acetylphosphate | 3,348,130 | 3,581,780 | 2,763,060 | 2,475,165 |
| 1105 | adenine | 27,343,090 | 22,142,156 | 18,066,456 | 45,361,896 |
| 1106 | adenosine | 16,563 | 22,620 | 34,703 | 26,151 |
| 1116 | adenosine 5'-diphosphate (ADP) | 171,632 | 191,221 | 232,063 | 300,865 |
| 1232 | adenosine 5'diphosphoribose | 120,812 | 112,168 | 111,040 | 130,405 |
| 1114 | adenosine 5'-monophosphate (AMP) | 4,124,498 | 4,000,580 | 6,321,126 | 5,120,702 |
| 665 | adrenate (22:4n6) | 67,195 | 98,837 | 94,853 | 30,373 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 27 | alanine | 59,739,956 | 61,392,076 | 58,225,072 | 41,559,608 |
| 1150 | allantoin | 29,024 | 17,404 | 30,483 | 27,655 |
| 179 | alpha-hydroxyisocaproate | 100,719 | 221,084 | 384,224 | |
| 198 | alpha-hydroxyisovalerate | 438,288 | 501,453 | 660,874 | 464,662 |
| 1266 | alpha-tocopherol | 277,769 | 285,258 | 215,883 | 207,352 |
| 1034 | androsterone sulfate | 5,868 | 5,622 | 5,121 | 5,870 |
| 566 | arabinose | 422,619 | 325,189 | 357,407 | 330,072 |
| 546 | arabitol | 650,198 | 631,961 | 512,654 | 573,008 |
| 1202 | arabonate | 82,115 | 110,045 | 108,000 | 116,187 |
| 659 | arachidonate (20:4n6) | 686,066 | 821,476 | 1,533,608 | 875,136 |
| 241 | arginine | 888,856 | 726,576 | 1,393,776 | 799,142 |
| 25 | asparagine | 1,190,101 | 1,147,523 | 847,738 | 1,213,263 |
| 24 | aspartate | 6,475,535 | 7,133,001 | 6,279,271 | 5,994,289 |
| 721 | azelate (nonanedioate) | 32,441 | 41,591 | 54,554 | 7,597 |
| 26 | beta-alanine | 94,272 | 92,691 | 63,966 | 52,945 |
| 7 | beta-hydroxypyruvate | 312,144 | 199,096 | 304,607 | 291,640 |
| 22 | betaine | 1,224,881 | 1,213,351 | 1,091,302 | 1,268,964 |
| 1057 | beta-sitosterol | 15,749 | 34,902 | 16,481 | 25,809 |
| 1216 | biliverdin | | 40,654 | 22,159 | 20,846 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 811 | butyrylcarnitine | 18,440 | 12,914 | | 18,606 |
| 1612 | caffeine | 2,755,255 | 2,649,273 | 2,555,892 | 2,809,313 |
| 1059 | campesterol | 228,484 | 178,116 | | 274,885 |
| 622 | caprate (10:0) | 37,090 | 31,072 | 29,263 | 13,557 |
| 618 | caproate (6:0) | 61,238 | 43,343 | 41,458 | 87,353 |
| 620 | caprylate (8:0) | 61,964 | 42,845 | 49,939 | 32,025 |
| 820 | carnitine | 823,844 | 802,720 | 810,327 | 748,275 |
| 1300 | catechol sulfate | 91,434 | 84,050 | 82,170 | 87,304 |
| 164 | C-glycosyltryptophan* | 27,003 | 27,122 | 27,774 | 30,009 |
| 1020 | cholesterol | 36,413,804 | 37,031,008 | 33,649,312 | 32,803,384 |
| 881 | choline | 758,785 | 844,880 | 906,633 | 782,707 |
| 582 | cis-aconitate | 971,813 | 965,590 | 1,091,042 | 634,631 |
| 641 | cis-vaccenate (18:1n7) | 103,745 | 137,179 | 194,116 | 115,498 |
| 579 | citrate | 324,530,176 | 289,676,608 | 256,915,088 | 380,581,440 |
| 248 | citrulline | 158,595 | 144,180 | 165,608 | 173,532 |
| 259 | creatine | 3,155,329 | 3,110,639 | 3,065,868 | 3,188,870 |
| 260 | creatinine | 368,395 | 396,776 | 310,196 | 370,502 |
| 213 | cysteine | 854,325 | 1,614,778 | 1,506,844 | 421,175 |
| 819 | deoxycarnitine | 540,779 | 475,548 | 514,399 | 578,492 |
| 655 | dihomo-linoleate (20:2n6) | 41,016 | 41,834 | 77,060 | 32,538 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 72,443 | 85,727 | 153,773 | 82,068 |
| 531 | dihydroxyacetone phosphate (DHAP) | 20,946 | 40,825 | | 3,139,871 |
| 3 | dimethylglycine | 246,687 | 437,855 | 240,986 | 191,525 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 158,153 | 210,643 | 370,969 | 137,766 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 79,287 | 82,416 | 143,061 | 55,064 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 140,590 | 215,800 | 301,430 | 193,132 |
| 1565 | ergothioneine | 497,357 | 461,335 | 520,948 | 539,562 |
| 735 | erucamide | 206,975 | 497,591 | 207,158 | 129,960 |
| 1632 | erythritol | 1,549,809 | 1,873,237 | 1,975,202 | 986,028 |
| 453 | erythronate* | 456,321 | 497,722 | 470,756 | 313,095 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 876 | ethanolamine | 714,292 | 651,519 | 519,216 | 393,396 |
| 472 | fructose | 80,913,064 | 86,507,560 | 78,355,280 | 53,150,484 |
| 524 | fructose-6-phosphate | 504,742 | 395,047 | 424,315 | 261,733 |
| 594 | fumarate | 271,306 | 297,773 | 418,249 | 312,444 |
| 404 | gamma-glutamylleucine | 23,286 | 31,492 | 23,785 | 26,039 |
| 521 | glucose | 1,053,598,976 | 1,032,565,824 | 1,029,962,432 | 1,050,528,832 |
| 519 | glucose-6-phosphate (G6P) | 1,583,868 | 930,779 | 1,246,771 | 114,535 |
| 39 | glutamate | 5,364,870 | 5,119,386 | 5,471,777 | 6,288,394 |
| 44 | glutamine | 1,462,849 | 1,421,720 | 1,185,657 | 1,966,634 |
| 80 | glutaroyl carnitine | 9,352 | | | 12,120 |
| 283 | glutathione, oxidized (GSSG) | 1,146,104 | 1,135,917 | 833,181 | 1,568,169 |
| 280 | glutathione, reduced (GSH) | 26,106,000 | 22,982,382 | 17,035,302 | 26,459,132 |
| 517 | glycerate | 470,668 | 586,381 | 575,996 | 309,751 |
| 882 | glycerol 3-phosphate (G3P) | 295,061 | 213,688 | 282,810 | 1,280,181 |
| 883 | glycerophosphorylcholine (GPC) | 148,839 | 150,884 | 168,429 | 155,419 |
| 1 | glycine | 43,565,284 | 53,847,536 | 62,256,112 | 28,291,758 |
| 851 | glycochenodeoxycholate | 15,191 | 13,326 | 16,755 | 16,503 |
| 840 | glycocholate | 8,157 | 7,388 | | 7,500 |
| 849 | glycodeoxycholate | | 11,419 | 10,286 | |
| 1318 | glycolate (hydroxyacetate) | 465,396 | 478,215 | 395,415 | 380,381 |
| 1128 | guanosine | 41,014 | 34,133 | 38,393 | 41,859 |
| 1212 | heme* | 946,633 | 6,250,787 | 1,578,698 | 865,836 |
| 619 | heptanoate (7:0) | 24,130 | 10,702 | 13,956 | 18,239 |
| 823 | hexanoylcarnitine | 43,055 | 33,403 | 54,792 | 65,873 |
| 1288 | hippurate | 55,127 | 55,540 | 59,143 | 54,622 |
| 50 | histidine | 34,184 | 52,873 | 45,252 | 54,626 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 231 | homocysteine | 48,090 | 76,061 | 65,983 | 19,970 |
| 1585 | homostachydrine* | 47,338 | 40,840 | 38,924 | 50,487 |
| 206 | hydroxyisovaleroyl carnitine | 209,280 | 189,954 | 206,345 | 201,272 |
| 1098 | hypoxanthine | 1,190,940 | 3,661,084 | 6,129,222 | 366,999 |
| 1101 | inosine 5'-monophosphate (IMP) | 269,325 | 175,203 | 195,010 | 82,146 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 71,000 | 58,710 | 67,460 | 329,423 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 57,383 | 93,775 | 46,916 | 502,465 |
| 496 | Isobar: sorbitol, mannitol | 20,448,232 | 19,889,494 | 17,503,946 | 19,898,894 |
| 200 | isobutyrylcarnitine | 137,471 | 127,764 | 121,604 | 169,915 |
| 180 | isoleucine | 4,536,709 | 4,544,457 | 4,538,633 | 4,536,955 |
| 478 | isomaltose | 2,297,650 | 1,930,628 | 1,563,279 | 1,479,343 |
| 205 | isovalerylcarnitine | 91,865 | 90,039 | 121,197 | 96,932 |
| 144 | kynurenine | 141,188 | 136,305 | 105,439 | 139,786 |
| 536 | lactate | 1,195,250,304 | 1,454,435,840 | 1,537,938,432 | 316,614,048 |
| 1018 | lathosterol | 116,987 | 77,676 | 76,679 | 68,518 |
| 625 | laurate (12:0) | 133,004 | 138,376 | 150,163 | 119,533 |
| 181 | leucine | 8,524,241 | 9,170,862 | 9,180,339 | 8,183,361 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 604 | linoleate (18:2n6) | 2,017,285 | 2,277,671 | 3,763,954 | 1,935,023 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 523,412 | 511,629 | 726,080 | 530,840 |
| 69 | lysine | 2,449,239 | 3,920,848 | 1,805,843 | 1,908,045 |
| 598 | malate | 1,151,802 | 1,247,215 | 1,410,160 | 722,792 |
| 482 | maltose | 1,244,747 | 1,238,197 | 1,089,176 | 1,109,965 |
| 487 | mannose | 13,836,418 | 14,351,988 | 13,004,333 | 14,288,494 |
| 489 | mannose-6-phosphate | 278,036 | 224,649 | 208,880 | 122,657 |
| 635 | margarate (17:0) | 454,264 | 358,713 | 548,762 | 290,791 |
| 658 | mead acid (20:3n9) | 10,342 | 12,297 | 36,027 | 19,527 |
| 225 | methionine | 591,278 | 442,776 | 412,237 | 910,720 |
| 890 | myo-inositol | 2,045,021 | 1,886,213 | 1,508,486 | 1,871,010 |
| 629 | myristate (14:0) | 846,052 | 704,453 | 856,844 | 365,057 |
| 630 | myristoleate (14:1n5) | | 15,417 | 37,796 | |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 299,484 | 200,879 | 219,238 | 247,312 |
| 75 | N-6-trimethyllysine | 125,710 | 108,226 | 88,378 | 81,227 |
| 4 | N-acetylglycine | 134,378 | 91,499 | 61,104 | 89,444 |
| 227 | N-acetylmethionine | | | 4,068 | 5,000 |
| 455 | N-acetylneuraminate | 82,934 | 111,325 | 81,073 | 41,976 |
| 1221 | nicotinamide | 2,839,631 | 3,421,625 | 2,577,569 | 2,419,713 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 3,646 | 7,612 | 3,594 | 5,164 |
| 825 | octanoylcarnitine | 66,639 | 68,985 | 65,843 | 49,823 |
| 639 | oleate (18:1n9) | 500,954 | 694,796 | 702,021 | 503,361 |
| 835 | oleoylcarnitine | 90,717 | 827,520 | 359,730 | 55,847 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 285 | ophthalmate | | 13,260 | | 126,322 |
| 244 | ornithine | 13,330,256 | 13,348,461 | 10,498,763 | 11,406,275 |
| 632 | palmitate (16:0) | 7,403,884 | 6,930,497 | 9,877,068 | 5,599,008 |
| 633 | palmitoleate (16:1n7) | 402,673 | 383,126 | 609,074 | 357,008 |
| 1004 | palmitoyl sphingomyelin | 15,296,857 | 15,483,889 | 13,799,316 | 13,666,355 |
| 833 | palmitoylcarnitine | 92,269 | 520,404 | 258,440 | 93,974 |
| 1243 | pantothenate | 96,511 | 88,079 | 92,747 | 97,366 |
| 1613 | paraxanthine | 581,962 | 600,267 | 498,181 | 517,976 |
| 88 | p-cresol sulfate | 77,606 | 71,521 | 78,245 | 79,054 |
| 621 | pelargonate (9:0) | 541,888 | 358,157 | 388,027 | 226,300 |
| 631 | pentadecanoate (15:0) | 230,847 | 218,632 | 297,162 | 159,741 |
| 135 | phenol sulfate | 21,654 | 19,965 | 19,700 | 23,306 |
| 128 | phenylacetylglutamine | 80,956 | 88,051 | 80,666 | 79,332 |
| 83 | phenylalanine | 10,777,701 | 10,596,395 | 9,766,167 | 9,265,584 |
| 602 | phosphate | 1,290,286,208 | 1,289,449,088 | 1,203,603,456 | 825,421,632 |
| 534 | phosphoenolpyruvate (PEP) | 55,665 | 22,811 | 39,021 | 519,173 |
| 877 | phosphoethanolamine | 99,221 | | 65,013 | 95,268 |
| 74 | pipecolate | 84,844 | 118,053 | 94,549 | 87,897 |
| 1531 | piperine | 63,157 | 80,667 | 69,635 | 96,486 |
| 246 | proline | 2,022,186 | 1,977,697 | 2,209,844 | 1,864,009 |
| 809 | propionylcarnitine | 707,248 | 591,287 | 635,194 | 769,841 |
| 1181 | pseudouridine | 10,690 | 9,596 | 11,550 | 8,068 |
| 45 | pyroglutamine* | 48,951 | 52,472 | 52,241 | 47,545 |
| 603 | pyrophosphate (PPi) | 120,252 | 94,482 | 36,279 | 160,293 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 535 | pyruvate | 3,584,718 | 1,392,119 | 883,286 | 104,646 |
| 1469 | ranitidine | 353,255 | 323,947 | 395,306 | 356,947 |
| 548 | ribitol | 264,230 | 170,760 | 262,227 | 199,769 |
| 557 | ribose 5-phosphate | 125,607 | 110,047 | 92,336 | 327,343 |
| 559 | ribulose | 21,528 | 29,620 | 5,901 | 36,306 |
| 224 | S-adenosylhomocysteine (SAH) | 218,707 | 180,852 | 240,547 | 136,466 |
| 551 | sedoheptulose-7-phosphate | 155,997 | 106,611 | 27,985 | |
| 8 | serine | 6,923,332 | 7,240,069 | 6,777,029 | 5,980,283 |
| 216 | S-methylcysteine | 207,436 | 225,249 | 203,359 | 155,595 |
| 281 | S-methylglutathione | 27,584 | 38,256 | 30,161 | 39,962 |
| 270 | spermidine | 1,226,414 | 1,160,830 | 1,181,574 | 993,676 |
| 1584 | stachydrine | 195,394 | 208,634 | 222,209 | 201,641 |
| 637 | stearate (18:0) | 7,954,844 | 7,000,055 | 9,915,066 | 5,389,298 |
| 1005 | stearoyl sphingomyelin | 1,229,736 | 1,340,268 | 1,390,094 | 1,200,951 |
| 834 | stearoylcarnitine | 78,930 | 363,625 | 178,108 | |
| 591 | succinylcarnitine | 366,863 | 359,724 | 404,492 | 323,401 |
| 1662 | terephthalic acid | 204,796 | 226,146 | 211,575 | 199,968 |
| 1614 | theobromine | 354,120 | 262,534 | 291,833 | 324,486 |
| 1615 | theophylline | 119,772 | 69,244 | 109,118 | 126,037 |
| 549 | threitol | 1,389,832 | 1,438,844 | 1,303,130 | 1,083,124 |
| 1199 | threonate | 577,713 | 520,950 | 565,903 | 422,204 |
| 17 | threonine | 168,561 | 167,515 | 185,889 | 162,617 |
| 252 | trans-4-hydroxyproline | 36,611 | 42,912 | 37,583 | 41,882 |

| | | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | 997743 | 997745 | 997721 | 997727 |
| | | 991348 | 991349 | 991350 | 991351 |
| | | NHSCi 2003 T2 D14 | NHSCi 2003 T2 D21 | NHSCi 2003 T2 D28 | NHSCi 2003 T1 D0 |
| | | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 501 | trehalose | 799,631 | 1,060,889 | 843,654 | 89,895 |
| 1242 | trigonelline (N'-methylnicotinate) | 250,669 | 258,900 | 252,621 | 274,003 |
| 145 | tryptophan | 4,758,198 | 4,512,919 | 4,266,043 | 4,030,519 |
| 151 | tryptophan betaine | 1,525,838 | 1,428,182 | 1,520,371 | 1,534,749 |
| 99 | tyrosine | 2,487,868 | 2,334,271 | 2,438,636 | 2,198,833 |
| 1149 | urate | 166,337 | 150,014 | 177,883 | 186,934 |
| 245 | urea | 34,699,208 | 32,933,632 | 30,938,074 | 30,904,742 |
| 1180 | uridine | 22,838 | 25,675 | 34,453 | 23,251 |
| 190 | valine | 9,654,649 | 9,108,516 | 9,098,879 | 9,146,812 |
| 565 | xylitol | | | | |
| 570 | xylonate | 81,607 | 73,825 | 102,421 | 100,853 |
| 569 | xylose | 56,695 | 78,572 | 100,976 | 48,763 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 905 | 1,2-propanediol | 5,094,592 | 7,900,588 | 11,946,278 | 9,815,234 |
| 532 | 1,3-dihydroxyacetone | 75,294 | 98,903 | 120,530 | 107,862 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 8,514,238 | 7,066,326 | 11,814,922 | 6,724,714 |
| 523 | 1,6-anhydroglucose | 393,854 | 400,508 | 409,846 | 316,366 |
| 636 | 10-heptadecenoate (17:1n7) | 77,209 | 76,842 | 89,804 | 68,109 |
| 742 | 13-methylmyristic acid | 112,010 | 145,087 | 167,105 | 144,375 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 183,732 | 244,720 | 287,861 | 217,988 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 26,056 | 27,509 | 36,945 | 20,343 |
| 938 | 1-linoleoylglycerophosphocholine | 228,535 | 240,843 | 503,766 | 217,971 |
| 926 | 1-myristoylglycerophosphocholine | 27,955 | 198,316 | 171,105 | 384,103 |
| 936 | 1-oleoylglycerophosphocholine | 249,026 | 805,615 | 1,160,093 | 1,969,326 |
| 915 | 1-oleoylglycerophosphoethanolamine | 24,152 | 5,933 | 32,349 | 11,154 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 28,985 | 44,659 | 32,712 | 41,689 |
| 929 | 1-palmitoylglycerophosphocholine | 1,681,923 | 4,234,489 | 7,516,405 | 8,921,981 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 21,884 | 15,622 | 42,151 | 18,028 |
| 934 | 1-stearoylglycerophosphocholine | 557,194 | 3,471,942 | 2,495,278 | 5,419,792 |
| 533 | 2,3-diphosphoglycerate | 514,005 | 406,442 | 275,816 | 82,205 |
| 263 | 2-aminobutyrate | 1,499,061 | 1,522,610 | 1,906,989 | 1,587,369 |
| 945 | 2-arachidonoylglycerophosphocholine* | 69,971 | 428,855 | 179,266 | 806,039 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 438,495 | 2,678,412 | 1,323,412 | 3,686,134 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 134,999 | 727,344 | 447,247 | 1,125,461 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 185,020 | 841,336 | 370,519 | 939,739 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 49,315 | 40,013 | 34,710 | 17,847 |
| 229 | 2-hydroxybutyrate (AHB) | 1,380,591 | 1,329,590 | 1,652,279 | 1,242,529 |
| 714 | 2-hydroxyglutarate | 115,986 | 115,174 | 184,819 | 166,854 |
| 706 | 2-hydroxypalmitate | 40,420 | 47,330 | 120,951 | 46,619 |
| 939 | 2-linoleoylglycerophosphocholine* | | 666,996 | 288,542 | 912,955 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 202 | 2-methylbutyroylcarnitine | 47,597 | 30,227 | 58,976 | 41,719 |
| 937 | 2-oleoylglycerophosphocholine* | 55,909 | 227,409 | 218,731 | 484,871 |
| 930 | 2-palmitoylglycerophosphocholine* | 107,736 | 850,966 | 500,430 | 1,320,038 |
| 935 | 2-stearoylglycerophosphocholine* | 52,478 | 224,465 | 116,539 | 342,063 |
| 821 | 3-dehydrocarnitine* | 1,016,691 | 982,362 | 1,153,383 | 1,023,845 |
| 170 | 3-indoxyl sulfate | 8,908 | 10,598 | 10,032 | 8,388 |
| 172 | 3-methyl-2-oxobutyrate | 10,308 | | 8,238 | 12,970 |
| 173 | 3-methyl-2-oxovalerate | 22,455 | 12,098 | 14,312 | 12,557 |
| 529 | 3-phosphoglycerate | 3,001,350 | 2,379,128 | 1,254,461 | 684,644 |
| 193 | 4-methyl-2-oxopentanoate | 45,223 | 20,461 | 30,765 | 24,861 |
| 266 | 5-methylthioadenosine (MTA) | 106,068 | 141,550 | 121,991 | 116,200 |
| 282 | 5-oxoproline | 248,409 | 316,581 | 487,200 | 465,612 |
| 545 | 6-phosphogluconate | 87,787 | 116,731 | 157,278 | 50,683 |
| 1024 | 7-beta-hydroxycholesterol | 24,651 | 24,894 | 51,849 | 48,199 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 80,921 | 148,527 | 137,264 | 145,151 |
| 672 | 9,10-epoxystearate | 5,273,860 | 7,416,512 | 10,051,883 | 7,850,631 |
| 822 | acetylcarnitine | 3,482,386 | 2,957,871 | 2,943,287 | 2,463,402 |
| 601 | acetylphosphate | 3,116,020 | 2,916,298 | 3,536,594 | 2,858,083 |
| 1105 | adenine | 42,820,164 | 35,164,124 | 32,958,494 | 22,692,290 |
| 1106 | adenosine | 39,606 | 50,679 | 53,112 | 47,176 |
| 1116 | adenosine 5'-diphosphate (ADP) | 174,757 | 112,277 | 180,872 | 116,869 |
| 1232 | adenosine 5'diphosphoribose | 140,137 | 133,202 | 129,905 | 108,365 |
| 1114 | adenosine 5'-monophosphate (AMP) | 3,384,504 | 1,818,121 | 5,602,308 | 3,526,180 |
| 665 | adrenate (22:4n6) | 134,402 | 40,015 | 65,717 | 54,909 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 27 | alanine | 46,026,540 | 46,403,848 | 61,844,304 | 50,513,772 |
| 1150 | allantoin | 15,691 | 16,447 | 36,580 | 12,260 |
| 179 | alpha-hydroxyisocaproate | 144,415 | 197,291 | 312,352 | 293,435 |
| 198 | alpha-hydroxyisovalerate | 1,037,016 | 1,425,137 | 2,069,952 | 1,720,625 |
| 1266 | alpha-tocopherol | 183,533 | 274,439 | 378,019 | 239,099 |
| 1034 | androsterone sulfate | 4,883 | | 5,621 | 5,827 |
| 566 | arabinose | 464,449 | 421,330 | 533,174 | 357,514 |
| 546 | arabitol | 858,582 | 791,148 | 995,548 | 828,324 |
| 1202 | arabonate | 112,045 | 106,724 | 177,292 | 90,025 |
| 659 | arachidonate (20:4n6) | 819,615 | 672,532 | 1,159,407 | 996,120 |
| 241 | arginine | 996,958 | 819,233 | 1,031,571 | 935,909 |
| 25 | asparagine | 1,076,330 | 1,060,803 | 1,280,762 | 1,024,284 |
| 24 | aspartate | 7,078,996 | 7,557,151 | 9,547,111 | 7,674,739 |
| 721 | azelate (nonanedioate) | 19,025 | 33,353 | 46,882 | 54,019 |
| 26 | beta-alanine | 53,465 | 67,742 | 104,855 | 91,048 |
| 7 | beta-hydroxypyruvate | 324,165 | 304,194 | 330,819 | 262,537 |
| 22 | betaine | 1,264,345 | 1,284,799 | 1,309,027 | 1,337,286 |
| 1057 | beta-sitosterol | | 49,466 | 44,720 | 28,975 |
| 1216 | biliverdin | 25,074 | 75,380 | 30,880 | 69,288 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 811 | butyrylcarnitine | 18,993 | | 18,555 | |
| 1612 | caffeine | 2,671,487 | 2,501,316 | 3,004,181 | 2,617,700 |
| 1059 | campesterol | | 126,048 | 183,062 | 105,610 |
| 622 | caprate (10:0) | 28,993 | 30,427 | 35,743 | 29,978 |
| 618 | caproate (6:0) | 77,649 | 53,301 | 53,011 | 25,272 |
| 620 | caprylate (8:0) | 42,353 | 55,138 | 42,464 | 25,735 |
| 820 | carnitine | 792,332 | 801,493 | 733,487 | 761,177 |
| 1300 | catechol sulfate | 83,229 | 82,922 | 90,053 | 89,518 |
| 164 | C-glycosyltryptophan* | 27,480 | 21,865 | 20,682 | 27,881 |
| 1020 | cholesterol | 32,736,830 | 35,737,660 | 43,877,268 | 38,579,980 |
| 881 | choline | 949,016 | 852,487 | 985,493 | 889,188 |
| 582 | cis-aconitate | 890,339 | 909,508 | 1,152,958 | 1,029,934 |
| 641 | cis-vaccenate (18:1n7) | | | 250,397 | 221,962 |
| 579 | citrate | 345,310,752 | 317,354,048 | 344,202,304 | 207,944,592 |
| 248 | citrulline | 151,995 | 152,676 | 158,868 | 178,615 |
| 259 | creatine | 3,105,707 | 3,087,004 | 3,193,254 | 3,029,256 |
| 260 | creatinine | 269,770 | 372,679 | 391,820 | 385,472 |
| 213 | cysteine | 480,046 | 758,948 | 1,519,907 | 1,160,282 |
| 819 | deoxycarnitine | 497,989 | 534,404 | 555,496 | 466,422 |
| 655 | dihomo-linoleate (20:2n6) | 49,672 | 43,052 | 64,917 | 48,778 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 84,867 | 72,285 | 120,602 | 97,726 |
| 531 | dihydroxyacetone phosphate (DHAP) | 3,737,129 | 740,411 | 162,486 | 64,234 |
| 3 | dimethylglycine | 258,305 | 296,444 | 240,992 | |
| 613 | docosahexaenoate (DHA; 22:6n3) | 168,444 | 163,981 | 235,179 | 226,132 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 57,715 | 68,934 | 88,767 | 84,895 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 233,741 | 195,426 | 233,767 | 259,059 |
| 1565 | ergothioneine | 489,496 | 433,692 | 555,621 | 455,299 |
| 735 | erucamide | | 552,061 | 176,649 | 785,073 |
| 1632 | erythritol | 1,346,993 | 2,164,535 | 4,162,346 | 4,280,122 |
| 453 | erythronate* | 446,768 | 738,985 | 1,482,815 | 1,356,493 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 876 | ethanolamine | 555,903 | 686,214 | 1,165,937 | 1,020,568 |
| 472 | fructose | 50,109,964 | 55,323,568 | 102,091,968 | 98,700,936 |
| 524 | fructose-6-phosphate | 296,830 | 641,289 | 646,186 | 519,872 |
| 594 | fumarate | 369,912 | 414,751 | 760,435 | 408,083 |
| 404 | gamma-glutamylleucine | 27,997 | 32,365 | 26,144 | 25,162 |
| 521 | glucose | 1,020,776,448 | 997,357,184 | 1,139,034,240 | 964,054,976 |
| 519 | glucose-6-phosphate (G6P) | 180,720 | 736,716 | 1,722,416 | 1,327,185 |
| 39 | glutamate | 5,533,269 | 5,249,449 | 6,124,830 | 4,963,277 |
| 44 | glutamine | 1,389,451 | 1,211,024 | 897,463 | 921,205 |
| 80 | glutaroyl carnitine | | 20,420 | 17,809 | |
| 283 | glutathione, oxidized (GSSG) | 1,267,565 | 958,516 | 877,904 | 797,820 |
| 280 | glutathione, reduced (GSH) | 23,101,658 | 22,202,784 | 15,096,875 | 15,510,460 |
| 517 | glycerate | 1,121,733 | 2,107,712 | 3,489,274 | 3,304,614 |
| 882 | glycerol 3-phosphate (G3P) | 1,634,444 | 877,318 | 549,688 | 297,549 |
| 883 | glycerophosphorylcholine (GPC) | 130,572 | 140,299 | 155,496 | 159,310 |
| 1 | glycine | 33,825,676 | 36,850,828 | 54,430,340 | 51,906,536 |
| 851 | glycochenodeoxycholate | 16,089 | 15,842 | 20,762 | 16,422 |
| 840 | glycocholate | 4,709 | | 3,415 | 6,331 |
| 849 | glycodeoxycholate | | 12,180 | 15,682 | |
| 1318 | glycolate (hydroxyacetate) | 439,427 | 365,340 | 568,437 | 448,191 |
| 1128 | guanosine | 48,753 | 35,829 | 44,277 | 27,753 |
| 1212 | heme* | 2,080,469 | 11,383,302 | 2,772,017 | 9,742,363 |
| 619 | heptanoate (7:0) | 19,019 | 19,535 | 18,253 | 9,481 |
| 823 | hexanoylcarnitine | 32,860 | 35,522 | 61,577 | 62,579 |
| 1288 | hippurate | 56,806 | 55,854 | 64,295 | 55,423 |
| 50 | histidine | 35,235 | 35,498 | 53,561 | 46,513 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 231 | homocysteine | 31,950 | 68,226 | 136,585 | 78,872 |
| 1585 | homostachydrine* | 33,072 | 52,929 | 41,901 | 49,128 |
| 206 | hydroxyisovaleroyl carnitine | 197,479 | 198,639 | 214,187 | 192,114 |
| 1098 | hypoxanthine | 22,240,624 | 23,073,438 | 30,759,420 | 24,490,568 |
| 1101 | inosine 5'-monophosphate (IMP) | 157,625 | 295,160 | 429,261 | 364,028 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 487,307 | 90,518 | 45,262 | 36,914 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 425,998 | 310,659 | 84,013 | 43,295 |
| 496 | Isobar: sorbitol, mannitol | 19,533,746 | 19,461,080 | 17,323,574 | 18,599,532 |
| 200 | isobutyrylcarnitine | 136,413 | 107,830 | 135,775 | 109,241 |
| 180 | isoleucine | 5,410,337 | 5,613,187 | 5,777,075 | 5,520,644 |
| 478 | isomaltose | 2,415,596 | 1,876,714 | 2,429,082 | 1,792,855 |
| 205 | isovalerylcarnitine | 92,686 | 88,859 | 98,716 | 96,003 |
| 144 | kynurenine | 148,929 | 165,805 | 118,761 | 132,904 |
| 536 | lactate | 1,020,426,624 | 1,586,645,376 | 2,372,599,808 | 2,221,599,488 |
| 1018 | lathosterol | 94,639 | 79,268 | 69,071 | 114,548 |
| 625 | laurate (12:0) | 122,574 | 129,266 | 124,453 | 124,539 |
| 181 | leucine | 9,541,025 | 10,279,834 | 11,479,407 | 10,036,593 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 604 | linoleate (18:2n6) | 2,334,804 | 2,267,921 | 3,710,364 | 2,700,794 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 538,085 | 528,911 | 643,149 | 647,742 |
| 69 | lysine | 2,062,752 | 2,778,876 | 3,292,959 | 3,042,442 |
| 598 | malate | 1,538,423 | 2,000,477 | 3,044,240 | 1,877,331 |
| 482 | maltose | 1,299,784 | 1,205,586 | 1,626,218 | 1,099,212 |
| 487 | mannose | 12,503,923 | 12,644,893 | 16,777,872 | 12,748,232 |
| 489 | mannose-6-phosphate | 155,536 | 266,746 | 403,017 | 210,633 |
| 635 | margarate (17:0) | 374,345 | 469,249 | 508,347 | 340,769 |
| 658 | mead acid (20:3n9) | 21,454 | 17,829 | 22,165 | 15,984 |
| 225 | methionine | 675,726 | 518,109 | 424,411 | 379,467 |
| 890 | myo-inositol | 1,830,739 | 1,937,274 | 2,220,758 | 1,926,134 |
| 629 | myristate (14:0) | 614,971 | 753,272 | 899,579 | 658,672 |
| 630 | myristoleate (14:1n5) | | 20,243 | 25,641 | 24,885 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 255,045 | 328,963 | 197,700 | 208,504 |
| 75 | N-6-trimethyllysine | 118,028 | 104,812 | 88,531 | 117,878 |
| 4 | N-acetylglycine | 129,534 | 82,324 | 129,186 | 81,418 |
| 227 | N-acetylmethionine | | | 4,569 | 3,814 |
| 455 | N-acetylneuraminate | 81,863 | 71,474 | 145,262 | 161,975 |
| 1221 | nicotinamide | 3,091,146 | 2,345,408 | 2,440,477 | 3,025,345 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 5,818 | 3,417 | 3,167 | 2,659 |
| 825 | octanoylcarnitine | 50,620 | 58,888 | 74,802 | 70,794 |
| 639 | oleate (18:1n9) | 668,373 | 1,037,370 | 869,825 | 727,692 |
| 835 | oleoylcarnitine | 176,499 | 1,896,469 | 814,920 | 3,297,641 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 285 | ophthalmate | 48,362 | 17,632 | | |
| 244 | ornithine | 11,180,306 | 12,310,781 | 16,416,260 | 13,502,701 |
| 632 | palmitate (16:0) | 6,535,080 | 8,036,350 | 11,042,204 | 7,455,168 |
| 633 | palmitoleate (16:1n7) | 468,814 | 489,618 | 894,550 | 476,559 |
| 1004 | palmitoyl sphingomyelin | 14,373,302 | 14,891,052 | 19,737,722 | 15,219,238 |
| 833 | palmitoylcarnitine | 167,796 | 994,773 | 477,062 | 2,072,686 |
| 1243 | pantothenate | 93,473 | 99,085 | 117,185 | 124,715 |
| 1613 | paraxanthine | 521,128 | 623,131 | 518,359 | 563,460 |
| 88 | p-cresol sulfate | 73,964 | 76,929 | 90,547 | 75,245 |
| 621 | pelargonate (9:0) | 416,123 | 432,364 | 388,122 | 260,585 |
| 631 | pentadecanoate (15:0) | 199,998 | 216,880 | 280,835 | 198,601 |
| 135 | phenol sulfate | 19,545 | 21,133 | 20,674 | 19,955 |
| 128 | phenylacetylglutamine | 89,135 | 83,598 | 87,730 | 73,734 |
| 83 | phenylalanine | 10,171,755 | 10,241,136 | 9,943,871 | 10,824,778 |
| 602 | phosphate | 761,357,696 | 801,848,512 | 1,235,966,976 | 1,119,354,496 |
| 534 | phosphoenolpyruvate (PEP) | 407,874 | 315,930 | 207,764 | 91,637 |
| 877 | phosphoethanolamine | | | 71,275 | |
| 74 | pipecolate | 101,955 | 110,178 | 89,147 | 101,775 |
| 1531 | piperine | 85,404 | 67,334 | 100,405 | 80,905 |
| 246 | proline | 1,854,912 | 1,822,370 | 2,373,863 | 2,105,123 |
| 809 | propionylcarnitine | 660,785 | 510,463 | 599,475 | 418,053 |
| 1181 | pseudouridine | 7,088 | 10,312 | 14,090 | 9,576 |
| 45 | pyroglutamine* | 64,256 | 38,425 | 68,071 | 80,202 |
| 603 | pyrophosphate (PPi) | 61,129 | 76,329 | 82,322 | 35,852 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 535 | pyruvate | 161,832 | 212,563 | 3,380,472 | 5,669,102 |
| 1469 | ranitidine | 353,058 | 350,556 | 432,854 | 336,545 |
| 548 | ribitol | 952,774 | 1,106,672 | 1,510,853 | 1,272,448 |
| 557 | ribose 5-phosphate | 336,985 | 312,301 | 206,851 | 114,607 |
| 559 | ribulose | 78,066 | 39,733 | 36,408 | 22,491 |
| 224 | S-adenosylhomocysteine (SAH) | 183,611 | 166,709 | 197,505 | 193,656 |
| 551 | sedoheptulose-7-phosphate | | 4,142 | 19,453 | 65,317 |
| 8 | serine | 6,583,504 | 7,134,192 | 9,398,409 | 8,111,226 |
| 216 | S-methylcysteine | 159,794 | 245,038 | 297,871 | 220,667 |
| 281 | S-methylglutathione | 39,255 | 34,424 | 28,687 | 20,016 |
| 270 | spermidine | 912,683 | 1,012,005 | 1,172,137 | 1,056,876 |
| 1584 | stachydrine | 191,830 | 175,462 | 203,083 | 135,447 |
| 637 | stearate (18:0) | 7,362,772 | 8,346,579 | 10,687,071 | 7,035,826 |
| 1005 | stearoyl sphingomyelin | 1,292,053 | 1,407,098 | 1,641,171 | 1,275,791 |
| 834 | stearoylcarnitine | 79,051 | 869,075 | 364,794 | 1,557,840 |
| 591 | succinylcarnitine | 332,049 | 320,544 | 413,784 | 373,895 |
| 1662 | terephthalic acid | 222,330 | 245,689 | 286,506 | 196,772 |
| 1614 | theobromine | 250,330 | 232,698 | 297,421 | 237,998 |
| 1615 | theophylline | 108,799 | 214,130 | 95,077 | 96,974 |
| 549 | threitol | 1,268,397 | 1,470,554 | 2,292,753 | 1,636,328 |
| 1199 | threonate | 581,345 | 551,125 | 784,763 | 646,381 |
| 17 | threonine | 163,837 | 209,384 | 184,000 | 169,344 |
| 252 | trans-4-hydroxyproline | 40,261 | 46,285 | 37,145 | 44,134 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 |
|---|---|---|---|---|---|
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | 997730 | 997747 | 997713 | 997751 |
| | | 991352 | 991353 | 991354 | 991355 |
| | | NHSCi 2003 T1 D7 | NHSCi 2003 T1 D14 | NHSCi 2003 T1 D21 | NHSCi 2003 T1 D28 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 |
| 501 | trehalose | 264,414 | 733,871 | 1,123,262 | 1,108,517 |
| 1242 | trigonelline (N'-methylnicotinate) | 256,829 | 250,492 | 299,135 | 223,820 |
| 145 | tryptophan | 4,409,522 | 4,518,646 | 4,357,563 | 4,664,176 |
| 151 | tryptophan betaine | 1,491,360 | 1,372,023 | 1,696,189 | 1,418,543 |
| 99 | tyrosine | 2,320,444 | 2,352,258 | 2,152,174 | 2,627,710 |
| 1149 | urate | 181,639 | 126,371 | 171,076 | 130,226 |
| 245 | urea | 31,577,746 | 31,722,304 | 40,273,300 | 32,665,470 |
| 1180 | uridine | 31,039 | 32,081 | 31,602 | 35,827 |
| 190 | valine | 9,045,619 | 9,410,652 | 9,143,607 | 9,538,689 |
| 565 | xylitol | 91,194 | 102,298 | 48,166 | 22,405 |
| 570 | xylonate | 61,581 | 91,428 | 145,463 | 106,285 |
| 569 | xylose | 92,996 | 241,030 | 498,976 | 395,727 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 905 | 1,2-propanediol | 745,465 | 5,542,436 | 11,739,036 | 11,456,830 |
| 532 | 1,3-dihydroxyacetone | 91,317 | 83,511 | 86,058 | 71,210 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 7,733,593 | 9,084,731 | 11,977,017 | 7,683,883 |
| 523 | 1,6-anhydroglucose | 539,458 | 309,368 | 490,427 | 309,208 |
| 636 | 10-heptadecenoate (17:1n7) | 47,620 | 56,219 | 63,134 | 101,628 |
| 742 | 13-methylmyristic acid | 70,477 | 113,970 | 135,348 | 190,039 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 123,330 | 180,985 | 260,928 | 318,573 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 58,155 | 26,798 | 32,254 | 24,288 |
| 938 | 1-linoleoylglycerophosphocholine | 418,360 | 241,666 | 330,506 | 270,487 |
| 926 | 1-myristoylglycerophosphocholine | | 47,843 | 56,395 | 68,330 |
| 936 | 1-oleoylglycerophosphocholine | 35,233 | 115,736 | 365,962 | 467,280 |
| 915 | 1-oleoylglycerophosphoethanolamine | 28,746 | 24,256 | 25,848 | 23,897 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 37,837 | 72,295 | 25,089 | 33,892 |
| 929 | 1-palmitoylglycerophosphocholine | 264,700 | 731,470 | 2,458,075 | 3,139,559 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 51,268 | 25,055 | 29,190 | 23,716 |
| 934 | 1-stearoylglycerophosphocholine | 126,564 | 382,165 | 866,049 | 1,215,477 |
| 533 | 2,3-diphosphoglycerate | 343,615 | 179,751 | 53,276 | 15,958 |
| 263 | 2-aminobutyrate | 1,550,880 | 1,483,557 | 1,833,759 | 1,388,255 |
| 945 | 2-arachidonoylglycerophosphocholine* | | 63,550 | 59,448 | 90,251 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 86,205 | 562,167 | 373,379 | 685,989 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | | 80,033 | 110,317 | 178,156 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | | 68,694 | 110,196 | 184,748 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 59,909 | 44,382 | 38,362 | 50,924 |
| 229 | 2-hydroxybutyrate (AHB) | 1,394,679 | 1,303,673 | 1,566,481 | 1,387,970 |
| 714 | 2-hydroxyglutarate | 57,644 | 92,289 | 111,144 | 106,544 |
| 706 | 2-hydroxypalmitate | 67,999 | 43,894 | 86,230 | 49,435 |
| 939 | 2-linoleoylglycerophosphocholine* | | | | 267,360 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 202 | 2-methylbutyroylcarnitine | 65,535 | 58,670 | 64,952 | 48,802 |
| 937 | 2-oleoylglycerophosphocholine* | | 50,257 | 103,141 | 120,696 |
| 930 | 2-palmitoylglycerophosphocholine* | 33,346 | 107,667 | 165,617 | 261,996 |
| 935 | 2-stearoylglycerophosphocholine* | | 36,493 | 85,896 | 108,863 |
| 821 | 3-dehydrocarnitine* | 906,418 | 961,604 | 1,059,317 | 1,106,133 |
| 170 | 3-indoxyl sulfate | 8,937 | 10,009 | 10,315 | 9,144 |
| 172 | 3-methyl-2-oxobutyrate | 45,886 | 35,004 | 49,798 | 65,092 |
| 173 | 3-methyl-2-oxovalerate | 44,605 | 59,005 | 72,995 | 73,524 |
| 529 | 3-phosphoglycerate | 2,267,315 | 1,175,531 | 1,150,217 | 730,233 |
| 193 | 4-methyl-2-oxopentanoate | 85,775 | 111,910 | 133,265 | 143,553 |
| 266 | 5-methylthioadenosine (MTA) | 34,671 | 98,330 | 101,348 | 104,721 |
| 282 | 5-oxoproline | 49,723 | 157,770 | 267,387 | 359,615 |
| 545 | 6-phosphogluconate | 233,923 | 136,218 | 102,403 | 82,150 |
| 1024 | 7-beta-hydroxycholesterol | 23,520 | 18,829 | 35,962 | |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 9,135 | 117,159 | 162,516 | 211,099 |
| 672 | 9,10-epoxystearate | 152,282 | 6,645,405 | 11,809,674 | 11,676,105 |
| 822 | acetylcarnitine | 3,567,269 | 3,127,408 | 3,163,545 | 3,080,800 |
| 601 | acetylphosphate | 3,521,678 | 3,464,525 | 3,399,281 | 2,765,531 |
| 1105 | adenine | 47,024,196 | 38,403,428 | 36,290,012 | 34,509,272 |
| 1106 | adenosine | 28,575 | 11,067 | 43,115 | 22,989 |
| 1116 | adenosine 5'-diphosphate (ADP) | 220,561 | 182,418 | 245,581 | 225,829 |
| 1232 | adenosine 5'diphosphoribose | 115,107 | 123,778 | 126,905 | 120,626 |
| 1114 | adenosine 5'-monophosphate (AMP) | 3,096,745 | 2,175,974 | 5,159,040 | 5,843,866 |
| 665 | adrenate (22:4n6) | 263,500 | 71,867 | 80,618 | 49,774 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 27 | alanine | 49,976,828 | 53,066,216 | 66,933,316 | 57,356,184 |
| 1150 | allantoin | 17,028 | 23,332 | 14,181 | 57,372 |
| 179 | alpha-hydroxyisocaproate | 84,320 | | 161,549 | 249,219 |
| 198 | alpha-hydroxyisovalerate | 384,817 | 378,194 | 541,972 | 614,961 |
| 1266 | alpha-tocopherol | 350,343 | 286,868 | 314,688 | 216,179 |
| 1034 | androsterone sulfate | 5,255 | 4,742 | 5,528 | 3,904 |
| 566 | arabinose | 413,890 | 309,074 | 507,504 | 315,544 |
| 546 | arabitol | 642,209 | 511,500 | 766,245 | 570,469 |
| 1202 | arabonate | 119,653 | 105,824 | 146,365 | 111,321 |
| 659 | arachidonate (20:4n6) | 516,035 | 546,934 | 640,309 | 1,048,029 |
| 241 | arginine | 617,204 | 676,944 | 698,446 | 1,699,196 |
| 25 | asparagine | 1,352,633 | 1,164,342 | 1,243,612 | 963,227 |
| 24 | aspartate | 6,387,902 | 6,871,906 | 7,341,442 | 6,570,116 |
| 721 | azelate (nonanedioate) | 6,262 | 21,906 | 50,306 | 53,504 |
| 26 | beta-alanine | 121,915 | 104,975 | 118,882 | 47,145 |
| 7 | beta-hydroxypyruvate | 331,478 | 293,631 | 292,325 | 314,497 |
| 22 | betaine | 1,161,682 | 1,207,833 | 1,186,017 | 1,278,111 |
| 1057 | beta-sitosterol | | 32,645 | 52,307 | 32,088 |
| 1216 | biliverdin | | 23,055 | | 20,790 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 811 | butyrylcarnitine | 17,822 | | | 13,327 |
| 1612 | caffeine | 2,753,506 | 2,504,050 | 2,881,762 | 2,832,695 |
| 1059 | campesterol | | 171,898 | | |
| 622 | caprate (10:0) | 15,020 | 29,587 | 37,076 | 36,725 |
| 618 | caproate (6:0) | 111,794 | 69,044 | 57,352 | 45,725 |
| 620 | caprylate (8:0) | 39,167 | 29,957 | 35,741 | 43,038 |
| 820 | carnitine | 663,728 | 766,394 | 777,366 | 761,035 |
| 1300 | catechol sulfate | 84,164 | 84,270 | 91,729 | 88,452 |
| 164 | C-glycosyltryptophan* | 27,059 | 32,641 | 27,023 | 30,397 |
| 1020 | cholesterol | 39,581,568 | 36,543,404 | 44,544,656 | 33,920,932 |
| 881 | choline | 697,453 | 753,068 | 881,484 | 887,555 |
| 582 | cis-aconitate | 579,430 | 702,831 | 918,649 | 828,881 |
| 641 | cis-vaccenate (18:1n7) | | 86,998 | 170,842 | 189,347 |
| 579 | citrate | 428,947,008 | 362,284,064 | 377,317,120 | 279,634,336 |
| 248 | citrulline | 148,677 | 158,868 | 160,536 | 161,807 |
| 259 | creatine | 3,147,259 | 3,091,284 | 3,350,623 | 3,254,799 |
| 260 | creatinine | 380,758 | 276,826 | 392,966 | 376,113 |
| 213 | cysteine | 689,943 | 830,427 | 857,522 | 1,219,648 |
| 819 | deoxycarnitine | 487,288 | 414,342 | 479,753 | 591,856 |
| 655 | dihomo-linoleate (20:2n6) | 25,349 | 30,826 | 36,360 | 41,644 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 61,147 | 43,586 | 76,840 | 107,997 |
| 531 | dihydroxyacetone phosphate (DHAP) | 132,668 | 16,113 | 224,498 | |
| 3 | dimethylglycine | 247,818 | | 246,137 | 304,134 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 71,607 | 118,299 | 114,267 | 202,076 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 28,612 | 45,242 | 49,538 | 96,471 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 109,876 | 158,018 | 141,551 | 263,634 |
| 1565 | ergothioneine | 551,497 | 432,934 | 558,397 | 548,245 |
| 735 | erucamide | 276,552 | 261,619 | 409,745 | |
| 1632 | erythritol | 1,020,082 | 1,201,194 | 1,627,422 | 1,826,592 |
| 453 | erythronate* | 431,639 | 380,390 | 575,805 | 476,161 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 876 | ethanolamine | 444,644 | 606,292 | 933,204 | 469,203 |
| 472 | fructose | 73,592,448 | 73,038,224 | 90,798,496 | 81,384,712 |
| 524 | fructose-6-phosphate | 506,707 | 494,636 | 793,079 | 687,997 |
| 594 | fumarate | 337,383 | 272,994 | 404,529 | 462,639 |
| 404 | gamma-glutamylleucine | 23,370 | 28,570 | 25,586 | 27,710 |
| 521 | glucose | 1,145,662,464 | 1,051,588,224 | 1,154,292,480 | 1,007,674,112 |
| 519 | glucose-6-phosphate (G6P) | 1,270,766 | 1,393,362 | 2,158,723 | 1,834,501 |
| 39 | glutamate | 6,607,252 | 4,784,893 | 6,068,648 | 4,895,959 |
| 44 | glutamine | 1,854,655 | 1,664,139 | 1,394,841 | 1,282,836 |
| 80 | glutaroyl carnitine | | 15,536 | 11,361 | 20,885 |
| 283 | glutathione, oxidized (GSSG) | 1,536,976 | 1,434,289 | 1,156,997 | 1,022,837 |
| 280 | glutathione, reduced (GSH) | 22,156,660 | 26,058,072 | 23,415,274 | 22,568,236 |
| 517 | glycerate | 283,370 | 482,091 | 856,981 | 642,495 |
| 882 | glycerol 3-phosphate (G3P) | 384,380 | 295,793 | 381,099 | 290,030 |
| 883 | glycerophosphorylcholine (GPC) | 168,187 | 167,300 | 148,713 | 145,989 |
| 1 | glycine | 30,459,652 | 34,107,052 | 46,871,188 | 52,295,720 |
| 851 | glycochenodeoxycholate | 21,412 | 14,671 | 17,295 | 19,348 |
| 840 | glycocholate | 5,351 | | 7,725 | 4,318 |
| 849 | glycodeoxycholate | 8,586 | | | |
| 1318 | glycolate (hydroxyacetate) | 462,094 | 495,049 | 539,603 | 434,382 |
| 1128 | guanosine | 33,726 | 35,356 | 38,938 | 37,136 |
| 1212 | heme* | 615,413 | 1,819,243 | 1,145,810 | 1,617,094 |
| 619 | heptanoate (7:0) | 15,218 | 20,165 | 20,617 | 16,034 |
| 823 | hexanoylcarnitine | 73,941 | 37,478 | 35,725 | 45,020 |
| 1288 | hippurate | 52,619 | 63,026 | 57,530 | 65,282 |
| 50 | histidine | 40,988 | 39,117 | 36,693 | 40,185 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 231 | homocysteine | 38,651 | 63,085 | 55,863 | 86,413 |
| 1585 | homostachydrine* | 45,480 | 41,047 | 42,057 | 38,489 |
| 206 | hydroxyisovaleroyl carnitine | 174,483 | 190,571 | 217,050 | 206,799 |
| 1098 | hypoxanthine | 357,857 | 443,716 | 1,540,916 | 2,909,897 |
| 1101 | inosine 5'-monophosphate (IMP) | 122,450 | 208,400 | 343,818 | 191,524 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 59,763 | 58,065 | 66,455 | 63,162 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 189,553 | 84,681 | 151,269 | 100,797 |
| 496 | Isobar: sorbitol, mannitol | 17,664,290 | 18,459,064 | 18,831,410 | 18,104,376 |
| 200 | isobutyrylcarnitine | 162,344 | 134,814 | 118,448 | 137,637 |
| 180 | isoleucine | 3,655,383 | 4,322,716 | 4,500,956 | 4,277,236 |
| 478 | isomaltose | 1,830,657 | 1,377,313 | 2,987,101 | 2,023,536 |
| 205 | isovalerylcarnitine | 97,051 | 93,569 | 112,835 | 94,010 |
| 144 | kynurenine | 130,991 | 117,032 | 121,182 | 113,468 |
| 536 | lactate | 219,773,488 | 668,204,544 | 1,320,499,968 | 1,502,399,360 |
| 1018 | lathosterol | 115,097 | 81,692 | 91,381 | 66,549 |
| 625 | laurate (12:0) | 101,642 | 115,661 | 87,744 | 130,280 |
| 181 | leucine | 6,983,435 | 7,804,498 | 8,769,108 | 8,426,035 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 604 | linoleate (18:2n6) | 1,365,113 | 1,457,105 | 2,026,197 | 2,989,312 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 246,779 | 436,841 | 398,413 | 526,144 |
| 69 | lysine | 2,180,764 | 2,605,770 | 4,363,680 | 1,926,589 |
| 598 | malate | 974,764 | 1,099,388 | 1,767,475 | 1,549,931 |
| 482 | maltose | 1,659,091 | 1,100,590 | 1,351,060 | 1,142,318 |
| 487 | mannose | 17,039,670 | 15,669,026 | 16,297,070 | 13,653,562 |
| 489 | mannose-6-phosphate | 239,608 | 267,211 | 398,044 | 351,789 |
| 635 | margarate (17:0) | 262,592 | 310,883 | 453,330 | 447,568 |
| 658 | mead acid (20:3n9) | 20,893 | 5,950 | 18,337 | 16,707 |
| 225 | methionine | 748,963 | 705,926 | 508,402 | 503,209 |
| 890 | myo-inositol | 2,280,102 | 2,075,890 | 2,385,278 | 1,672,674 |
| 629 | myristate (14:0) | 401,070 | 723,104 | 820,138 | 976,880 |
| 630 | myristoleate (14:1n5) | 14,424 | | | 45,316 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 292,361 | 299,107 | 196,349 | 249,327 |
| 75 | N-6-trimethyllysine | 105,525 | 147,909 | 124,055 | 109,690 |
| 4 | N-acetylglycine | 147,937 | 139,741 | 117,156 | 73,590 |
| 227 | N-acetylmethionine | 4,876 | | 4,207 | 5,168 |
| 455 | N-acetylneuraminate | 29,955 | 60,023 | 117,358 | 87,067 |
| 1221 | nicotinamide | 2,483,235 | 2,287,273 | 3,061,721 | 3,744,597 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 2,866 | 3,965 | 3,071 | 3,529 |
| 825 | octanoylcarnitine | 45,746 | 59,572 | 60,687 | 75,646 |
| 639 | oleate (18:1n9) | 988,918 | 704,987 | 851,576 | 686,319 |
| 835 | oleoylcarnitine | 72,832 | 193,833 | 241,106 | 338,804 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 285 | ophthalmate | 86,150 | 22,320 | | |
| 244 | ornithine | 13,754,966 | 13,368,233 | 15,370,339 | 10,388,709 |
| 632 | palmitate (16:0) | 5,660,507 | 6,226,841 | 8,189,210 | 8,121,497 |
| 633 | palmitoleate (16:1n7) | 236,778 | 415,979 | 355,046 | 539,108 |
| 1004 | palmitoyl sphingomyelin | 16,914,186 | 14,422,895 | 19,492,446 | 14,503,270 |
| 833 | palmitoylcarnitine | | 129,497 | 189,146 | 274,127 |
| 1243 | pantothenate | 108,096 | 83,864 | 119,207 | 106,866 |
| 1613 | paraxanthine | 436,920 | 611,989 | 548,293 | 495,671 |
| 88 | p-cresol sulfate | 81,349 | 74,739 | 86,044 | 79,590 |
| 621 | pelargonate (9:0) | 226,548 | 347,348 | 377,646 | 289,970 |
| 631 | pentadecanoate (15:0) | 152,004 | 226,215 | 220,682 | 263,728 |
| 135 | phenol sulfate | 20,851 | 19,109 | 23,186 | 25,279 |
| 128 | phenylacetylglutamine | 77,384 | 77,265 | 87,105 | 85,953 |
| 83 | phenylalanine | 7,762,848 | 9,454,861 | 9,785,504 | 10,072,558 |
| 602 | phosphate | 1,153,601,152 | 1,140,459,264 | 1,533,833,216 | 1,283,482,240 |
| 534 | phosphoenolpyruvate (PEP) | 377,326 | 230,271 | 80,526 | 62,062 |
| 877 | phosphoethanolamine | | 67,997 | 130,290 | |
| 74 | pipecolate | 114,108 | 123,954 | 109,387 | 110,645 |
| 1531 | piperine | 131,170 | 70,842 | 72,463 | 83,012 |
| 246 | proline | 1,958,820 | 1,803,254 | 2,195,216 | 2,064,586 |
| 809 | propionylcarnitine | 757,385 | 636,318 | 705,852 | 663,757 |
| 1181 | pseudouridine | 10,591 | 8,542 | 11,482 | 16,321 |
| 45 | pyroglutamine* | 82,600 | 49,694 | 74,796 | 56,790 |
| 603 | pyrophosphate (PPi) | 192,657 | 169,938 | 51,439 | 16,184 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 535 | pyruvate | 2,754,908 | 2,835,749 | 3,752,118 | 1,589,179 |
| 1469 | ranitidine | 377,435 | 305,239 | 414,925 | 385,438 |
| 548 | ribitol | 238,729 | 163,572 | 277,166 | 207,410 |
| 557 | ribose 5-phosphate | 231,690 | 175,353 | 169,389 | 108,367 |
| 559 | ribulose | | 23,478 | 13,883 | 18,999 |
| 224 | S-adenosylhomocysteine (SAH) | 121,506 | 191,402 | 226,296 | 252,239 |
| 551 | sedoheptulose-7-phosphate | 18,716 | 141,133 | 35,476 | 66,973 |
| 8 | serine | 6,690,800 | 6,545,978 | 7,781,857 | 6,767,347 |
| 216 | S-methylcysteine | 215,932 | 268,168 | 275,732 | 219,059 |
| 281 | S-methylglutathione | 31,160 | 30,894 | 30,219 | 28,836 |
| 270 | spermidine | 893,702 | 1,022,620 | 1,170,312 | 1,280,653 |
| 1584 | stachydrine | 197,827 | 178,193 | 184,074 | 248,399 |
| 637 | stearate (18:0) | 5,334,110 | 6,137,328 | 8,682,885 | 8,213,118 |
| 1005 | stearoyl sphingomyelin | 1,509,931 | 1,352,906 | 1,595,698 | 1,321,143 |
| 834 | stearoylcarnitine | 39,964 | 70,787 | 114,185 | 140,880 |
| 591 | succinylcarnitine | 339,675 | 297,560 | 364,784 | 399,232 |
| 1662 | terephthalic acid | 291,667 | 259,547 | 236,052 | 232,314 |
| 1614 | theobromine | 330,840 | 250,101 | 299,885 | 304,534 |
| 1615 | theophylline | 72,301 | 99,675 | 182,464 | 135,783 |
| 549 | threitol | 1,118,487 | 1,241,592 | 1,603,978 | 1,310,499 |
| 1199 | threonate | 613,251 | 486,071 | 626,715 | 513,435 |
| 17 | threonine | 175,088 | 150,748 | 161,778 | 183,176 |
| 252 | trans-4-hydroxyproline | 39,439 | 44,770 | 40,694 | 39,766 |

| | | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | 997716 | 997752 | 997719 | 997724 |
| | | 991356 | 991357 | 991358 | 991359 |
| | | NHSCi 2003 C D0 | NHSCi 2003 C D7 | NHSCi 2003 C D14 | NHSCi 2003 C D21 |
| | | C D0 | C D7 | C D14 | C D21 |
| | | 193.847 | 179.605 | 175.15 | 167.535 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D0 | C D7 | C D14 | C D21 |
| 501 | trehalose | 97,806 | 518,969 | 1,111,288 | 837,693 |
| 1242 | trigonelline (N'-methylnicotinate) | 264,197 | 236,175 | 265,502 | 278,679 |
| 145 | tryptophan | 3,631,722 | 4,102,700 | 4,409,757 | 4,285,182 |
| 151 | tryptophan betaine | 1,431,999 | 1,407,965 | 1,578,823 | 1,595,563 |
| 99 | tyrosine | 1,799,546 | 2,228,006 | 2,271,666 | 2,324,717 |
| 1149 | urate | 181,254 | 155,272 | 189,889 | 168,887 |
| 245 | urea | 33,063,718 | 31,198,160 | 34,479,028 | 30,550,978 |
| 1180 | uridine | 17,807 | 22,788 | 21,241 | 24,467 |
| 190 | valine | 7,813,211 | 8,622,408 | 8,899,696 | 9,083,185 |
| 565 | xylitol | | | | |
| 570 | xylonate | 37,575 | 49,461 | 102,285 | 98,514 |
| 569 | xylose | 75,703 | 60,204 | 107,993 | 93,872 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 905 | 1,2-propanediol | 14,866,116 | 4,732,242 | 8,877,082 | 11,024,061 |
| 532 | 1,3-dihydroxyacetone | 71,487 | 72,315 | 88,302 | 97,843 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 9,799,194 | 6,314,912 | 8,753,204 | 7,350,232 |
| 523 | 1,6-anhydroglucose | 378,368 | 331,929 | 288,474 | 281,344 |
| 636 | 10-heptadecenoate (17:1n7) | 99,983 | 52,221 | 74,115 | 78,955 |
| 742 | 13-methylmyristic acid | 174,351 | 57,251 | 95,666 | 116,603 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 338,906 | 139,630 | 214,022 | 265,868 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 20,429 | 64,481 | 26,055 | 25,200 |
| 938 | 1-linoleoylglycerophosphocholine | 239,615 | 470,973 | 236,606 | 229,663 |
| 926 | 1-myristoylglycerophosphocholine | 108,714 | | 66,246 | 74,117 |
| 936 | 1-oleoylglycerophosphocholine | 878,497 | 187,460 | 562,279 | 471,502 |
| 915 | 1-oleoylglycerophosphoethanolamine | 16,921 | 50,751 | 34,814 | 11,474 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 30,950 | 38,448 | 15,764 | 31,982 |
| 929 | 1-palmitoylglycerophosphocholine | 5,900,696 | 1,036,902 | 2,900,194 | 2,563,844 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 24,537 | 43,399 | 16,194 | 13,889 |
| 934 | 1-stearoylglycerophosphocholine | 1,988,020 | 371,740 | 1,164,406 | 1,296,232 |
| 533 | 2,3-diphosphoglycerate | 17,146 | 347,674 | 100,045 | 17,657 |
| 263 | 2-aminobutyrate | 1,589,408 | 2,218,991 | 2,722,774 | 2,667,683 |
| 945 | 2-arachidonoylglycerophosphocholine* | 192,300 | 35,575 | 168,711 | 202,691 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 1,437,579 | 323,714 | 1,573,934 | 1,967,320 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 340,603 | 111,767 | 269,754 | 426,141 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 395,785 | 89,351 | 335,291 | 391,305 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 32,439 | 44,590 | 38,235 | 32,175 |
| 229 | 2-hydroxybutyrate (AHB) | 1,364,453 | 1,460,712 | 1,701,494 | 1,801,408 |
| 714 | 2-hydroxyglutarate | 115,945 | 107,074 | 126,439 | 174,700 |
| 706 | 2-hydroxypalmitate | 47,298 | 74,240 | 39,214 | 43,962 |
| 939 | 2-linoleoylglycerophosphocholine* | 419,326 | | 351,103 | 307,996 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 202 | 2-methylbutyroylcarnitine | 61,392 | 79,619 | 56,933 | 56,908 |
| 937 | 2-oleoylglycerophosphocholine* | 184,264 | 93,762 | 195,387 | 179,311 |
| 930 | 2-palmitoylglycerophosphocholine* | 410,775 | 110,801 | 303,985 | 360,238 |
| 935 | 2-stearoylglycerophosphocholine* | 112,720 | | 112,650 | 90,132 |
| 821 | 3-dehydrocarnitine* | 1,138,316 | 1,034,712 | 1,034,847 | 1,061,604 |
| 170 | 3-indoxyl sulfate | 8,839 | 4,230 | 4,984 | 3,892 |
| 172 | 3-methyl-2-oxobutyrate | 39,850 | 50,607 | 57,731 | 52,980 |
| 173 | 3-methyl-2-oxovalerate | 63,333 | 46,637 | 56,752 | 56,915 |
| 529 | 3-phosphoglycerate | 694,597 | 1,172,991 | 1,040,874 | 476,708 |
| 193 | 4-methyl-2-oxopentanoate | 107,035 | 106,251 | 132,158 | 136,134 |
| 266 | 5-methylthioadenosine (MTA) | 107,301 | 40,681 | 101,342 | 123,505 |
| 282 | 5-oxoproline | 442,655 | 56,665 | 183,699 | 294,942 |
| 545 | 6-phosphogluconate | 44,588 | 47,121 | 84,215 | 40,442 |
| 1024 | 7-beta-hydroxycholesterol | 15,910 | 45,740 | 12,939 | 29,835 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 247,076 | 6,772 | 104,834 | 140,798 |
| 672 | 9,10-epoxystearate | 13,436,268 | 231,764 | 5,225,775 | 6,967,034 |
| 822 | acetylcarnitine | 3,041,098 | 4,375,307 | 3,964,733 | 3,815,497 |
| 601 | acetylphosphate | 3,160,937 | 3,260,516 | 3,741,576 | 4,005,335 |
| 1105 | adenine | 33,779,032 | 41,717,592 | 29,851,106 | 19,291,972 |
| 1106 | adenosine | 23,027 | 18,010 | 16,994 | 15,771 |
| 1116 | adenosine 5'-diphosphate (ADP) | 198,708 | 244,579 | 182,650 | 185,946 |
| 1232 | adenosine 5'diphosphoribose | 117,490 | 95,636 | 105,344 | 99,959 |
| 1114 | adenosine 5'-monophosphate (AMP) | 6,139,028 | 4,370,879 | 4,075,112 | 4,442,594 |
| 665 | adrenate (22:4n6) | 30,848 | 98,456 | 110,541 | 54,285 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 27 | alanine | 61,188,412 | 52,278,748 | 65,398,400 | 70,100,184 |
| 1150 | allantoin | 40,558 | 51,408 | 13,998 | 16,388 |
| 179 | alpha-hydroxyisocaproate | 331,016 | | | 188,710 |
| 198 | alpha-hydroxyisovalerate | 793,435 | 309,467 | 289,582 | 363,053 |
| 1266 | alpha-tocopherol | 230,446 | 168,019 | 165,014 | 149,210 |
| 1034 | androsterone sulfate | 4,606 | 8,676 | 6,634 | 7,606 |
| 566 | arabinose | 349,319 | 339,400 | 330,925 | 390,921 |
| 546 | arabitol | 680,380 | 573,597 | 548,209 | 500,688 |
| 1202 | arabonate | 126,756 | 74,847 | 111,315 | 94,048 |
| 659 | arachidonate (20:4n6) | 1,000,687 | 462,961 | 570,460 | 730,649 |
| 241 | arginine | 1,208,572 | 383,363 | 862,572 | 699,121 |
| 25 | asparagine | 933,457 | 1,574,333 | 1,538,009 | 1,474,817 |
| 24 | aspartate | 7,139,496 | 2,427,314 | 2,836,212 | 3,263,091 |
| 721 | azelate (nonanedioate) | 73,267 | 6,300 | 18,510 | 27,122 |
| 26 | beta-alanine | 88,894 | 176,953 | 157,935 | 201,987 |
| 7 | beta-hydroxypyruvate | 297,446 | 163,622 | 322,000 | 307,210 |
| 22 | betaine | 1,323,155 | 1,565,390 | 1,629,721 | 1,668,581 |
| 1057 | beta-sitosterol | | 61,653 | | |
| 1216 | biliverdin | 21,234 | 27,466 | 28,173 | 60,384 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 811 | butyrylcarnitine | 16,837 | | 15,149 | 35,750 |
| 1612 | caffeine | 2,399,502 | 3,775,415 | 3,358,247 | 3,312,058 |
| 1059 | campesterol | 284,834 | 225,673 | 229,713 | 301,398 |
| 622 | caprate (10:0) | 35,912 | 16,425 | 27,932 | 36,590 |
| 618 | caproate (6:0) | 56,028 | 70,295 | 72,782 | 40,854 |
| 620 | caprylate (8:0) | 32,087 | 22,626 | 39,802 | 41,971 |
| 820 | carnitine | 653,067 | 859,212 | 991,410 | 1,012,787 |
| 1300 | catechol sulfate | 84,580 | 79,972 | 80,017 | 77,623 |
| 164 | C-glycosyltryptophan* | 38,375 | 28,156 | 26,892 | 42,941 |
| 1020 | cholesterol | 35,386,532 | 33,105,708 | 36,210,112 | 39,926,704 |
| 881 | choline | 892,647 | 2,108,159 | 2,168,710 | 1,975,017 |
| 582 | cis-aconitate | 660,396 | 654,765 | 848,362 | 895,162 |
| 641 | cis-vaccenate (18:1n7) | 142,832 | 92,262 | 192,807 | |
| 579 | citrate | 271,567,296 | 279,913,504 | 256,853,264 | 229,689,984 |
| 248 | citrulline | 164,472 | 99,062 | 118,712 | 103,896 |
| 259 | creatine | 3,249,477 | 3,702,736 | 3,753,894 | 3,788,817 |
| 260 | creatinine | 373,217 | 416,801 | 391,170 | 393,564 |
| 213 | cysteine | 1,439,629 | 402,681 | 606,589 | 971,630 |
| 819 | deoxycarnitine | 523,098 | 603,374 | 582,634 | 695,545 |
| 655 | dihomo-linoleate (20:2n6) | 54,579 | 43,078 | 50,055 | 58,270 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 97,308 | 55,866 | 57,143 | 59,631 |
| 531 | dihydroxyacetone phosphate (DHAP) | | | 36,202 | |
| 3 | dimethylglycine | 306,640 | 193,695 | 256,734 | 276,553 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 193,359 | 74,426 | 110,271 | 175,133 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 99,741 | 33,554 | 56,770 | 79,940 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 286,520 | 58,980 | 132,608 | 147,182 |
| 1565 | ergothioneine | 527,747 | 973,519 | 839,918 | 835,805 |
| 735 | erucamide | 348,482 | 990,856 | 106,333 | 279,766 |
| 1632 | erythritol | 2,388,445 | 762,988 | 1,085,846 | 1,349,400 |
| 453 | erythronate* | 564,772 | 349,645 | 407,211 | 553,933 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 876 | ethanolamine | 641,402 | 553,372 | 603,424 | 942,185 |
| 472 | fructose | 91,205,144 | 62,306,108 | 74,201,088 | 79,748,064 |
| 524 | fructose-6-phosphate | 602,655 | 417,025 | 472,346 | 477,267 |
| 594 | fumarate | 445,347 | 321,557 | 363,352 | 402,505 |
| 404 | gamma-glutamylleucine | 19,611 | 27,674 | 16,689 | 21,436 |
| 521 | glucose | 1,038,950,976 | 1,010,169,664 | 1,061,818,688 | 1,085,405,312 |
| 519 | glucose-6-phosphate (G6P) | 1,796,014 | 1,160,047 | 1,612,947 | 1,263,673 |
| 39 | glutamate | 4,997,358 | 7,168,533 | 7,080,612 | 7,595,470 |
| 44 | glutamine | 1,192,279 | 1,877,726 | 1,544,420 | 1,460,887 |
| 80 | glutaroyl carnitine | 17,852 | 16,176 | 19,782 | 16,720 |
| 283 | glutathione, oxidized (GSSG) | 852,735 | 1,442,111 | 1,228,827 | 1,032,453 |
| 280 | glutathione, reduced (GSH) | 21,059,756 | 23,449,578 | 20,390,998 | 24,802,908 |
| 517 | glycerate | 920,270 | 221,452 | 412,063 | 505,355 |
| 882 | glycerol 3-phosphate (G3P) | 305,658 | 387,761 | 302,234 | 298,426 |
| 883 | glycerophosphorylcholine (GPC) | 157,840 | 144,957 | 145,898 | 143,193 |
| 1 | glycine | 59,083,828 | 23,479,246 | 37,560,636 | 47,368,668 |
| 851 | glycochenodeoxycholate | 16,296 | 150,818 | 98,974 | 89,512 |
| 840 | glycocholate | 6,863 | 58,682 | 49,881 | 51,519 |
| 849 | glycodeoxycholate | 8,151 | 43,610 | 39,689 | 37,498 |
| 1318 | glycolate (hydroxyacetate) | 412,571 | 323,106 | 432,862 | 445,637 |
| 1128 | guanosine | 40,252 | 36,267 | 35,052 | 29,112 |
| 1212 | heme* | 2,458,107 | 1,337,160 | 3,359,267 | 4,162,878 |
| 619 | heptanoate (7:0) | 20,413 | 12,629 | 19,636 | 14,543 |
| 823 | hexanoylcarnitine | 57,650 | 44,588 | 29,539 | 29,724 |
| 1288 | hippurate | 52,762 | 54,942 | 49,193 | 49,802 |
| 50 | histidine | 39,191 | 48,469 | 45,404 | 44,749 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 231 | homocysteine | 101,404 | 18,296 | 28,609 | 63,628 |
| 1585 | homostachydrine* | 42,532 | 35,635 | 33,901 | 34,260 |
| 206 | hydroxyisovaleroyl carnitine | 199,428 | 433,188 | 383,050 | 364,332 |
| 1098 | hypoxanthine | 5,726,936 | 184,379 | 188,554 | 1,010,152 |
| 1101 | inosine 5'-monophosphate (IMP) | 210,439 | 164,643 | 340,178 | 524,568 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 60,260 | 59,340 | 62,915 | 52,665 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 95,608 | 81,353 | 87,471 | 80,990 |
| 496 | Isobar: sorbitol, mannitol | 17,766,824 | 18,403,908 | 18,956,124 | 18,274,208 |
| 200 | isobutyrylcarnitine | 136,153 | 179,779 | 169,293 | 147,503 |
| 180 | isoleucine | 4,660,911 | 4,070,097 | 4,618,131 | 4,576,028 |
| 478 | isomaltose | 2,150,195 | 1,501,424 | 2,617,697 | 2,077,336 |
| 205 | isovalerylcarnitine | 105,522 | 98,832 | 101,153 | 87,227 |
| 144 | kynurenine | 125,784 | 118,545 | 162,325 | 121,238 |
| 536 | lactate | 1,801,197,568 | 282,948,320 | 856,344,512 | 1,232,642,048 |
| 1018 | lathosterol | 77,125 | | 45,256 | 49,652 |
| 625 | laurate (12:0) | 131,042 | 90,667 | 103,770 | 118,520 |
| 181 | leucine | 8,996,487 | 8,485,215 | 9,793,614 | 10,022,278 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 604 | linoleate (18:2n6) | 2,854,648 | 2,121,206 | 2,520,759 | 2,934,382 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 684,028 | 289,340 | 520,360 | 555,806 |
| 69 | lysine | 1,159,421 | 2,689,346 | 2,846,649 | 2,973,361 |
| 598 | malate | 1,817,132 | 1,183,954 | 1,605,431 | 1,604,171 |
| 482 | maltose | 1,300,158 | 1,004,487 | 1,156,125 | 1,235,795 |
| 487 | mannose | 13,775,427 | 12,921,835 | 13,585,284 | 14,283,581 |
| 489 | mannose-6-phosphate | 295,219 | 205,612 | 214,854 | 215,244 |
| 635 | margarate (17:0) | 473,674 | 327,403 | 397,583 | 450,271 |
| 658 | mead acid (20:3n9) | 27,230 | 17,690 | 13,632 | 7,257 |
| 225 | methionine | 400,754 | 871,642 | 851,631 | 627,433 |
| 890 | myo-inositol | 1,943,253 | 2,177,501 | 2,240,130 | 2,466,853 |
| 629 | myristate (14:0) | 842,193 | 456,894 | 671,825 | 734,894 |
| 630 | myristoleate (14:1n5) | 25,634 | 19,786 | | 27,574 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 226,365 | 128,853 | 112,583 | 131,173 |
| 75 | N-6-trimethyllysine | 129,954 | 207,432 | 199,288 | 154,487 |
| 4 | N-acetylglycine | | 60,738 | 81,754 | 90,906 |
| 227 | N-acetylmethionine | 5,332 | 7,472 | 4,206 | |
| 455 | N-acetylneuraminate | 148,623 | 41,797 | 82,781 | 83,927 |
| 1221 | nicotinamide | 2,757,552 | 2,102,704 | 2,434,348 | 2,266,781 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 2,285 | 3,452 | 4,281 | 8,362 |
| 825 | octanoylcarnitine | 69,006 | 84,208 | 85,071 | 82,106 |
| 639 | oleate (18:1n9) | 620,775 | 727,388 | 690,991 | 942,979 |
| 835 | oleoylcarnitine | 588,338 | 344,844 | 1,004,542 | 1,699,879 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 285 | ophthalmate | | 184,491 | 61,277 | 22,451 |
| 244 | ornithine | 12,108,834 | 11,520,120 | 13,073,590 | 14,296,622 |
| 632 | palmitate (16:0) | 8,343,986 | 7,214,126 | 7,140,379 | 7,853,787 |
| 633 | palmitoleate (16:1n7) | 643,264 | 251,585 | 372,897 | 380,516 |
| 1004 | palmitoyl sphingomyelin | 15,744,304 | 14,751,954 | 15,966,146 | 17,801,990 |
| 833 | palmitoylcarnitine | 448,923 | 231,236 | 538,860 | 916,355 |
| 1243 | pantothenate | 111,153 | 94,658 | 100,994 | 100,503 |
| 1613 | paraxanthine | 511,703 | 388,352 | 525,707 | 512,656 |
| 88 | p-cresol sulfate | 76,301 | 45,396 | 45,541 | 45,250 |
| 621 | pelargonate (9:0) | 327,609 | 172,490 | 370,622 | 309,845 |
| 631 | pentadecanoate (15:0) | 222,446 | 166,204 | 200,364 | 228,140 |
| 135 | phenol sulfate | 19,582 | 19,408 | 18,741 | 17,671 |
| 128 | phenylacetylglutamine | 80,435 | 42,162 | 41,085 | 44,814 |
| 83 | phenylalanine | 10,595,847 | 6,835,470 | 8,864,478 | 9,102,095 |
| 602 | phosphate | 1,339,702,400 | 1,002,410,304 | 1,223,869,696 | 1,298,603,008 |
| 534 | phosphoenolpyruvate (PEP) | 43,910 | 239,214 | 108,179 | 32,033 |
| 877 | phosphoethanolamine | 65,341 | 74,125 | 80,273 | 110,292 |
| 74 | pipecolate | 106,018 | 81,418 | 105,961 | 86,742 |
| 1531 | piperine | 91,726 | 171,368 | 158,498 | 96,931 |
| 246 | proline | 2,149,858 | 2,163,042 | 2,082,362 | 2,052,232 |
| 809 | propionylcarnitine | 626,733 | 1,427,119 | 1,222,332 | 1,100,619 |
| 1181 | pseudouridine | 11,694 | 8,866 | 9,968 | 8,311 |
| 45 | pyroglutamine* | 62,240 | 173,894 | 187,319 | 172,320 |
| 603 | pyrophosphate (PPi) | 35,022 | 148,198 | 171,827 | 84,463 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 535 | pyruvate | 1,383,204 | 3,683,327 | 3,732,736 | 1,684,570 |
| 1469 | ranitidine | 378,825 | | | |
| 548 | ribitol | 254,906 | 169,871 | 273,815 | 134,022 |
| 557 | ribose 5-phosphate | 140,262 | 125,677 | 110,459 | 111,884 |
| 559 | ribulose | 17,431 | 29,385 | 17,277 | 18,080 |
| 224 | S-adenosylhomocysteine (SAH) | 243,619 | 134,789 | 219,723 | 194,554 |
| 551 | sedoheptulose-7-phosphate | 84,948 | 18,377 | 71,220 | 85,223 |
| 8 | serine | 7,395,738 | 7,074,594 | 8,687,528 | 8,759,669 |
| 216 | S-methylcysteine | 206,354 | 71,654 | 72,071 | 53,316 |
| 281 | S-methylglutathione | 28,458 | 20,277 | 43,484 | 27,756 |
| 270 | spermidine | 1,335,984 | 1,430,269 | 1,618,862 | 1,603,250 |
| 1584 | stachydrine | 183,012 | 3,405,363 | 3,532,005 | 3,353,102 |
| 637 | stearate (18:0) | 7,997,423 | 6,666,030 | 7,771,983 | 8,372,065 |
| 1005 | stearoyl sphingomyelin | 1,438,372 | 1,084,208 | 1,064,038 | 1,322,722 |
| 834 | stearoylcarnitine | 318,485 | 146,101 | 380,748 | 709,417 |
| 591 | succinylcarnitine | 399,279 | 571,063 | 601,544 | 613,988 |
| 1662 | terephthalic acid | 222,876 | 384,837 | 347,127 | 428,126 |
| 1614 | theobromine | 362,523 | 169,101 | 139,337 | 341,773 |
| 1615 | theophylline | 127,469 | 94,936 | 86,851 | 92,224 |
| 549 | threitol | 1,508,355 | 671,375 | 827,647 | 962,741 |
| 1199 | threonate | 535,658 | 478,661 | 532,947 | 529,854 |
| 17 | threonine | 182,269 | 190,291 | 237,555 | 262,031 |
| 252 | trans-4-hydroxyproline | 43,731 | 27,048 | 23,987 | 26,953 |

| | | DARM-00015 | DARM-00016 | DARM-00017 | DARM-00018 |
|---|---|---|---|---|---|
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | 997729 | 997715 | 997736 | 997748 |
| | | 991360 | 991361 | 991362 | 991363 |
| | | NHSCi 2003 C D28 | NHSCI 1866 T2 D0 | NHSCI 1866 T2 D7 | NHSCI 1866 T2 D14 |
| | | C D28 | T2 D0 | T2 D7 | T2 D14 |
| | | 175.121 | 176.276 | 164.34 | 172.339 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D28 | T2 D0 | T2 D7 | T2 D14 |
| 501 | trehalose | 996,469 | 157,424 | 621,208 | 1,077,238 |
| 1242 | trigonelline (N'-methylnicotinate) | 259,666 | 490,459 | 492,993 | 486,486 |
| 145 | tryptophan | 4,533,571 | 3,590,607 | 4,486,706 | 4,359,510 |
| 151 | tryptophan betaine | 1,521,566 | 4,557,345 | 4,402,292 | 4,252,671 |
| 99 | tyrosine | 2,238,650 | 2,410,461 | 2,769,754 | 2,872,390 |
| 1149 | urate | 153,368 | 214,504 | 183,618 | 163,812 |
| 245 | urea | 34,159,176 | 23,854,346 | 28,532,186 | 28,787,614 |
| 1180 | uridine | 20,164 | 27,493 | 30,559 | 35,443 |
| 190 | valine | 9,392,703 | 9,301,228 | 10,405,112 | 11,047,712 |
| 565 | xylitol | 12,425 | | | |
| 570 | xylonate | 87,714 | 63,458 | 48,256 | 75,641 |
| 569 | xylose | 83,277 | | 124,820 | 91,754 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 905 | 1,2-propanediol | 12,988,405 | 17,579,018 | 4,883,337 | 11,158,786 |
| 532 | 1,3-dihydroxyacetone | 71,598 | 87,438 | 95,508 | 58,140 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 7,769,879 | 6,815,589 | 6,894,500 | 6,652,106 |
| 523 | 1,6-anhydroglucose | 313,780 | 298,975 | 327,056 | 482,878 |
| 636 | 10-heptadecenoate (17:1n7) | 99,381 | 121,017 | 58,306 | 82,459 |
| 742 | 13-methylmyristic acid | 118,800 | 195,899 | 82,759 | 99,940 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 275,938 | 439,076 | 117,415 | 189,105 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 31,432 | 25,317 | 23,213 | 19,593 |
| 938 | 1-linoleoylglycerophosphocholine | 272,364 | 335,274 | 233,853 | 239,863 |
| 926 | 1-myristoylglycerophosphocholine | 64,906 | 79,486 | | 87,388 |
| 936 | 1-oleoylglycerophosphocholine | 392,551 | 976,080 | 132,943 | 1,797,474 |
| 915 | 1-oleoylglycerophosphoethanolamine | 17,977 | 22,455 | 16,684 | 9,933 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 44,231 | 63,395 | 20,584 | 45,829 |
| 929 | 1-palmitoylglycerophosphocholine | 2,302,004 | 5,330,005 | 762,895 | 8,022,161 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 16,633 | 24,392 | 13,802 | 15,749 |
| 934 | 1-stearoylglycerophosphocholine | 1,479,612 | 2,051,804 | 261,966 | 3,126,313 |
| 533 | 2,3-diphosphoglycerate | 3,820 | | 424,122 | 476,646 |
| 263 | 2-aminobutyrate | 2,866,594 | 2,636,668 | 2,360,075 | 2,292,059 |
| 945 | 2-arachidonoylglycerophosphocholine* | 182,369 | 214,159 | 83,937 | 406,006 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 1,710,407 | 1,987,412 | 404,129 | 3,423,001 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 325,072 | 350,497 | 120,514 | 822,177 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 504,217 | 540,002 | 150,283 | 1,058,896 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 29,405 | 27,464 | 21,764 | 38,147 |
| 229 | 2-hydroxybutyrate (AHB) | 1,824,982 | 1,624,975 | 1,755,588 | 1,668,014 |
| 714 | 2-hydroxyglutarate | 183,311 | 267,356 | 86,275 | 293,229 |
| 706 | 2-hydroxypalmitate | 41,185 | 53,740 | 34,513 | 45,504 |
| 939 | 2-linoleoylglycerophosphocholine* | 358,967 | 266,997 | | 603,328 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 202 | 2-methylbutyroylcarnitine | 59,511 | 65,353 | 59,371 | 54,524 |
| 937 | 2-oleoylglycerophosphocholine* | 125,320 | 187,515 | 83,221 | 408,239 |
| 930 | 2-palmitoylglycerophosphocholine* | 382,178 | 456,156 | 41,157 | 677,752 |
| 935 | 2-stearoylglycerophosphocholine* | 137,857 | 141,873 | 17,302 | 168,910 |
| 821 | 3-dehydrocarnitine* | 1,041,111 | 1,180,521 | 919,964 | 1,024,916 |
| 170 | 3-indoxyl sulfate | 4,891 | 4,909 | 3,088 | 3,604 |
| 172 | 3-methyl-2-oxobutyrate | 43,501 | 35,532 | 26,163 | |
| 173 | 3-methyl-2-oxovalerate | 62,630 | 58,615 | 45,616 | 28,256 |
| 529 | 3-phosphoglycerate | 339,502 | 337,094 | 2,994,259 | 1,768,015 |
| 193 | 4-methyl-2-oxopentanoate | 116,109 | 100,533 | 91,059 | 43,289 |
| 266 | 5-methylthioadenosine (MTA) | 131,980 | 100,486 | 50,073 | 124,318 |
| 282 | 5-oxoproline | 389,006 | 561,164 | 60,006 | 215,000 |
| 545 | 6-phosphogluconate | | 59,070 | 65,019 | 49,694 |
| 1024 | 7-beta-hydroxycholesterol | | 31,852 | 39,027 | 25,325 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 184,958 | 230,491 | 15,807 | 112,411 |
| 672 | 9,10-epoxystearate | 8,035,032 | 10,290,958 | 262,413 | 5,419,621 |
| 822 | acetylcarnitine | 3,643,731 | 3,616,617 | 3,699,032 | 3,956,132 |
| 601 | acetylphosphate | 3,549,777 | 3,362,782 | 3,269,842 | 3,340,224 |
| 1105 | adenine | 14,296,981 | 10,888,939 | 38,773,896 | 39,361,264 |
| 1106 | adenosine | 27,384 | 30,660 | 16,531 | 33,120 |
| 1116 | adenosine 5'-diphosphate (ADP) | 173,006 | 179,982 | 169,042 | 148,837 |
| 1232 | adenosine 5'diphosphoribose | 90,260 | 75,788 | 97,530 | 119,749 |
| 1114 | adenosine 5'-monophosphate (AMP) | 5,220,412 | 7,785,904 | 2,825,064 | 3,599,888 |
| 665 | adrenate (22:4n6) | 139,089 | 129,986 | 251,158 | 40,106 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 27 | alanine | 69,618,664 | 70,075,624 | 49,597,364 | 52,059,648 |
| 1150 | allantoin | 33,353 | 34,494 | 13,333 | 22,227 |
| 179 | alpha-hydroxyisocaproate | 272,954 | 388,477 | | 257,854 |
| 198 | alpha-hydroxyisovalerate | 610,933 | 905,115 | 501,450 | 1,242,532 |
| 1266 | alpha-tocopherol | 164,265 | 147,588 | 161,150 | 130,569 |
| 1034 | androsterone sulfate | 7,775 | 8,716 | 7,495 | 8,312 |
| 566 | arabinose | 327,335 | 363,255 | 359,675 | 409,806 |
| 546 | arabitol | 650,758 | 587,747 | 492,839 | 781,818 |
| 1202 | arabonate | 87,604 | 111,541 | 91,880 | 107,463 |
| 659 | arachidonate (20:4n6) | 1,035,176 | 1,445,696 | 415,619 | 641,629 |
| 241 | arginine | 823,418 | 2,158,228 | 674,520 | 847,895 |
| 25 | asparagine | 1,355,122 | 1,037,958 | 1,632,671 | 1,672,673 |
| 24 | aspartate | 4,061,158 | 3,382,174 | 4,605,921 | 4,713,740 |
| 721 | azelate (nonanedioate) | 42,878 | 49,992 | 5,912 | 17,650 |
| 26 | beta-alanine | 150,330 | 58,525 | 155,782 | 151,518 |
| 7 | beta-hydroxypyruvate | 263,380 | 307,563 | 255,303 | 262,860 |
| 22 | betaine | 1,661,101 | 1,652,498 | 1,592,822 | 1,685,309 |
| 1057 | beta-sitosterol | 51,142 | 46,068 | 45,816 | 46,029 |
| 1216 | biliverdin | 60,683 | 49,190 | 18,414 | 86,882 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 811 | butyrylcarnitine | 15,882 | 14,181 | 28,350 | 16,237 |
| 1612 | caffeine | 3,541,355 | 3,056,576 | 2,968,486 | 3,125,682 |
| 1059 | campesterol | 229,315 | | | 205,461 |
| 622 | caprate (10:0) | 31,823 | 34,835 | 16,366 | 25,727 |
| 618 | caproate (6:0) | 43,562 | 51,821 | 43,667 | 57,151 |
| 620 | caprylate (8:0) | 60,793 | 54,301 | 19,984 | 62,170 |
| 820 | carnitine | 975,356 | 1,027,886 | 972,927 | 989,284 |
| 1300 | catechol sulfate | 78,314 | 80,056 | 80,586 | 83,616 |
| 164 | C-glycosyltryptophan* | 36,197 | 26,920 | 26,946 | 24,759 |
| 1020 | cholesterol | 37,924,164 | 36,418,236 | 37,268,052 | 36,268,140 |
| 881 | choline | 2,121,928 | 2,141,355 | 2,136,781 | 2,176,103 |
| 582 | cis-aconitate | 948,779 | 1,049,116 | 548,775 | 845,962 |
| 641 | cis-vaccenate (18:1n7) | 191,206 | 122,033 | 156,317 | 335,037 |
| 579 | citrate | 214,941,248 | 182,096,240 | 301,815,680 | 271,697,088 |
| 248 | citrulline | 132,630 | 112,217 | 110,256 | 101,075 |
| 259 | creatine | 3,726,428 | 3,760,821 | 3,528,599 | 3,766,965 |
| 260 | creatinine | 453,973 | 421,680 | 407,646 | 370,191 |
| 213 | cysteine | 1,469,723 | 1,499,818 | 486,877 | 418,808 |
| 819 | deoxycarnitine | 567,749 | 604,672 | 516,383 | 581,091 |
| 655 | dihomo-linoleate (20:2n6) | 68,472 | 97,515 | 36,918 | 60,112 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 85,816 | 106,351 | 47,939 | 59,294 |
| 531 | dihydroxyacetone phosphate (DHAP) | 36,450 | 14,876 | 1,726,288 | 3,554,937 |
| 3 | dimethylglycine | 490,315 | 405,000 | 270,058 | 234,698 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 198,626 | 240,531 | 72,313 | 153,300 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 93,726 | 133,260 | 35,471 | 61,087 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 191,871 | 211,947 | 154,648 | 145,613 |
| 1565 | ergothioneine | 825,681 | 947,207 | 730,661 | 812,798 |
| 735 | erucamide | 322,761 | 205,025 | 864,326 | 368,533 |
| 1632 | erythritol | 1,583,447 | 1,723,622 | 864,946 | 1,406,027 |
| 453 | erythronate* | 544,325 | 632,895 | 349,267 | 573,851 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 876 | ethanolamine | 817,581 | 449,802 | 398,511 | 614,570 |
| 472 | fructose | 84,917,432 | 76,978,512 | 61,459,480 | 46,021,040 |
| 524 | fructose-6-phosphate | 348,462 | 558,766 | 199,972 | 460,074 |
| 594 | fumarate | 452,332 | 677,878 | 298,892 | 557,441 |
| 404 | gamma-glutamylleucine | 20,341 | | 29,980 | 33,534 |
| 521 | glucose | 1,036,868,032 | 1,081,754,368 | 1,063,524,672 | 1,053,441,792 |
| 519 | glucose-6-phosphate (G6P) | 992,712 | 1,678,752 | 325,699 | 219,862 |
| 39 | glutamate | 6,926,577 | 7,878,551 | 7,916,416 | 8,248,287 |
| 44 | glutamine | 1,349,251 | 1,070,462 | 1,897,135 | 1,391,232 |
| 80 | glutaroyl carnitine | 20,693 | 17,280 | 13,402 | 12,278 |
| 283 | glutathione, oxidized (GSSG) | 904,246 | 913,998 | 1,700,524 | 1,169,490 |
| 280 | glutathione, reduced (GSH) | 22,826,626 | 19,206,434 | 24,510,320 | 18,046,108 |
| 517 | glycerate | 705,096 | 710,916 | 335,496 | 2,455,053 |
| 882 | glycerol 3-phosphate (G3P) | 336,971 | 295,156 | 760,290 | 1,057,582 |
| 883 | glycerophosphorylcholine (GPC) | 145,826 | 139,502 | 153,165 | 146,334 |
| 1 | glycine | 54,611,724 | 70,597,176 | 27,344,856 | 32,933,818 |
| 851 | glycochenodeoxycholate | 105,234 | 93,996 | 95,013 | 106,437 |
| 840 | glycocholate | 58,328 | 60,700 | 51,839 | 55,294 |
| 849 | glycodeoxycholate | 46,414 | 44,025 | 27,804 | 32,978 |
| 1318 | glycolate (hydroxyacetate) | 377,606 | 350,231 | 366,458 | 371,036 |
| 1128 | guanosine | 17,236 | 25,314 | 28,931 | 31,015 |
| 1212 | heme* | 2,404,961 | 2,028,298 | 2,018,425 | 9,060,939 |
| 619 | heptanoate (7:0) | 17,772 | 19,096 | 7,078 | 16,347 |
| 823 | hexanoylcarnitine | 26,931 | 41,797 | 32,801 | 40,053 |
| 1288 | hippurate | 48,748 | 48,988 | 46,846 | 53,650 |
| 50 | histidine | 42,787 | 40,189 | 48,047 | 41,588 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 231 | homocysteine | 83,562 | 69,119 | 26,772 | 35,380 |
| 1585 | homostachydrine* | 41,734 | 25,645 | 39,915 | 25,749 |
| 206 | hydroxyisovaleroyl carnitine | 403,540 | 361,707 | 321,621 | 371,607 |
| 1098 | hypoxanthine | 3,746,092 | 7,582,735 | 218,018 | 15,006,904 |
| 1101 | inosine 5'-monophosphate (IMP) | 435,611 | 507,463 | 199,428 | 242,285 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 46,635 | 47,458 | 159,838 | 470,896 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 62,697 | 92,875 | 415,389 | 526,939 |
| 496 | Isobar: sorbitol, mannitol | 19,596,932 | 18,810,812 | 20,693,838 | 19,441,930 |
| 200 | isobutyrylcarnitine | 147,053 | 145,159 | 155,481 | 139,957 |
| 180 | isoleucine | 4,776,263 | 4,879,193 | 4,081,148 | 5,524,639 |
| 478 | isomaltose | 1,987,299 | 1,835,022 | 3,797,408 | 1,921,827 |
| 205 | isovalerylcarnitine | 94,873 | 94,547 | 94,705 | 102,380 |
| 144 | kynurenine | 159,947 | 123,647 | 171,047 | 150,418 |
| 536 | lactate | 1,464,920,448 | 1,629,336,448 | 410,955,296 | 1,221,739,776 |
| 1018 | lathosterol | 52,650 | | | |
| 625 | laurate (12:0) | 126,880 | 135,917 | 107,314 | 130,118 |
| 181 | leucine | 10,317,954 | 11,209,174 | 7,826,979 | 11,076,082 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 604 | linoleate (18:2n6) | 3,488,389 | 4,216,679 | 1,893,378 | 3,325,434 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 585,315 | 797,433 | 463,198 | 632,529 |
| 69 | lysine | 2,735,003 | 2,312,196 | 2,787,946 | 2,883,800 |
| 598 | malate | 1,849,524 | 2,396,799 | 982,479 | 2,436,818 |
| 482 | maltose | 1,114,331 | 1,071,442 | 1,199,963 | 1,161,170 |
| 487 | mannose | 13,174,139 | 12,421,385 | 14,402,010 | 12,403,063 |
| 489 | mannose-6-phosphate | 178,214 | 239,605 | 108,630 | 284,746 |
| 635 | margarate (17:0) | 490,851 | 747,239 | 285,902 | 422,281 |
| 658 | mead acid (20:3n9) | 23,696 | 9,927 | 6,654 | 11,098 |
| 225 | methionine | 519,521 | 442,595 | 884,048 | 788,060 |
| 890 | myo-inositol | 2,382,103 | 1,935,200 | 2,619,273 | 2,420,938 |
| 629 | myristate (14:0) | 884,099 | 963,766 | 382,467 | 737,971 |
| 630 | myristoleate (14:1n5) | 31,564 | 38,529 | 17,273 | 26,865 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 225,900 | 140,357 | 207,537 | 107,726 |
| 75 | N-6-trimethyllysine | 203,543 | 175,609 | 224,147 | 175,826 |
| 4 | N-acetylglycine | 58,161 | 82,589 | 82,780 | 67,347 |
| 227 | N-acetylmethionine | 7,385 | 5,726 | 4,067 | 6,335 |
| 455 | N-acetylneuraminate | 91,039 | 89,395 | 31,680 | 84,752 |
| 1221 | nicotinamide | 2,276,759 | 2,900,386 | 2,084,399 | 2,805,582 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 8,043 | 3,893 | 8,691 | 9,748 |
| 825 | octanoylcarnitine | 88,502 | 75,900 | 58,972 | 69,756 |
| 639 | oleate (18:1n9) | 1,009,422 | 828,776 | 907,505 | 910,789 |
| 835 | oleoylcarnitine | 1,544,235 | 1,489,540 | 313,945 | 2,955,699 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 285 | ophthalmate | 19,017 | | 227,185 | 97,437 |
| 244 | ornithine | 13,163,223 | 9,595,782 | 10,832,294 | 12,721,358 |
| 632 | palmitate (16:0) | 8,226,684 | 11,159,390 | 5,431,364 | 7,438,743 |
| 633 | palmitoleate (16:1n7) | 635,560 | 557,851 | 364,918 | 477,093 |
| 1004 | palmitoyl sphingomyelin | 16,440,715 | 15,896,092 | 14,012,885 | 16,431,550 |
| 833 | palmitoylcarnitine | 807,041 | 825,461 | 200,078 | 1,440,512 |
| 1243 | pantothenate | 115,021 | 101,784 | 99,612 | 104,805 |
| 1613 | paraxanthine | 514,252 | 471,959 | 438,211 | 501,931 |
| 88 | p-cresol sulfate | 48,933 | 42,918 | 40,529 | 45,665 |
| 621 | pelargonate (9:0) | 354,666 | 398,180 | 123,418 | 303,302 |
| 631 | pentadecanoate (15:0) | 245,416 | 308,371 | 174,751 | 229,888 |
| 135 | phenol sulfate | 18,254 | 18,729 | 19,500 | 21,576 |
| 128 | phenylacetylglutamine | 40,842 | 48,882 | 43,617 | 43,380 |
| 83 | phenylalanine | 9,432,172 | 9,297,807 | 7,104,701 | 9,035,316 |
| 602 | phosphate | 1,310,245,504 | 1,264,968,192 | 877,120,960 | 742,547,264 |
| 534 | phosphoenolpyruvate (PEP) | 25,115 | 16,771 | 465,258 | 302,786 |
| 877 | phosphoethanolamine | 92,849 | 90,439 | 133,297 | 61,514 |
| 74 | pipecolate | 88,160 | 112,236 | 97,249 | 105,482 |
| 1531 | piperine | 113,691 | 84,138 | 101,004 | 157,842 |
| 246 | proline | 2,234,918 | 2,418,336 | 1,905,368 | 2,043,748 |
| 809 | propionylcarnitine | 1,073,437 | 1,039,936 | 1,208,132 | 1,089,995 |
| 1181 | pseudouridine | 8,164 | 9,365 | 5,590 | 8,771 |
| 45 | pyroglutamine* | 178,501 | 201,908 | 184,215 | 189,017 |
| 603 | pyrophosphate (PPi) | 76,524 | 37,001 | 260,564 | 108,258 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 535 | pyruvate | 1,061,162 | 1,217,532 | 112,132 | 63,634 |
| 1469 | ranitidine | | | | |
| 548 | ribitol | 229,530 | 235,520 | 179,868 | 1,032,010 |
| 557 | ribose 5-phosphate | 134,948 | 98,268 | 303,035 | 437,942 |
| 559 | ribulose | 19,378 | 36,687 | 24,209 | 138,348 |
| 224 | S-adenosylhomocysteine (SAH) | 210,327 | 256,069 | 119,533 | 190,459 |
| 551 | sedoheptulose-7-phosphate | 40,991 | 69,361 | | 5,191 |
| 8 | serine | 8,690,862 | 8,589,556 | 7,383,090 | 8,659,009 |
| 216 | S-methylcysteine | 130,226 | 89,804 | 69,732 | 81,016 |
| 281 | S-methylglutathione | 31,276 | 20,929 | 24,198 | 38,620 |
| 270 | spermidine | 1,619,453 | 1,654,982 | 1,261,554 | 1,494,457 |
| 1584 | stachydrine | 3,444,752 | 3,618,930 | 3,174,276 | 3,434,351 |
| 637 | stearate (18:0) | 8,879,079 | 11,802,712 | 5,153,922 | 7,450,746 |
| 1005 | stearoyl sphingomyelin | 1,134,866 | 1,103,962 | 1,173,464 | 1,378,934 |
| 834 | stearoylcarnitine | 685,867 | 635,931 | 113,319 | 1,081,304 |
| 591 | succinylcarnitine | 602,811 | 669,668 | 508,744 | 554,379 |
| 1662 | terephthalic acid | 430,156 | 428,498 | 401,573 | 429,262 |
| 1614 | theobromine | 197,378 | 237,016 | 160,705 | 172,203 |
| 1615 | theophylline | 133,270 | 118,079 | 74,393 | 90,281 |
| 549 | threitol | 968,914 | 957,934 | 834,558 | 1,089,986 |
| 1199 | threonate | 567,150 | 551,803 | 506,499 | 462,111 |
| 17 | threonine | 238,672 | 233,172 | 205,602 | 223,507 |
| 252 | trans-4-hydroxyproline | 32,518 | 25,701 | 19,313 | 28,263 |

| | | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 | NHSCI 1866 T1 D7 |
| | | 997740 | 997720 | 997746 | 997738 |
| | | 991364 | 991365 | 991366 | 991367 |
| | | NHSCI 1866 T2 D21 | NHSCI 1866 T2 D28 | NHSCI 1866 T1 D0 | NHSCI 1866 T1 D7 |
| | | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| | | 203.125 | 169.237 | 179.08 | 165.545 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T2 D21 | T2 D28 | T1 D0 | T1 D7 |
| 501 | trehalose | 1,325,007 | 1,042,991 | 190,060 | 462,741 |
| 1242 | trigonelline (N'-methylnicotinate) | 501,302 | 462,348 | 484,522 | 505,470 |
| 145 | tryptophan | 4,679,503 | 4,174,408 | 3,589,194 | 4,354,362 |
| 151 | tryptophan betaine | 4,354,753 | 4,427,971 | 3,840,391 | 4,271,965 |
| 99 | tyrosine | 3,029,753 | 2,886,537 | 2,522,695 | 2,872,657 |
| 1149 | urate | 166,881 | 174,699 | 187,677 | 178,192 |
| 245 | urea | 27,915,962 | 27,365,086 | 24,941,684 | 27,766,150 |
| 1180 | uridine | 39,013 | 46,772 | 27,367 | 43,315 |
| 190 | valine | 10,775,019 | 10,639,117 | 9,167,983 | 10,653,256 |
| 565 | xylitol | 19,881 | | | 279,174 |
| 570 | xylonate | 75,060 | 59,895 | 49,776 | 82,130 |
| 569 | xylose | | 149,690 | 86,756 | 123,024 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 905 | 1,2-propanediol | 9,222,896 | 11,653,529 | 16,395,251 | 5,359,018 |
| 532 | 1,3-dihydroxyacetone | 79,639 | 75,059 | 66,607 | 71,270 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 6,016,202 | 8,553,883 | 6,683,827 | 7,625,753 |
| 523 | 1,6-anhydroglucose | 511,979 | 293,938 | 390,658 | 422,889 |
| 636 | 10-heptadecenoate (17:1n7) | 87,318 | 106,381 | 101,766 | 68,349 |
| 742 | 13-methylmyristic acid | 132,142 | 143,027 | 170,341 | 76,519 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 213,039 | 263,284 | 309,137 | 125,661 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 20,053 | 20,043 | 19,307 | 35,154 |
| 938 | 1-linoleoylglycerophosphocholine | 244,569 | 246,194 | 237,103 | 247,500 |
| 926 | 1-myristoylglycerophosphocholine | 102,061 | 198,228 | 59,542 | |
| 936 | 1-oleoylglycerophosphocholine | 1,587,265 | 3,673,508 | 779,136 | 38,365 |
| 915 | 1-oleoylglycerophosphoethanolamine | 17,824 | 10,839 | 23,412 | 26,206 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 44,045 | 41,357 | 28,608 | 27,195 |
| 929 | 1-palmitoylglycerophosphocholine | 7,190,304 | 13,289,885 | 4,358,269 | 125,397 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 11,739 | 17,475 | 9,695 | 18,804 |
| 934 | 1-stearoylglycerophosphocholine | 2,980,702 | 6,212,239 | 1,742,057 | 48,748 |
| 533 | 2,3-diphosphoglycerate | 333,988 | 130,003 | 25,572 | 314,605 |
| 263 | 2-aminobutyrate | 2,537,859 | 2,450,284 | 2,724,597 | 2,469,166 |
| 945 | 2-arachidonoylglycerophosphocholine* | 404,946 | 742,997 | 153,659 | |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 3,413,996 | 5,115,768 | 1,716,124 | 88,717 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 828,081 | 1,285,999 | 352,568 | 41,806 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 919,153 | 1,583,575 | 432,783 | |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 19,731 | 22,683 | 18,451 | 30,919 |
| 229 | 2-hydroxybutyrate (AHB) | 1,690,633 | 1,630,246 | 1,556,682 | 1,588,466 |
| 714 | 2-hydroxyglutarate | 296,627 | 318,966 | 354,627 | 105,231 |
| 706 | 2-hydroxypalmitate | 47,416 | 56,921 | 57,935 | 36,965 |
| 939 | 2-linoleoylglycerophosphocholine* | 676,049 | 1,129,196 | 409,232 | |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 202 | 2-methylbutyroylcarnitine | 40,669 | 47,016 | 51,127 | 74,990 |
| 937 | 2-oleoylglycerophosphocholine* | 337,856 | 708,052 | 164,772 | |
| 930 | 2-palmitoylglycerophosphocholine* | 639,670 | 1,237,807 | 330,006 | 34,141 |
| 935 | 2-stearoylglycerophosphocholine* | 164,754 | 385,602 | 113,450 | |
| 821 | 3-dehydrocarnitine* | 1,019,193 | 932,404 | 1,018,342 | 940,934 |
| 170 | 3-indoxyl sulfate | 3,053 | 4,915 | 3,975 | 4,098 |
| 172 | 3-methyl-2-oxobutyrate | 6,240 | 8,786 | | 56,751 |
| 173 | 3-methyl-2-oxovalerate | 17,025 | 16,565 | 22,984 | 53,631 |
| 529 | 3-phosphoglycerate | 1,478,279 | 598,853 | 542,490 | 1,123,098 |
| 193 | 4-methyl-2-oxopentanoate | 24,801 | 30,725 | 41,940 | 113,635 |
| 266 | 5-methylthioadenosine (MTA) | 140,884 | 117,209 | 109,639 | 47,611 |
| 282 | 5-oxoproline | 350,384 | 385,959 | 418,018 | 55,881 |
| 545 | 6-phosphogluconate | 80,351 | 33,268 | 31,567 | 115,280 |
| 1024 | 7-beta-hydroxycholesterol | 28,826 | 19,054 | 22,345 | 19,557 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 152,463 | 157,052 | 213,245 | 13,769 |
| 672 | 9,10-epoxystearate | 8,368,615 | 8,289,198 | 11,156,853 | 400,963 |
| 822 | acetylcarnitine | 3,473,271 | 3,330,010 | 3,275,070 | 4,034,797 |
| 601 | acetylphosphate | 3,284,806 | 3,234,368 | 3,255,410 | 2,935,023 |
| 1105 | adenine | 33,155,058 | 25,601,084 | 16,469,920 | 42,802,920 |
| 1106 | adenosine | 35,262 | 30,706 | 31,773 | 37,023 |
| 1116 | adenosine 5'-diphosphate (ADP) | 134,937 | 95,612 | 94,216 | 218,446 |
| 1232 | adenosine 5'diphosphoribose | 102,409 | 82,110 | 68,008 | 94,292 |
| 1114 | adenosine 5'-monophosphate (AMP) | 2,832,129 | 3,536,550 | 5,477,438 | 3,445,505 |
| 665 | adrenate (22:4n6) | 68,604 | 106,317 | 109,502 | 35,631 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 27 | alanine | 50,100,840 | 51,392,724 | 60,260,428 | 56,876,548 |
| 1150 | allantoin | 9,816 | 25,160 | 28,017 | 46,315 |
| 179 | alpha-hydroxyisocaproate | 429,098 | 315,064 | 410,059 | |
| 198 | alpha-hydroxyisovalerate | 1,381,199 | 1,310,523 | 1,658,694 | 288,261 |
| 1266 | alpha-tocopherol | 121,546 | 109,708 | 171,439 | 174,305 |
| 1034 | androsterone sulfate | 4,983 | 6,402 | 7,721 | 5,431 |
| 566 | arabinose | 296,164 | 346,448 | 386,519 | 297,138 |
| 546 | arabitol | 866,851 | 800,143 | 957,866 | 585,899 |
| 1202 | arabonate | 80,462 | 73,555 | 76,541 | 67,569 |
| 659 | arachidonate (20:4n6) | 697,589 | 1,008,060 | 1,476,199 | 695,282 |
| 241 | arginine | 988,248 | 1,240,274 | 1,372,072 | 530,412 |
| 25 | asparagine | 1,323,333 | 1,203,043 | 1,392,988 | 1,406,645 |
| 24 | aspartate | 4,816,711 | 4,305,496 | 3,695,279 | 3,381,338 |
| 721 | azelate (nonanedioate) | 24,727 | 32,976 | 48,723 | 4,398 |
| 26 | beta-alanine | 147,916 | 116,475 | 167,238 | 151,480 |
| 7 | beta-hydroxypyruvate | 260,419 | 192,934 | 265,273 | 303,406 |
| 22 | betaine | 1,720,901 | 1,677,453 | 1,717,075 | 1,639,042 |
| 1057 | beta-sitosterol | 57,786 | 49,832 | 45,102 | 30,940 |
| 1216 | biliverdin | 73,846 | 121,908 | 32,588 | 19,615 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 811 | butyrylcarnitine | 9,986 | 25,941 | 12,620 | 16,262 |
| 1612 | caffeine | 3,204,983 | 3,235,623 | 3,163,755 | 3,387,228 |
| 1059 | campesterol | 207,988 | 410,371 | 375,275 | 240,252 |
| 622 | caprate (10:0) | 27,899 | 19,115 | 25,526 | 15,349 |
| 618 | caproate (6:0) | 21,964 | 22,321 | 20,907 | 43,003 |
| 620 | caprylate (8:0) | 19,582 | 37,463 | 24,080 | 27,589 |
| 820 | carnitine | 1,068,483 | 1,025,964 | 1,009,222 | 938,032 |
| 1300 | catechol sulfate | 77,652 | 76,520 | 75,564 | 79,676 |
| 164 | C-glycosyltryptophan* | 31,863 | 33,420 | 27,721 | 31,840 |
| 1020 | cholesterol | 34,291,188 | 32,623,754 | 36,720,168 | 35,122,852 |
| 881 | choline | 2,249,203 | 2,107,602 | 2,141,094 | 2,123,580 |
| 582 | cis-aconitate | 914,380 | 926,615 | 922,791 | 622,362 |
| 641 | cis-vaccenate (18:1n7) | 105,201 | 216,159 | 363,117 | 227,686 |
| 579 | citrate | 198,625,488 | 145,882,720 | 120,670,864 | 295,909,920 |
| 248 | citrulline | 114,735 | 112,684 | 119,573 | 100,053 |
| 259 | creatine | 3,761,597 | 3,710,686 | 3,729,844 | 3,638,218 |
| 260 | creatinine | 434,766 | 401,605 | 448,956 | 412,470 |
| 213 | cysteine | 649,481 | 956,357 | 1,064,491 | 468,283 |
| 819 | deoxycarnitine | 583,392 | 556,648 | 589,514 | 569,406 |
| 655 | dihomo-linoleate (20:2n6) | 75,468 | 80,418 | 93,527 | 45,828 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 71,432 | 88,102 | 117,655 | 69,155 |
| 531 | dihydroxyacetone phosphate (DHAP) | 711,366 | | | 33,072 |
| 3 | dimethylglycine | 296,146 | 181,282 | 349,965 | 364,534 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 146,753 | 184,351 | 231,315 | 118,229 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 82,788 | 103,119 | 131,731 | 49,019 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 178,067 | 200,501 | 213,780 | 156,298 |
| 1565 | ergothioneine | 787,115 | 784,154 | 822,103 | 898,558 |
| 735 | erucamide | 260,022 | 265,707 | | 570,717 |
| 1632 | erythritol | 2,037,034 | 2,614,540 | 3,672,486 | 837,725 |
| 453 | erythronate* | 955,566 | 1,345,808 | 1,403,580 | 389,326 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 876 | ethanolamine | 616,450 | 513,979 | 740,718 | 449,686 |
| 472 | fructose | 48,251,748 | 73,835,424 | 99,218,608 | 62,642,476 |
| 524 | fructose-6-phosphate | 601,632 | 269,948 | 398,915 | 553,908 |
| 594 | fumarate | 617,688 | 639,637 | 604,120 | 415,915 |
| 404 | gamma-glutamylleucine | 26,263 | 27,469 | | 24,169 |
| 521 | glucose | 947,113,472 | 896,353,088 | 993,111,232 | 1,118,494,208 |
| 519 | glucose-6-phosphate (G6P) | 1,117,890 | 1,420,377 | 1,316,496 | 1,412,532 |
| 39 | glutamate | 6,378,748 | 5,257,395 | 6,198,704 | 6,831,711 |
| 44 | glutamine | 1,097,059 | 959,056 | 880,151 | 1,941,536 |
| 80 | glutaroyl carnitine | 12,938 | 13,182 | 11,913 | 17,870 |
| 283 | glutathione, oxidized (GSSG) | 986,813 | 779,092 | 691,372 | 1,474,703 |
| 280 | glutathione, reduced (GSH) | 22,980,926 | 21,671,654 | 19,504,774 | 26,064,682 |
| 517 | glycerate | 4,681,174 | 5,326,287 | 6,292,381 | 249,083 |
| 882 | glycerol 3-phosphate (G3P) | 564,928 | 252,624 | 273,805 | 395,807 |
| 883 | glycerophosphorylcholine (GPC) | 160,595 | 156,805 | 166,682 | 171,745 |
| 1 | glycine | 34,244,468 | 39,616,372 | 53,382,244 | 27,236,388 |
| 851 | glycochenodeoxycholate | 99,498 | 89,799 | 94,180 | 120,061 |
| 840 | glycocholate | 50,337 | 48,685 | 56,512 | 58,620 |
| 849 | glycodeoxycholate | 44,255 | 34,620 | 41,816 | 32,563 |
| 1318 | glycolate (hydroxyacetate) | 371,105 | 340,540 | 409,050 | 393,353 |
| 1128 | guanosine | 32,032 | 32,000 | 19,652 | 25,082 |
| 1212 | heme* | 5,497,433 | 10,833,596 | 1,124,794 | 187,384 |
| 619 | heptanoate (7:0) | 6,033 | 7,009 | 7,562 | 9,017 |
| 823 | hexanoylcarnitine | 25,003 | 30,915 | 26,561 | 61,494 |
| 1288 | hippurate | 52,463 | 50,955 | 50,157 | 48,853 |
| 50 | histidine | 41,985 | 54,803 | 44,890 | 37,045 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 231 | homocysteine | 102,438 | 92,077 | 125,847 | 25,998 |
| 1585 | homostachydrine* | 31,065 | 34,000 | 36,082 | 41,178 |
| 206 | hydroxyisovaleroyl carnitine | 348,729 | 335,775 | 343,590 | 361,571 |
| 1098 | hypoxanthine | 13,937,754 | 12,358,769 | 14,866,583 | 279,881 |
| 1101 | inosine 5'-monophosphate (IMP) | 405,409 | 605,083 | 679,813 | 134,957 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 79,205 | 30,139 | 25,676 | 53,309 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 261,361 | 42,323 | 43,696 | 81,386 |
| 496 | Isobar: sorbitol, mannitol | 20,631,362 | 19,962,346 | 16,509,542 | 17,943,808 |
| 200 | isobutyrylcarnitine | 135,366 | 132,992 | 130,810 | 143,152 |
| 180 | isoleucine | 5,791,709 | 5,323,534 | 5,687,231 | 4,385,777 |
| 478 | isomaltose | 1,489,502 | 1,627,792 | 2,074,130 | 1,946,129 |
| 205 | isovalerylcarnitine | 98,113 | 90,526 | 96,377 | 107,873 |
| 144 | kynurenine | 147,800 | 127,429 | 112,213 | 138,889 |
| 536 | lactate | 1,643,635,584 | 1,936,001,408 | 2,385,103,360 | 283,727,616 |
| 1018 | lathosterol | 46,234 | 52,225 | | |
| 625 | laurate (12:0) | 139,308 | 110,852 | 109,737 | 108,254 |
| 181 | leucine | 11,146,261 | 10,841,503 | 11,718,432 | 9,206,251 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 604 | linoleate (18:2n6) | 3,454,248 | 4,061,245 | 4,524,522 | 2,696,804 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 562,984 | 707,330 | 698,064 | 570,880 |
| 69 | lysine | 2,899,100 | 2,479,688 | 3,217,801 | 2,485,539 |
| 598 | malate | 2,705,658 | 2,812,607 | 2,370,052 | 1,111,300 |
| 482 | maltose | 1,068,441 | 1,122,334 | 1,304,029 | 1,355,155 |
| 487 | mannose | 11,294,361 | 11,001,329 | 11,860,068 | 14,083,007 |
| 489 | mannose-6-phosphate | 276,375 | 240,282 | 255,265 | 219,228 |
| 635 | margarate (17:0) | 399,697 | 472,678 | 520,903 | 294,869 |
| 658 | mead acid (20:3n9) | 16,461 | 14,273 | 18,625 | 20,403 |
| 225 | methionine | 641,689 | 481,944 | 453,751 | 881,990 |
| 890 | myo-inositol | 1,999,987 | 1,791,128 | 2,181,631 | 2,326,825 |
| 629 | myristate (14:0) | 671,065 | 690,413 | 788,174 | 401,086 |
| 630 | myristoleate (14:1n5) | 37,469 | | | 48,279 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 104,601 | 139,784 | 161,098 | 112,680 |
| 75 | N-6-trimethyllysine | 164,703 | 182,702 | 171,199 | 180,387 |
| 4 | N-acetylglycine | 69,833 | | 85,540 | 80,848 |
| 227 | N-acetylmethionine | 3,741 | 5,469 | 5,033 | 5,502 |
| 455 | N-acetylneuraminate | 60,076 | 115,440 | 144,073 | 30,853 |
| 1221 | nicotinamide | 2,466,889 | 2,901,258 | 2,575,339 | 2,649,055 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 3,127 | 2,604 | 2,771 | 3,624 |
| 825 | octanoylcarnitine | 76,524 | 85,048 | 64,582 | 74,458 |
| 639 | oleate (18:1n9) | 873,971 | 917,018 | 996,987 | 597,759 |
| 835 | oleoylcarnitine | 3,057,726 | 7,241,210 | 1,733,185 | 39,832 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 285 | ophthalmate | 52,223 | 23,753 | | 204,163 |
| 244 | ornithine | 12,768,683 | 10,862,977 | 12,987,170 | 11,518,017 |
| 632 | palmitate (16:0) | 7,773,711 | 8,460,192 | 9,093,167 | 6,094,743 |
| 633 | palmitoleate (16:1n7) | 594,583 | 511,705 | 554,747 | 472,426 |
| 1004 | palmitoyl sphingomyelin | 15,122,169 | 13,045,416 | 15,386,679 | 15,587,769 |
| 833 | palmitoylcarnitine | 1,413,824 | 3,149,368 | 859,247 | |
| 1243 | pantothenate | 103,143 | 88,135 | 94,692 | 91,492 |
| 1613 | paraxanthine | 501,549 | 447,541 | 491,750 | 489,402 |
| 88 | p-cresol sulfate | 39,727 | 40,431 | 41,708 | 46,335 |
| 621 | pelargonate (9:0) | 191,865 | 173,659 | 218,977 | 107,227 |
| 631 | pentadecanoate (15:0) | 214,252 | 261,516 | 282,267 | 161,375 |
| 135 | phenol sulfate | 18,658 | 17,398 | 19,028 | 20,850 |
| 128 | phenylacetylglutamine | 39,670 | 43,365 | 36,500 | 36,932 |
| 83 | phenylalanine | 9,345,391 | 8,765,870 | 9,414,596 | 7,616,771 |
| 602 | phosphate | 675,251,968 | 845,790,656 | 1,104,383,744 | 1,071,254,272 |
| 534 | phosphoenolpyruvate (PEP) | 209,038 | 70,826 | 27,817 | 263,933 |
| 877 | phosphoethanolamine | 89,288 | 67,771 | 50,592 | |
| 74 | pipecolate | 97,968 | 103,222 | 91,430 | 92,603 |
| 1531 | piperine | 119,521 | 138,843 | 81,002 | 126,860 |
| 246 | proline | 2,112,336 | 2,086,547 | 2,257,323 | 2,024,499 |
| 809 | propionylcarnitine | 933,796 | 841,561 | 812,781 | 1,267,591 |
| 1181 | pseudouridine | 10,952 | 7,553 | 9,629 | 10,650 |
| 45 | pyroglutamine* | 204,814 | 172,022 | 163,727 | 146,838 |
| 603 | pyrophosphate (PPi) | 95,057 | 58,494 | 61,654 | 114,575 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 535 | pyruvate | 181,161 | 3,408,564 | 7,034,338 | 3,892,667 |
| 1469 | ranitidine | | | | |
| 548 | ribitol | 1,410,089 | 1,256,211 | 1,640,570 | 170,112 |
| 557 | ribose 5-phosphate | 242,187 | 85,959 | 71,897 | 101,950 |
| 559 | ribulose | 111,852 | 32,986 | 54,531 | |
| 224 | S-adenosylhomocysteine (SAH) | 229,461 | 169,683 | 232,285 | 134,742 |
| 551 | sedoheptulose-7-phosphate | | 34,028 | 86,705 | 52,333 |
| 8 | serine | 8,534,447 | 8,305,055 | 9,531,856 | 7,174,827 |
| 216 | S-methylcysteine | 58,931 | 71,970 | 82,448 | 58,170 |
| 281 | S-methylglutathione | 44,493 | 28,444 | 21,097 | 25,339 |
| 270 | spermidine | 1,420,840 | 1,392,796 | 1,501,036 | 1,423,610 |
| 1584 | stachydrine | 3,378,943 | 3,452,362 | 3,444,646 | 3,534,442 |
| 637 | stearate (18:0) | 7,597,692 | 8,274,300 | 9,011,432 | 5,454,827 |
| 1005 | stearoyl sphingomyelin | 1,127,528 | 1,100,591 | 1,194,281 | 1,087,408 |
| 834 | stearoylcarnitine | 993,279 | 2,405,598 | 560,078 | |
| 591 | succinylcarnitine | 598,940 | 620,805 | 693,106 | 531,937 |
| 1662 | terephthalic acid | 353,476 | 376,418 | 333,558 | 425,030 |
| 1614 | theobromine | 159,734 | 187,818 | 233,955 | 166,447 |
| 1615 | theophylline | 90,363 | 47,447 | 112,746 | 144,988 |
| 549 | threitol | 1,163,937 | 1,112,152 | 1,222,698 | 659,998 |
| 1199 | threonate | 542,629 | 553,646 | 619,076 | 503,317 |
| 17 | threonine | 234,652 | 220,304 | 262,908 | 187,534 |
| 252 | trans-4-hydroxyproline | 30,124 | 24,840 | 22,725 | 22,861 |

| | | DARM-00023 | DARM-00024 | DARM-00025 | DARM-00026 |
|---|---|---|---|---|---|
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 CONTROL |
| | | 997739 | 997737 | 997732 | 997735 |
| | | 991368 | 991369 | 991370 | 991371 |
| | | NHSCI 1866 T1 D14 | NHSCI 1866 T1 D21 | NHSCI 1866 T1 D28 | NHSCI 1866 C D0 |
| | | T1 D14 | T1 D21 | T1 D28 | C D0 |
| | | 173.574 | 171.422 | 155.949 | 177.522 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | T1 D14 | T1 D21 | T1 D28 | C D0 |
| 501 | trehalose | 630,175 | 939,834 | 1,063,138 | 159,979 |
| 1242 | trigonelline (N'-methylnicotinate) | 495,616 | 479,519 | 479,042 | 508,849 |
| 145 | tryptophan | 4,375,374 | 4,166,448 | 4,322,376 | 4,000,641 |
| 151 | tryptophan betaine | 4,143,583 | 4,125,602 | 4,432,113 | 4,396,314 |
| 99 | tyrosine | 2,919,663 | 2,787,029 | 2,726,773 | 2,677,883 |
| 1149 | urate | 147,324 | 149,184 | 138,873 | 206,944 |
| 245 | urea | 24,829,290 | 24,798,716 | 28,481,742 | 27,163,684 |
| 1180 | uridine | 40,633 | 36,538 | 42,784 | 25,665 |
| 190 | valine | 10,208,828 | 10,230,705 | 10,366,040 | 9,614,625 |
| 565 | xylitol | 290,929 | 161,397 | 92,652 | |
| 570 | xylonate | 93,594 | 107,315 | 66,169 | 56,895 |
| 569 | xylose | 310,196 | 365,001 | 468,016 | 137,822 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 905 | 1,2-propanediol | 7,541,707 | 11,474,456 | 10,838,376 | 13,819,999 |
| 532 | 1,3-dihydroxyacetone | 62,248 | 81,743 | 59,754 | 91,977 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 5,766,874 | 6,650,703 | 6,459,022 | 6,144,440 |
| 523 | 1,6-anhydroglucose | 297,838 | 302,773 | 259,616 | 338,037 |
| 636 | 10-heptadecenoate (17:1n7) | 88,236 | 87,893 | 108,649 | 80,277 |
| 742 | 13-methylmyristic acid | 132,301 | 146,198 | 137,503 | 130,180 |
| 744 | 15-methylpalmitate (isobar with 2-methylpalmitate) | 225,093 | 224,138 | 335,268 | 247,699 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 34,056 | 27,537 | 29,738 | 22,073 |
| 938 | 1-linoleoylglycerophosphocholine | 324,502 | 263,673 | 323,220 | 217,008 |
| 926 | 1-myristoylglycerophosphocholine | 30,883 | 67,891 | 51,273 | 248,555 |
| 936 | 1-oleoylglycerophosphocholine | 147,482 | 464,838 | 754,374 | 2,874,057 |
| 915 | 1-oleoylglycerophosphoethanolamine | 21,281 | 15,809 | 25,668 | 16,655 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 33,967 | 52,041 | 40,849 | 48,834 |
| 929 | 1-palmitoylglycerophosphocholine | 934,112 | 2,595,194 | 4,493,467 | 10,554,460 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 19,991 | 20,085 | 15,198 | 12,864 |
| 934 | 1-stearoylglycerophosphocholine | 333,108 | 990,782 | 1,407,856 | 6,352,232 |
| 533 | 2,3-diphosphoglycerate | 114,587 | 21,834 | 4,300 | 4,070 |
| 263 | 2-aminobutyrate | 2,332,484 | 2,724,088 | 2,244,825 | 2,475,433 |
| 945 | 2-arachidonoylglycerophosphocholine* | 54,086 | 117,454 | 158,278 | 724,160 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 420,211 | 1,181,052 | 1,627,422 | 4,628,157 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 166,924 | 357,590 | 337,392 | 1,231,888 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 128,120 | 386,344 | 441,543 | 1,306,412 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 37,268 | 35,103 | 20,464 | 21,554 |
| 229 | 2-hydroxybutyrate (AHB) | 1,598,860 | 1,717,726 | 1,384,226 | 1,725,043 |
| 714 | 2-hydroxyglutarate | 97,025 | 148,145 | 169,055 | 237,560 |
| 706 | 2-hydroxypalmitate | 51,366 | 43,684 | 57,502 | 41,992 |
| 939 | 2-linoleoylglycerophosphocholine* | 206,348 | 268,697 | 400,028 | 1,322,133 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 202 | 2-methylbutyroylcarnitine | 76,855 | 61,196 | 87,420 | 43,965 |
| 937 | 2-oleoylglycerophosphocholine* | 66,600 | 128,114 | 161,528 | 651,263 |
| 930 | 2-palmitoylglycerophosphocholine* | 111,258 | 257,942 | 316,727 | 1,425,490 |
| 935 | 2-stearoylglycerophosphocholine* | | 61,539 | 72,930 | 470,915 |
| 821 | 3-dehydrocarnitine* | 1,067,343 | 1,042,639 | 1,044,675 | 1,045,926 |
| 170 | 3-indoxyl sulfate | 4,277 | 3,665 | 2,759 | 5,125 |
| 172 | 3-methyl-2-oxobutyrate | 53,364 | 51,377 | 38,252 | 34,658 |
| 173 | 3-methyl-2-oxovalerate | 55,305 | 63,694 | 59,705 | 51,366 |
| 529 | 3-phosphoglycerate | 862,740 | 781,792 | 434,652 | 392,112 |
| 193 | 4-methyl-2-oxopentanoate | 118,641 | 128,891 | 99,049 | 85,243 |
| 266 | 5-methylthioadenosine (MTA) | 71,125 | 111,907 | 98,027 | 108,532 |
| 282 | 5-oxoproline | 183,518 | 295,056 | 370,626 | 439,621 |
| 545 | 6-phosphogluconate | 59,949 | | | |
| 1024 | 7-beta-hydroxycholesterol | 21,900 | 34,141 | 30,496 | 14,146 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 98,325 | 124,208 | 180,865 | 188,284 |
| 672 | 9,10-epoxystearate | 5,387,020 | 6,655,581 | 9,202,128 | 8,887,839 |
| 822 | acetylcarnitine | 3,972,325 | 3,750,447 | 3,889,831 | 3,619,613 |
| 601 | acetylphosphate | 3,052,876 | 3,555,621 | 2,839,613 | 3,265,498 |
| 1105 | adenine | 36,307,960 | 26,311,536 | 23,192,424 | 21,060,490 |
| 1106 | adenosine | 24,392 | 24,654 | 44,702 | 23,869 |
| 1116 | adenosine 5'-diphosphate (ADP) | 231,523 | 201,800 | 163,767 | 116,207 |
| 1232 | adenosine 5'diphosphoribose | 100,886 | 89,094 | 90,954 | 73,759 |
| 1114 | adenosine 5'-monophosphate (AMP) | 4,575,457 | 5,406,040 | 6,401,236 | 5,820,486 |
| 665 | adrenate (22:4n6) | 74,564 | 66,291 | 79,886 | 94,859 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 27 | alanine | 59,010,100 | 70,591,808 | 57,490,560 | 64,239,864 |
| 1150 | allantoin | 23,605 | | 15,289 | 23,737 |
| 179 | alpha-hydroxyisocaproate | | 133,295 | 223,270 | 320,248 |
| 198 | alpha-hydroxyisovalerate | 280,019 | 397,562 | 500,789 | 635,087 |
| 1266 | alpha-tocopherol | 136,646 | 191,922 | 114,256 | 130,652 |
| 1034 | androsterone sulfate | 8,112 | 7,077 | 6,701 | 9,389 |
| 566 | arabinose | 361,155 | 351,108 | 282,015 | 276,692 |
| 546 | arabitol | 477,814 | 510,724 | 462,336 | 631,655 |
| 1202 | arabonate | 109,597 | 103,372 | 72,624 | 110,717 |
| 659 | arachidonate (20:4n6) | 823,763 | 838,584 | 1,176,509 | 944,103 |
| 241 | arginine | 1,242,925 | 1,631,118 | 1,454,897 | 549,452 |
| 25 | asparagine | 1,254,520 | 1,397,682 | 1,004,096 | 1,295,981 |
| 24 | aspartate | 2,459,311 | 3,225,898 | 3,106,433 | 3,999,182 |
| 721 | azelate (nonanedioate) | 14,007 | 24,954 | 36,298 | 42,424 |
| 26 | beta-alanine | 77,848 | 84,345 | 74,068 | 184,491 |
| 7 | beta-hydroxypyruvate | 251,874 | 337,569 | 154,928 | 239,218 |
| 22 | betaine | 1,626,279 | 1,728,294 | 1,672,991 | 1,688,387 |
| 1057 | beta-sitosterol | 50,513 | 58,349 | 40,491 | 35,062 |
| 1216 | biliverdin | 26,329 | 18,371 | 36,174 | 52,215 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 811 | butyrylcarnitine | 25,466 | | 18,848 | 19,521 |
| 1612 | caffeine | 3,417,860 | 3,098,230 | 3,143,026 | 3,179,570 |
| 1059 | campesterol | 169,601 | 343,638 | 332,088 | 252,559 |
| 622 | caprate (10:0) | 22,388 | 32,120 | 25,005 | 22,274 |
| 618 | caproate (6:0) | 44,492 | 30,729 | 28,846 | 26,717 |
| 620 | caprylate (8:0) | 32,838 | 47,004 | 34,072 | 29,931 |
| 820 | carnitine | 886,367 | 989,525 | 907,057 | 1,017,687 |
| 1300 | catechol sulfate | 82,344 | 76,843 | 80,589 | 75,807 |
| 164 | C-glycosyltryptophan* | 34,204 | 32,858 | 32,617 | 33,572 |
| 1020 | cholesterol | 33,314,874 | 40,148,852 | 30,020,408 | 34,903,636 |
| 881 | choline | 2,131,830 | 2,210,468 | 2,180,703 | 2,098,193 |
| 582 | cis-aconitate | 791,270 | 840,415 | 873,276 | 778,737 |
| 641 | cis-vaccenate (18:1n7) | 203,724 | 188,204 | 194,304 | 256,726 |
| 579 | citrate | 239,197,344 | 233,029,664 | 175,058,144 | 150,407,968 |
| 248 | citrulline | 97,201 | 115,885 | 106,913 | 116,739 |
| 259 | creatine | 3,795,108 | 3,682,630 | 3,742,688 | 3,720,130 |
| 260 | creatinine | 298,824 | 329,233 | 412,330 | 413,987 |
| 213 | cysteine | 661,165 | 1,171,320 | 993,262 | 1,329,492 |
| 819 | deoxycarnitine | 591,736 | 576,227 | 567,295 | 549,537 |
| 655 | dihomo-linoleate (20:2n6) | 79,059 | 67,573 | 99,750 | 69,913 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 76,597 | 81,738 | 104,133 | 67,178 |
| 531 | dihydroxyacetone phosphate (DHAP) | 34,163 | | | 23,090 |
| 3 | dimethylglycine | 463,672 | 353,777 | 314,053 | 438,720 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 167,778 | 160,543 | 234,436 | 154,398 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 91,538 | 88,988 | 135,122 | 107,994 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 150,263 | 160,535 | 198,839 | 196,233 |
| 1565 | ergothioneine | 873,930 | 828,627 | 858,040 | 776,286 |
| 735 | erucamide | 246,738 | 386,464 | | 490,737 |
| 1632 | erythritol | 937,482 | 1,422,206 | 1,287,599 | 1,576,778 |
| 453 | erythronate* | 399,630 | 469,898 | 481,616 | 656,974 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 876 | ethanolamine | 325,509 | 451,993 | 363,962 | 959,334 |
| 472 | fructose | 68,505,920 | 81,753,176 | 71,085,720 | 84,452,280 |
| 524 | fructose-6-phosphate | 553,045 | 646,289 | 506,948 | 475,395 |
| 594 | fumarate | 522,600 | 574,550 | 537,816 | 501,266 |
| 404 | gamma-glutamylleucine | 21,952 | 16,951 | 24,416 | 18,848 |
| 521 | glucose | 1,039,883,456 | 1,089,999,360 | 951,012,160 | 997,553,728 |
| 519 | glucose-6-phosphate (G6P) | 1,502,941 | 1,664,616 | 1,464,321 | 1,516,292 |
| 39 | glutamate | 6,284,719 | 7,018,903 | 5,429,270 | 6,033,070 |
| 44 | glutamine | 1,723,548 | 1,384,945 | 1,212,226 | 1,184,348 |
| 80 | glutaroyl carnitine | 15,353 | 17,731 | 17,376 | 22,019 |
| 283 | glutathione, oxidized (GSSG) | 1,270,879 | 1,020,500 | 926,367 | 1,200,988 |
| 280 | glutathione, reduced (GSH) | 18,079,298 | 24,764,038 | 21,248,432 | 20,547,928 |
| 517 | glycerate | 499,548 | 620,731 | 732,564 | 908,512 |
| 882 | glycerol 3-phosphate (G3P) | 355,687 | 348,275 | 286,390 | 202,625 |
| 883 | glycerophosphorylcholine (GPC) | 148,260 | 168,340 | 157,523 | 160,346 |
| 1 | glycine | 33,644,972 | 49,065,748 | 46,324,516 | 51,901,188 |
| 851 | glycochenodeoxycholate | 103,526 | 99,755 | 93,377 | 78,893 |
| 840 | glycocholate | 60,575 | 49,236 | 52,828 | 44,676 |
| 849 | glycodeoxycholate | 26,398 | 41,886 | 34,653 | 42,344 |
| 1318 | glycolate (hydroxyacetate) | 379,420 | 463,703 | 355,768 | 433,516 |
| 1128 | guanosine | 26,356 | 27,701 | 25,858 | 24,958 |
| 1212 | heme* | 636,851 | 1,905,266 | 2,001,279 | 9,562,559 |
| 619 | heptanoate (7:0) | 10,281 | 8,621 | 9,196 | 10,045 |
| 823 | hexanoylcarnitine | 43,338 | 26,171 | 31,616 | 32,959 |
| 1288 | hippurate | 58,894 | 51,578 | 48,359 | 50,721 |
| 50 | histidine | 44,508 | 45,454 | 41,544 | 39,166 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 231 | homocysteine | 32,666 | 87,447 | 73,188 | 79,757 |
| 1585 | homostachydrine* | 27,786 | 36,490 | 27,568 | 32,484 |
| 206 | hydroxyisovaleroyl carnitine | 396,962 | 366,801 | 364,054 | 354,559 |
| 1098 | hypoxanthine | 237,200 | 785,728 | 2,546,911 | 6,082,068 |
| 1101 | inosine 5'-monophosphate (IMP) | 328,889 | 582,387 | 331,913 | 339,770 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 55,048 | 50,627 | 53,103 | 35,784 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 77,308 | 85,729 | 55,929 | 65,253 |
| 496 | Isobar: sorbitol, mannitol | 18,733,526 | 17,814,282 | 18,544,120 | 18,990,472 |
| 200 | isobutyrylcarnitine | 163,111 | 137,186 | 138,537 | 130,574 |
| 180 | isoleucine | 4,663,533 | 4,409,751 | 4,377,872 | 4,644,256 |
| 478 | isomaltose | 1,872,634 | 1,872,018 | 1,507,209 | 1,745,698 |
| 205 | isovalerylcarnitine | 101,548 | 111,929 | 113,812 | 89,564 |
| 144 | kynurenine | 136,839 | 121,669 | 158,329 | 128,163 |
| 536 | lactate | 743,800,768 | 1,301,145,344 | 1,372,414,208 | 1,640,015,488 |
| 1018 | lathosterol | 38,989 | 49,485 | | |
| 625 | laurate (12:0) | 127,706 | 142,753 | 143,001 | 121,349 |
| 181 | leucine | 9,521,423 | 9,576,510 | 9,373,946 | 10,474,238 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 604 | linoleate (18:2n6) | 3,532,413 | 3,434,276 | 4,306,622 | 3,115,737 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 544,045 | 655,342 | 676,656 | 560,640 |
| 69 | lysine | 1,985,777 | 2,449,953 | 1,618,185 | 3,332,711 |
| 598 | malate | 1,507,907 | 1,988,038 | 1,840,882 | 2,524,373 |
| 482 | maltose | 1,153,248 | 1,375,508 | 1,119,766 | 1,049,543 |
| 487 | mannose | 13,239,841 | 14,826,829 | 11,488,961 | 12,203,624 |
| 489 | mannose-6-phosphate | 199,106 | 251,148 | 233,714 | 264,289 |
| 635 | margarate (17:0) | 482,030 | 431,418 | 579,953 | 416,367 |
| 658 | mead acid (20:3n9) | 12,961 | 19,272 | 12,276 | 7,756 |
| 225 | methionine | 864,860 | 610,165 | 444,437 | 406,243 |
| 890 | myo-inositol | 1,971,318 | 2,201,784 | 1,795,906 | 1,954,884 |
| 629 | myristate (14:0) | 666,258 | 740,326 | 902,147 | 709,081 |
| 630 | myristoleate (14:1n5) | 19,377 | 28,689 | 32,995 | 24,186 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 169,135 | 171,621 | 76,472 | 147,074 |
| 75 | N-6-trimethyllysine | 274,891 | 182,982 | 223,191 | 178,198 |
| 4 | N-acetylglycine | 67,489 | 65,786 | 100,518 | 101,630 |
| 227 | N-acetylmethionine | 4,576 | 5,901 | 4,937 | 5,013 |
| 455 | N-acetylneuraminate | 39,246 | 97,244 | 91,567 | 81,988 |
| 1221 | nicotinamide | 2,519,914 | 2,606,459 | 2,753,504 | 2,514,949 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 3,656 | 3,817 | 3,607 | 7,409 |
| 825 | octanoylcarnitine | 66,818 | 69,316 | 73,599 | 73,250 |
| 639 | oleate (18:1n9) | 675,705 | 773,779 | 737,139 | 824,894 |
| 835 | oleoylcarnitine | 296,722 | 839,169 | 1,173,849 | 6,755,525 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 285 | ophthalmate | 50,721 | 28,414 | | |
| 244 | ornithine | 10,093,262 | 10,921,280 | 8,529,724 | 13,036,086 |
| 632 | palmitate (16:0) | 8,209,507 | 8,075,588 | 9,564,448 | 7,921,516 |
| 633 | palmitoleate (16:1n7) | 580,007 | 421,599 | 525,917 | 372,048 |
| 1004 | palmitoyl sphingomyelin | 14,827,738 | 16,726,182 | 12,126,371 | 14,610,131 |
| 833 | palmitoylcarnitine | 261,552 | 452,163 | 563,927 | 4,437,191 |
| 1243 | pantothenate | 95,089 | 94,199 | 147,169 | 99,677 |
| 1613 | paraxanthine | 443,009 | 461,396 | 465,535 | 461,229 |
| 88 | p-cresol sulfate | 47,429 | 44,307 | 44,968 | 42,116 |
| 621 | pelargonate (9:0) | 213,751 | 232,404 | 230,384 | 187,391 |
| 631 | pentadecanoate (15:0) | 237,729 | 249,538 | 320,664 | 238,384 |
| 135 | phenol sulfate | 17,688 | 21,920 | 20,488 | 16,515 |
| 128 | phenylacetylglutamine | 41,655 | 42,652 | 42,530 | 44,447 |
| 83 | phenylalanine | 8,497,740 | 8,430,026 | 8,708,808 | 9,319,272 |
| 602 | phosphate | 1,101,179,264 | 1,367,314,816 | 1,115,626,624 | 1,211,363,840 |
| 534 | phosphoenolpyruvate (PEP) | 116,097 | 66,183 | 21,439 | |
| 877 | phosphoethanolamine | | | | 50,346 |
| 74 | pipecolate | 86,158 | 85,900 | 94,000 | 107,875 |
| 1531 | piperine | 144,936 | 157,719 | 78,523 | 83,224 |
| 246 | proline | 2,276,136 | 2,143,683 | 2,344,439 | 2,205,136 |
| 809 | propionylcarnitine | 1,289,884 | 1,089,291 | 1,003,801 | 1,026,906 |
| 1181 | pseudouridine | 8,071 | 6,295 | 8,016 | 10,189 |
| 45 | pyroglutamine* | 217,914 | 153,990 | 165,113 | 199,223 |
| 603 | pyrophosphate (PPi) | 102,490 | 92,626 | 27,461 | 76,834 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 535 | pyruvate | 2,612,024 | 1,233,071 | 1,064,282 | 884,012 |
| 1469 | ranitidine | | | | |
| 548 | ribitol | 192,978 | 151,854 | 156,197 | 250,366 |
| 557 | ribose 5-phosphate | 103,861 | 156,431 | 155,592 | 65,059 |
| 559 | ribulose | 20,289 | 26,440 | 22,860 | 32,354 |
| 224 | S-adenosylhomocysteine (SAH) | 215,285 | 218,722 | 251,737 | 229,574 |
| 551 | sedoheptulose-7-phosphate | 34,147 | 45,388 | 73,991 | 149,773 |
| 8 | serine | 7,328,767 | 9,014,268 | 7,163,924 | 8,348,743 |
| 216 | S-methylcysteine | 60,126 | 107,130 | 58,716 | 85,171 |
| 281 | S-methylglutathione | 33,263 | 25,149 | 30,967 | 48,782 |
| 270 | spermidine | 1,483,578 | 1,562,241 | 1,630,592 | 1,594,886 |
| 1584 | stachydrine | 3,516,873 | 3,386,667 | 3,385,275 | 3,445,669 |
| 637 | stearate (18:0) | 8,055,712 | 7,885,242 | 9,392,982 | 7,982,961 |
| 1005 | stearoyl sphingomyelin | 985,680 | 1,102,903 | 1,171,900 | 992,645 |
| 834 | stearoylcarnitine | 105,241 | 339,318 | 430,841 | 2,472,239 |
| 591 | succinylcarnitine | 580,363 | 608,239 | 644,169 | 647,327 |
| 1662 | terephthalic acid | 386,525 | 336,663 | 361,405 | 375,317 |
| 1614 | theobromine | 219,573 | 207,816 | 229,773 | 168,888 |
| 1615 | theophylline | 141,504 | 87,686 | 160,482 | 73,034 |
| 549 | threitol | 774,444 | 1,009,916 | 766,303 | 965,406 |
| 1199 | threonate | 436,950 | 480,646 | 457,574 | 409,992 |
| 17 | threonine | 180,434 | 201,578 | 227,682 | 242,880 |
| 252 | trans-4-hydroxyproline | 25,854 | 27,239 | 27,820 | 23,271 |

| | | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D51 |
| | | 997723 | 997728 | 997722 | 997744 |
| | | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 C D7 | NHSCI 1866 C D14 | NHSCI 1866 C D21 | NHSCI 1866 C D28 |
| | | C D7 | C D14 | C D21 | C D28 |
| | | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORT ORDER** | **BIOCHEMICAL NAME** | C D7 | C D14 | C D21 | C D28 |
| 501 | trehalose | 476,243 | 998,895 | 791,556 | 1,379,798 |
| 1242 | trigonelline (N'-methylnicotinate) | 476,134 | 476,112 | 501,977 | 487,468 |
| 145 | tryptophan | 3,808,759 | 4,151,956 | 4,103,621 | 4,203,022 |
| 151 | tryptophan betaine | 4,345,513 | 4,368,475 | 4,281,072 | 4,256,259 |
| 99 | tyrosine | 2,597,682 | 2,713,701 | 2,648,452 | 2,987,171 |
| 1149 | urate | 189,204 | 172,683 | 170,845 | 138,051 |
| 245 | urea | 24,193,656 | 27,595,104 | 24,141,402 | 26,030,124 |
| 1180 | uridine | 29,864 | 34,372 | 40,913 | 41,433 |
| 190 | valine | 9,670,583 | 10,262,873 | 10,083,593 | 10,646,373 |
| 565 | xylitol | | 13,661 | | |
| 570 | xylonate | 58,551 | 77,409 | 56,203 | 71,113 |
| 569 | xylose | 151,298 | 112,753 | | 87,341 |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 905 | 1,2-propanediol | Lipid | Ketone bodies | 38002 | GC/MS | 1041 | 117 | 57-55-6; |
| 532 | 1,3-dihydroxyacetone | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 35981 | GC/MS | 1349 | 306.1 | 62147-49-3; |
| 515 | 1,5-anhydroglucitol (1,5-AG) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 20675 | GC/MS | 1788.7 | 217 | 154-58-5; |
| 523 | 1,6-anhydroglucose | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 21049 | GC/MS | 1679.5 | 204.1 | 498-07-7; |
| 636 | 10-heptadecenoate (17:1n7) | Lipid | Long chain fatty acid | 33971 | LC/MS Neg | 5558 | 267.3 | 29743-97-3; |
| 742 | 13-methylmyristic acid | Lipid | Fatty acid, branched | 38293 | LC/MS Neg | 5498 | 241.3 | 2485-71-4; |
| 744 | 15-methylpalmitate (isobar with 2- | Lipid | Fatty acid, branched | 38768 | LC/MS Neg | 5698 | 269.4 | |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | Lipid | Lysolipid | 35186 | LC/MS Neg | 5731 | 500.3 | |
| 938 | 1-linoleoylglycerophosphocholine | Lipid | Lysolipid | 34419 | LC/MS Neg | 5844 | 594 | |
| 926 | 1-myristoylglycerophosphocholine | Lipid | Lysolipid | 35626 | LC/MS Pos | 5481 | 468.3 | 20559-16-4; |
| 936 | 1-oleoylglycerophosphocholine | Lipid | Lysolipid | 33960 | LC/MS Pos | 5700 | 522.4 | 19420-56-5; |
| 915 | 1-oleoylglycerophosphoethanolamine | Lipid | Lysolipid | 35628 | LC/MS Neg | 5928 | 478.3 | |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | Lipid | Monoacylglycerol | 21127 | GC/MS | 2119.5 | 371.3 | 542-44-9; |
| 929 | 1-palmitoylglycerophosphocholine | Lipid | Lysolipid | 33955 | LC/MS Pos | 5671 | 496.4 | 17364-16-8; |
| 909 | 1-palmitoylglycerophosphoethanolamine | Lipid | Lysolipid | 35631 | LC/MS Neg | 5940 | 452.3 | |
| 934 | 1-stearoylglycerophosphocholine | Lipid | Lysolipid | 33961 | LC/MS Pos | 5844 | 524.4 | 19420-57-6; |
| 533 | 2,3-diphosphoglycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 15664 | LC/MS Neg | 580 | 264.9 | 102783-53-9; |
| 263 | 2-aminobutyrate | Amino acid | Butanoate metabolism | 1577 | GC/MS | 1215.7 | 130 | 1492-24-6; |
| 945 | 2-arachidonoylglycerophosphocholine* | Lipid | Lysolipid | 35256 | LC/MS Pos | 5524 | 544.3 | |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | Lipid | Lysolipid | 34656 | LC/MS Pos | 5525 | 502.3 | |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | Lipid | Lysolipid | 34258 | LC/MS Pos | 5512 | 526.2 | |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | Lipid | Lysolipid | 34875 | LC/MS Pos | 5548 | 528.2 | |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | Xenobiotics | Chemical | 35490 | LC/MS Neg | 3909 | 143.1 | |
| 229 | 2-hydroxybutyrate (AHB) | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 21044 | GC/MS | 1169.4 | 130.9 | 3347-90-8; |
| 714 | 2-hydroxyglutarate | Lipid | Fatty acid, dicarboxylate | 37253 | GC/MS | 1576 | 247 | 40951-21-1; |
| 706 | 2-hydroxypalmitate | Lipid | Fatty acid, monohydroxy | 35675 | LC/MS Neg | 5508 | 271.3 | 764-67-0; |
| 939 | 2-linoleoylglycerophosphocholine* | Lipid | Lysolipid | 35257 | LC/MS Pos | 5544 | 520.4 | |
| 202 | 2-methylbutyroylcarnitine | Amino acid | Valine, leucine and isoleucine | 35431 | LC/MS Pos | 2439 | 246.1 | 31023-25-3; |
| 937 | 2-oleoylglycerophosphocholine* | Lipid | Lysolipid | 35254 | LC/MS Pos | 5640 | 522.4 | |
| 930 | 2-palmitoylglycerophosphocholine* | Lipid | Lysolipid | 35253 | LC/MS Pos | 5604 | 496.3 | |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 935 | 2-stearoylglycerophosphocholine* | Lipid | Lysolipid | 35255 | LC/MS Pos | 5780 | 524.4 | |
| 821 | 3-dehydrocarnitine* | Lipid | Carnitine metabolism | 32654 | LC/MS Pos | 1020 | 160.2 | 10457-99-5; |
| 170 | 3-indoxyl sulfate | Amino acid | Tryptophan metabolism | 27672 | LC/MS Neg | 2258 | 212 | 2642-37-7; |
| 172 | 3-methyl-2-oxobutyrate | Amino acid | Valine, leucine and isoleucine | 21047 | LC/MS Neg | 1489 | 115.1 | 3715-29-5; |
| 173 | 3-methyl-2-oxovalerate | Amino acid | Valine, leucine and isoleucine | 15676 | LC/MS Neg | 2106 | 129.2 | 51829-07-3; |
| 529 | 3-phosphoglycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 1414 | GC/MS | 1754 | 299 | 80731-10-8; |
| 193 | 4-methyl-2-oxopentanoate | Amino acid | Valine, leucine and isoleucine | 22116 | LC/MS Neg | 2200 | 129.2 | 816-66-0; |
| 266 | 5-methylthioadenosine (MTA) | Amino acid | Polyamine metabolism | 1419 | LC/MS Pos | 2427 | 298.1 | 2457-80-9; |
| 282 | 5-oxoproline | Amino acid | Glutathione metabolism | 1494 | LC/MS Neg | 744 | 128.2 | 98-79-3; |
| 545 | 6-phosphogluconate | Carbohydrate | Nucleotide sugars, pentose | 15442 | GC/MS | 2060.4 | 387.2 | 921-62-0;53411-70-4; |
| 1024 | 7-beta-hydroxycholesterol | Lipid | Sterol/Steroid | 35092 | GC/MS | 2340 | 456.4 | 566-27-8; |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | Lipid | Long chain fatty acid | 38398 | LC/MS Neg | 5328 | 295.4 | |
| 672 | 9,10-epoxystearate | Lipid | Fatty acid, oxidized | 39627 | LC/MS Neg | 5386.6 | 297.4 | |
| 822 | acetylcarnitine | Lipid | Carnitine metabolism | 32198 | LC/MS Pos | 1203 | 204.2 | 5080-50-2; |
| 601 | acetylphosphate | Energy | Oxidative phosphorylation | 15488 | GC/MS | 1263 | 211 | 94249-01-1; |
| 1105 | adenine | Nucleotide | Purine metabolism, adenine | 554 | LC/MS Pos | 1003 | 136.1 | 73-24-5; |
| 1106 | adenosine | Nucleotide | Purine metabolism, adenine | 555 | LC/MS Pos | 1650 | 268.1 | 58-61-7; |
| 1116 | adenosine 5'-diphosphate (ADP) | Nucleotide | Purine metabolism, adenine | 3108 | LC/MS Neg | 800 | 426.1 | 20398-34-9; |
| 1232 | adenosine 5'diphosphoribose | Cofactors and vitamins | Nicotinate and nicotinamide | 558 | LC/MS Neg | 964 | 558.1 | 68414-18-6; |
| 1114 | adenosine 5'-monophosphate (AMP) | Nucleotide | Purine metabolism, adenine | 32342 | LC/MS Pos | 1210 | 348.1 | 149022-20-8; |
| 665 | adrenate (22:4n6) | Lipid | Long chain fatty acid | 32980 | LC/MS Neg | 5684 | 331.3 | 2091-25-0; |
| 27 | alanine | Amino acid | Alanine and aspartate | 1126 | GC/MS | 1147.6 | 115.9 | 56-41-7; |
| 1150 | allantoin | Nucleotide | Purine metabolism, urate | 1107 | GC/MS | 1809.8 | 518.3 | 97-59-6; |
| 179 | alpha-hydroxyisocaproate | Amino acid | Valine, leucine and isoleucine | 22132 | GC/MS | 1274 | 102.8 | 10303-64-7; |
| 198 | alpha-hydroxyisovalerate | Amino acid | Valine, leucine and isoleucine | 33937 | GC/MS | 1208 | 145.1 | 600-37-3; |
| 1266 | alpha-tocopherol | Cofactors and vitamins | Tocopherol metabolism | 1561 | GC/MS | 2305.4 | 502.5 | 59-02-9;10191-41-0; |
| 1034 | androsterone sulfate | Lipid | Sterol/Steroid | 31591 | LC/MS Neg | 5011 | 369.2 | 2479-86-9 ; |
| 566 | arabinose | Carbohydrate | Nucleotide sugars, pentose | 575 | GC/MS | 1631.6 | 217 | 28697-53-2; |
| 546 | arabitol | Carbohydrate | Nucleotide sugars, pentose | 15964 | GC/MS | 1687.5 | 217 | 488-82-4; |
| 1202 | arabonate | Cofactors and vitamins | Ascorbate and aldarate | 37516 | GC/MS | 1736 | 292.1 | 7643-75-7; |
| 659 | arachidonate (20:4n6) | Lipid | Long chain fatty acid | 1110 | LC/MS Neg | 5525 | 303.4 | 506-32-1; |
| 241 | arginine | Amino acid | Urea cycle; arginine-, proline-, | 1638 | GC/MS | 1608.5 | 142 | 1119-34-2; |
| 25 | asparagine | Amino acid | Alanine and aspartate | 512 | GC/MS | 1617.5 | 188 | 70-47-3; |
| 24 | aspartate | Amino acid | Alanine and aspartate | 15996 | GC/MS | 1529.7 | 232 | 56-84-8; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 721 | azelate (nonanedioate) | Lipid | Fatty acid, dicarboxylate | 18362 | LC/MS Neg | 1322 | 187.2 | 123-99-9; |
| 26 | beta-alanine | Amino acid | Alanine and aspartate | 55 | GC/MS | 1451.8 | 174 | 56-41-7;107-95-9; |
| 7 | beta-hydroxypyruvate | Amino acid | Glycine, serine and threonine | 15686 | GC/MS | 1425.1 | 221 | 3369-79-7; |
| 22 | betaine | Amino acid | Glycine, serine and threonine | 3141 | LC/MS Pos | 721 | 118.2 | 107-43-7; |
| 1057 | beta-sitosterol | Lipid | Sterol/Steroid | 27414 | GC/MS | 2380.8 | 357.4 | 83-46-5; |
| 1216 | biliverdin | Cofactors and vitamins | Hemoglobin and porphyrin | 2137 | LC/MS Pos | 4936 | 583.3 | 55482-27-4;55482-27-4 ; |
| 811 | butyrylcarnitine | Lipid | Fatty acid metabolism (also BCAA metabolism) | 32412 | LC/MS Pos | 2007 | 232.2 | 25576-40-3; |
| 1612 | caffeine | Xenobiotics | Xanthine metabolism | 569 | LC/MS Pos | 2820 | 195.1 | 58-08-2; |
| 1059 | campesterol | Lipid | Sterol/Steroid | 33997 | GC/MS | 2353 | 129 | 474-62-4; |
| 622 | caprate (10:0) | Lipid | Medium chain fatty acid | 1642 | LC/MS Neg | 5092 | 171.2 | 112-37-8; |
| 618 | caproate (6:0) | Lipid | Medium chain fatty acid | 32489 | LC/MS Neg | 2766 | 115.2 | 142-62-1; |
| 620 | caprylate (8:0) | Lipid | Medium chain fatty acid | 32492 | LC/MS Neg | 4367 | 143.2 | 124-07-2; |
| 820 | carnitine | Lipid | Carnitine metabolism | 15500 | LC/MS Pos | 702 | 162.2 | 461-05-2; |
| 1300 | catechol sulfate | Xenobiotics | Benzoate metabolism | 35320 | LC/MS Neg | 1928 | 188.9 | |
| 164 | C-glycosyltryptophan* | Amino acid | Tryptophan metabolism | 32675 | LC/MS Pos | 1912 | 367.1 | |
| 1020 | cholesterol | Lipid | Sterol/Steroid | 63 | GC/MS | 2316.9 | 329.3 | 57-88-5; |
| 881 | choline | Lipid | Glycerolipid metabolism | 15506 | LC/MS Pos | 674 | 104.2 | 67-48-1; |
| 582 | cis-aconitate | Energy | Krebs cycle | 12025 | LC/MS Neg | 603 | 173.1 | 585-84-2; |
| 641 | cis-vaccenate (18:1n7) | Lipid | Long chain fatty acid | 33970 | GC/MS | 1987 | 339.3 | 693-72-1; |
| 579 | citrate | Energy | Krebs cycle | 1564 | GC/MS | 1763.4 | 273.1 | 77-92-9; |
| 248 | citrulline | Amino acid | Urea cycle; arginine-, proline-, | 2132 | LC/MS Pos | 715 | 176.1 | 372-75-8; |
| 259 | creatine | Amino acid | Creatine metabolism | 27718 | LC/MS Pos | 758 | 132.1 | 57-00-1; |
| 260 | creatinine | Amino acid | Creatine metabolism | 513 | LC/MS Pos | 730 | 114.1 | 60-27-5; |
| 213 | cysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 31453 | GC/MS | 1560.1 | 218 | 52-90-4;56-89-3; |
| 819 | deoxycarnitine | Lipid | Carnitine metabolism | 36747 | LC/MS Pos | 759 | 146.1 | 6249-56-5; |
| 655 | dihomo-linoleate (20:2n6) | Lipid | Long chain fatty acid | 17805 | LC/MS Neg | 5722 | 307.3 | 2091-39-6; |
| 609 | dihomo-linolenate (20:3n3 or n6) | Lipid | Essential fatty acid | 35718 | LC/MS Neg | 5600 | 305.4 | |
| 531 | dihydroxyacetone phosphate (DHAP) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 15522 | GC/MS | 1737 | 315.1 | 102783-56-2; |
| 3 | dimethylglycine | Amino acid | Glycine, serine and threonine | 5086 | GC/MS | 1030 | 57.9 | 1118-68-9; |
| 613 | docosahexaenoate (DHA; 22:6n3) | Lipid | Essential fatty acid | 19323 | LC/MS Neg | 5518 | 327.3 | 6217-54-5; |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | Lipid | Essential fatty acid | 32504 | LC/MS Neg | 5574 | 329.4 | 2234-74-4 ; |
| 610 | eicosapentaenoate (EPA; 20:5n3) | Lipid | Essential fatty acid | 18467 | LC/MS Neg | 5442 | 301.3 | 10-2005-9;10417-94-4; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 1565 | ergothioneine | Xenobiotics | Food component/Plant | 37459 | LC/MS Pos | 847 | 230.2 | 58511-63-0; |
| 735 | erucamide | Lipid | Fatty acid, amide | 35177 | GC/MS | 2173 | 203 | 112-84-5; |
| 1632 | erythritol | Xenobiotics | Sugar, sugar substitute, starch | 20699 | GC/MS | 1517.5 | 217 | 149-32-6; |
| 453 | erythronate* | Carbohydrate | Aminosugars metabolism | 33477 | GC/MS | 1546.9 | 292.1 | 13752-84-6; |
| 876 | ethanolamine | Lipid | Glycerolipid metabolism | 1497 | GC/MS | 1304 | 174.1 | 141-43-5; |
| 472 | fructose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 31266 | GC/MS | 1762.7 | 204 | 57-48-7; |
| 524 | fructose-6-phosphate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 12021 | GC/MS | 1994.9 | 315.1 | 103213-47-4; |
| 594 | fumarate | Energy | Krebs cycle | 1643 | GC/MS | 1382.1 | 245 | 100-17-8; |
| 404 | gamma-glutamylleucine | Peptide | gamma-glutamyl | 18369 | LC/MS Pos | 2744 | 261.2 | 2566-39-4; |
| 521 | glucose | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 20488 | GC/MS | 1866.8 | 217.1 | 50-99-7; |
| 519 | glucose-6-phosphate (G6P) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 31260 | GC/MS | 2042.7 | 387.2 | 103192-55-8; |
| 39 | glutamate | Amino acid | Glutamate metabolism | 57 | GC/MS | 1611.9 | 246 | 56-86-0; |
| 44 | glutamine | Amino acid | Glutamate metabolism | 53 | LC/MS Pos | 684 | 147.2 | 56-85-9; |
| 80 | glutaroyl carnitine | Amino acid | Lysine metabolism | 35439 | LC/MS Pos | 1565 | 276.1 | 102636-82-8; |
| 283 | glutathione, oxidized (GSSG) | Amino acid | Glutathione metabolism | 27727 | LC/MS Pos | 1535 | 613.1 | 103239-24-3; |
| 280 | glutathione, reduced (GSH) | Amino acid | Glutathione metabolism | 2127 | LC/MS Pos | 1274 | 308.1 | 70-18-8; |
| 517 | glycerate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 1572 | GC/MS | 1360.7 | 189 | 600-19-1; |
| 882 | glycerol 3-phosphate (G3P) | Lipid | Glycerolipid metabolism | 15365 | GC/MS | 1719.7 | 357.1 | 29849-82-9; |
| 883 | glycerophosphorylcholine (GPC) | Lipid | Glycerolipid metabolism | 15990 | LC/MS Pos | 694 | 258.1 | 28319-77-9; |
| 1 | glycine | Amino acid | Glycine, serine and threonine | 11777 | GC/MS | 1166 | 101.9 | 56-40-6; |
| 851 | glycochenodeoxycholate | Lipid | Bile acid metabolism | 32346 | LC/MS Neg | 5245 | 448.4 | 16564-43-5; |
| 840 | glycocholate | Lipid | Bile acid metabolism | 18476 | LC/MS Neg | 5104 | 464.4 | 475-31-0;863-57-0; |
| 849 | glycodeoxycholate | Lipid | Bile acid metabolism | 18477 | LC/MS Neg | 5265 | 448.4 | 360-65-6; |
| 1318 | glycolate (hydroxyacetate) | Xenobiotics | Chemical | 15737 | GC/MS | 1119 | 177 | 79-14-1; |
| 1128 | guanosine | Nucleotide | Purine metabolism, guanine | 1573 | LC/MS Pos | 1676 | 284 | 118-00-3; |
| 1212 | heme* | Cofactors and vitamins | Hemoglobin and porphyrin | 32593 | LC/MS Pos | 4985 | 616.2 | 14875-96-8; |
| 619 | heptanoate (7:0) | Lipid | Medium chain fatty acid | 1644 | LC/MS Neg | 3695 | 129.2 | 111-14-8; |
| 823 | hexanoylcarnitine | Lipid | Carnitine metabolism | 32328 | LC/MS Pos | 3174 | 260.2 | 6920-35-0; |
| 1288 | hippurate | Xenobiotics | Benzoate metabolism | 15753 | LC/MS Neg | 2136 | 178.1 | 495-69-2; |
| 50 | histidine | Amino acid | Histidine metabolism | 59 | LC/MS Neg | 757 | 154.1 | 5934-29-2; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 231 | homocysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 40266 | GC/MS | 1648.2 | 234 | 454-29-5; |
| 1585 | homostachydrine* | Xenobiotics | Food component/Plant | 33009 | LC/MS Pos | 1199 | 158.2 | 1195-94-4; |
| 206 | hydroxyisovaleroyl carnitine | Amino acid | Valine, leucine and isoleucine | 35433 | LC/MS Pos | 1683 | 262.1 | 99159-87-2; |
| 1098 | hypoxanthine | Nucleotide | Purine metabolism, (hypo)xanthine/inosine | 3127 | GC/MS | 1759.2 | 265 | 68-94-0; |
| 1101 | inosine 5'-monophosphate (IMP) | Nucleotide | Purine metabolism, (hypo)xanthine/inosine | 2133 | GC/MS | 2254 | 315 | 4691-65-0; |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 36984 | LC/MS Neg | 572 | 339 | |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | Carbohydrate | Nucleotide sugars, pentose | 37288 | GC/MS | 1935 | 357.2 | |
| 496 | Isobar: sorbitol, mannitol | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 33004 | LC/MS Pos | 709 | 183.1 | |
| 200 | isobutyrylcarnitine | Amino acid | Valine, leucine and isoleucine | 33441 | LC/MS Pos | 1941 | 232.2 | 25518-49-4; |
| 180 | isoleucine | Amino acid | Valine, leucine and isoleucine | 1125 | LC/MS Pos | 1614 | 132.1 | 73-32-5; |
| 478 | isomaltose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 39777 | GC/MS | 2221.8 | 204.1 | 499-40-1; |
| 205 | isovalerylcarnitine | Amino acid | Valine, leucine and isoleucine | 34407 | LC/MS Pos | 2533 | 246.2 | |
| 144 | kynurenine | Amino acid | Tryptophan metabolism | 15140 | LC/MS Pos | 1902 | 209.1 | 2922-83-0; |
| 536 | lactate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 527 | GC/MS | 1102.8 | 116.9 | 79-33-4; |
| 1018 | lathosterol | Lipid | Sterol/Steroid | 39864 | GC/MS | 2337 | 255.2 | 80-99-9 ; |
| 625 | laurate (12:0) | Lipid | Medium chain fatty acid | 1645 | LC/MS Neg | 5288 | 199.3 | 143-07-7; |
| 181 | leucine | Amino acid | Valine, leucine and isoleucine | 60 | LC/MS Pos | 1674 | 132.2 | 61-90-5; |
| 604 | linoleate (18:2n6) | Lipid | Essential fatty acid | 1105 | LC/MS Neg | 5533 | 279.3 | 60-33-3; |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | Lipid | Essential fatty acid | 34035 | LC/MS Neg | 5450 | 277.3 | |
| 69 | lysine | Amino acid | Lysine metabolism | 1301 | GC/MS | 1836.7 | 317.2 | 56-87-1; |
| 598 | malate | Energy | Krebs cycle | 1303 | GC/MS | 1502 | 233 | 6915-15-7; |
| 482 | maltose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 15806 | GC/MS | 2142.1 | 204.1 | 6363-53-7; |
| 487 | mannose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 584 | GC/MS | 1753.5 | 203.9 | 3458-28-4; |
| 489 | mannose-6-phosphate | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 1470 | GC/MS | 2035.9 | 387.2 | 70442-25-0;104872-94-8; |
| 635 | margarate (17:0) | Lipid | Long chain fatty acid | 1121 | LC/MS Neg | 5733 | 269.3 | 506-12-7; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 658 | mead acid (20:3n9) | Lipid | Long chain fatty acid | 35174 | LC/MS Neg | 5642 | 305.4 | 20590-32-3; |
| 225 | methionine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 1302 | LC/MS Pos | 1252 | 150.1 | 63-68-3; |
| 890 | myo-inositol | Lipid | Inositol metabolism | 19934 | GC/MS | 1924.9 | 217 | 87-89-8; |
| 629 | myristate (14:0) | Lipid | Long chain fatty acid | 1365 | LC/MS Neg | 5439 | 227.3 | 544-63-8; |
| 630 | myristoleate (14:1n5) | Lipid | Long chain fatty acid | 32418 | LC/MS Neg | 5338 | 225.3 | 544-64-9 ; |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | Cofactors and vitamins | Nicotinate and nicotinamide | 40469 | LC/MS Pos | 1707.3 | 153.2 | 701-44-0; |
| 75 | N-6-trimethyllysine | Amino acid | Lysine metabolism | 1498 | LC/MS Pos | 650 | 189.2 | 23284-33-5; |
| 4 | N-acetylglycine | Amino acid | Glycine, serine and threonine | 27710 | GC/MS | 1396.4 | 143.9 | 543-24-8; |
| 227 | N-acetylmethionine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 1589 | LC/MS Neg | 1805 | 190.1 | 65-82-7; |
| 455 | N-acetylneuraminate | Carbohydrate | Aminosugars metabolism | 1592 | GC/MS | 2074.9 | 245 | 131-48-6; |
| 1221 | nicotinamide | Cofactors and vitamins | Nicotinate and nicotinamide | 594 | LC/MS Pos | 1267 | 123.1 | 98-92-0; |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | Cofactors and vitamins | Nicotinate and nicotinamide | 5278 | LC/MS Neg | 1411 | 661.8 | 53-84-9; |
| 825 | octanoylcarnitine | Lipid | Carnitine metabolism | 33936 | LC/MS Pos | 4100 | 288.3 | 3671-77-0; |
| 639 | oleate (18:1n9) | Lipid | Long chain fatty acid | 1359 | GC/MS | 1984.4 | 339.2 | 112-80-1; |
| 835 | oleoylcarnitine | Lipid | Carnitine metabolism | 35160 | LC/MS Pos | 5202 | 426.4 | |
| 285 | ophthalmate | Amino acid | Glutathione metabolism | 34592 | LC/MS Pos | 1457 | 290.1 | 495-27-2; |
| 244 | ornithine | Amino acid | Urea cycle; arginine-, proline-, | 1493 | GC/MS | 1763.8 | 141.9 | 3184-13-2; |
| 632 | palmitate (16:0) | Lipid | Long chain fatty acid | 1336 | LC/MS Neg | 5619 | 255.3 | 57-10-3; |
| 633 | palmitoleate (16:1n7) | Lipid | Long chain fatty acid | 33447 | LC/MS Neg | 5477 | 253.3 | 373-49-9; |
| 1004 | palmitoyl sphingomyelin | Lipid | Sphingolipid | 37506 | GC/MS | 2524 | 311.3 | |
| 833 | palmitoylcarnitine | Lipid | Carnitine metabolism | 22189 | LC/MS Pos | 5179 | 400.4 | 6865-14-1; |
| 1243 | pantothenate | Cofactors and vitamins | Pantothenate and CoA | 1508 | LC/MS Pos | 2218 | 220.1 | 137-08-6; |
| 1613 | paraxanthine | Xenobiotics | Xanthine metabolism | 18254 | LC/MS Pos | 2444 | 181.2 | 611-59-6; |
| 88 | p-cresol sulfate | Amino acid | Phenylalanine & tyrosine | 36103 | LC/MS Neg | 2896 | 187.1 | 3233-57-7; |
| 621 | pelargonate (9:0) | Lipid | Medium chain fatty acid | 12035 | LC/MS Neg | 4847 | 157.2 | 112-05-0; |
| 631 | pentadecanoate (15:0) | Lipid | Long chain fatty acid | 1361 | LC/MS Neg | 5522 | 241.3 | 1002-84-2; |
| 135 | phenol sulfate | Amino acid | Phenylalanine & tyrosine | 32553 | LC/MS Neg | 2199 | 173.1 | 937-34-8; |
| 128 | phenylacetylglutamine | Amino acid | Phenylalanine & tyrosine | 35126 | LC/MS Pos | 2868 | 265.2 | 28047-15-6; |
| 83 | phenylalanine | Amino acid | Phenylalanine & tyrosine | 64 | LC/MS Pos | 2056 | 166.1 | 63-91-2; |
| 602 | phosphate | Energy | Oxidative phosphorylation | 11438 | GC/MS | 1307.7 | 298.9 | 7664-38-2 ; |
| 534 | phosphoenolpyruvate (PEP) | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 597 | GC/MS | 1595.4 | 369 | 10526-80-4; |
| 877 | phosphoethanolamine | Lipid | Glycerolipid metabolism | 12102 | GC/MS | 1577.3 | 299.1 | 1071-23-4; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 74 | pipecolate | Amino acid | Lysine metabolism | 1444 | LC/MS Pos | 1120 | 130.1 | 4043-87-2; |
| 1531 | piperine | Xenobiotics | Food component/Plant | 33935 | LC/MS Pos | 5136 | 286.2 | 94-62-2; |
| 246 | proline | Amino acid | Urea cycle; arginine-, proline-, | 1898 | LC/MS Pos | 796 | 116.1 | 147-85-3; |
| 809 | propionylcarnitine | Lipid | Fatty acid metabolism (also BCAA metabolism) | 32452 | LC/MS Pos | 1589 | 218.2 | 17298-37-2 ; |
| 1181 | pseudouridine | Nucleotide | Pyrimidine metabolism, uracil | 33442 | LC/MS Neg | 1104 | 243.1 | 1445-07-4; |
| 45 | pyroglutamine* | Amino acid | Glutamate metabolism | 32672 | LC/MS Pos | 764 | 129.2 | |
| 603 | pyrophosphate (PPi) | Energy | Oxidative phosphorylation | 2078 | GC/MS | 1642.3 | 451 | 1466-09-3; |
| 535 | pyruvate | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 599 | GC/MS | 1130.6 | 217 | 127-17-3; |
| 1469 | ranitidine | Xenobiotics | Drug | 38595 | LC/MS Pos | 1967 | 315.1 | 66357-59-3; |
| 548 | ribitol | Carbohydrate | Nucleotide sugars, pentose | 15772 | GC/MS | 1692.4 | 217 | 488-81-3; |
| 557 | ribose 5-phosphate | Carbohydrate | Nucleotide sugars, pentose | 561 | GC/MS | 1928.4 | 315.1 | 18265-46-8;108321-05-7; |
| 559 | ribulose | Carbohydrate | Nucleotide sugars, pentose | 35855 | GC/MS | 1662 | 306.1 | 488-84-6; |
| 224 | S-adenosylhomocysteine (SAH) | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 15948 | LC/MS Pos | 1480 | 385.1 | 979-92-0; |
| 551 | sedoheptulose-7-phosphate | Carbohydrate | Nucleotide sugars, pentose | 35649 | GC/MS | 2070 | 691.35 | 2646-35-7; |
| 8 | serine | Amino acid | Glycine, serine and threonine | 1648 | GC/MS | 1389.1 | 204 | 56-45-1; |
| 216 | S-methylcysteine | Amino acid | Cysteine, methionine, SAM, taurine metabolism | 39592 | GC/MS | 1447.8 | 218.1 | 1187-84-4; |
| 281 | S-methylglutathione | Amino acid | Glutathione metabolism | 33944 | LC/MS Pos | 1610 | 322.1 | 2922-56-7; |
| 270 | spermidine | Amino acid | Polyamine metabolism | 485 | LC/MS Pos | 533 | 146.2 | 124-20-9; |
| 1584 | stachydrine | Xenobiotics | Food component/Plant | 34384 | LC/MS Pos | 860 | 144.1 | 4136-37-2; |
| 637 | stearate (18:0) | Lipid | Long chain fatty acid | 1358 | LC/MS Neg | 5886 | 283.4 | 57-11-4; |
| 1005 | stearoyl sphingomyelin | Lipid | Sphingolipid | 19503 | GC/MS | 2645 | 311.3 | 85187-10-6;85187-10-6 ; |
| 834 | stearoylcarnitine | Lipid | Carnitine metabolism | 34409 | LC/MS Pos | 5300 | 428.4 | 18822-91-8; |
| 591 | succinylcarnitine | Energy | Krebs cycle | 37058 | LC/MS Pos | 1401 | 262.1 | |
| 1662 | terephthalic acid | Xenobiotics | Phthalate | 20684 | GC/MS | 1746.7 | 295 | 100-21-0; |
| 1614 | theobromine | Xenobiotics | Xanthine metabolism | 18392 | LC/MS Pos | 2136 | 181.1 | 83-67-0; |
| 1615 | theophylline | Xenobiotics | Xanthine metabolism | 18394 | LC/MS Pos | 2495 | 181.1 | 58-55-9; |
| 549 | threitol | Carbohydrate | Nucleotide sugars, pentose | 35854 | GC/MS | 1513 | 217.1 | 2418-52-2; |
| 1199 | threonate | Cofactors and vitamins | Ascorbate and aldarate | 27738 | GC/MS | 1560.7 | 292.1 | 70753-61-6; |
| 17 | threonine | Amino acid | Glycine, serine and threonine | 1284 | LC/MS Pos | 713 | 120.1 | 72-19-5; |
| 252 | trans-4-hydroxyproline | Amino acid | Urea cycle; arginine-, proline-, | 32306 | LC/MS Pos | 705 | 132.1 | 51-35-4; |

| PATHWAY SORTORDER | BIOCHEMICAL NAME | SUPER PATHWAY | SUB PATHWAY | COMP ID | PLATFORM | RI | MASS | CAS |
|---|---|---|---|---|---|---|---|---|
| 501 | trehalose | Carbohydrate | Fructose, mannose, galactose, starch, and sucrose metabolism | 15573 | GC/MS | 2174.9 | 361.2 | 6138-23-4; |
| 1242 | trigonelline (N'-methylnicotinate) | Cofactors and vitamins | Nicotinate and nicotinamide | 32401 | LC/MS Pos | 757 | 138.1 | 6138-41-6 ; |
| 145 | tryptophan | Amino acid | Tryptophan metabolism | 54 | LC/MS Pos | 2445 | 205.1 | 73-22-3; |
| 151 | tryptophan betaine | Amino acid | Tryptophan metabolism | 37097 | LC/MS Pos | 2464 | 247.1 | 20671-76-5; |
| 99 | tyrosine | Amino acid | Phenylalanine & tyrosine | 1299 | LC/MS Pos | 1516 | 182.1 | 60-18-4; |
| 1149 | urate | Nucleotide | Purine metabolism, urate | 1604 | LC/MS Neg | 769 | 167.1 | 69-93-2;120K5305; |
| 245 | urea | Amino acid | Urea cycle; arginine-, proline-, | 1670 | GC/MS | 1223.9 | 171 | 57-13-6; |
| 1180 | uridine | Nucleotide | Pyrimidine metabolism, uracil | 606 | LC/MS Neg | 1467 | 243.1 | 58-96-8; |
| 190 | valine | Amino acid | Valine, leucine and isoleucine | 1649 | LC/MS Pos | 1040 | 118.1 | 72-18-4; |
| 565 | xylitol | Carbohydrate | Nucleotide sugars, pentose | 4966 | GC/MS | 1677.6 | 307.2 | 87-99-0; |
| 570 | xylonate | Carbohydrate | Nucleotide sugars, pentose | 35638 | GC/MS | 1722 | 292 | 73686-31-7; |
| 569 | xylose | Carbohydrate | Nucleotide sugars, pentose | 15835 | GC/MS | 1723.9 | 204 | 609-06-3; |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 905 | 1,2-propanediol | C00717,C0291 | HMDB01881 | 0.093989 | 0.401140 | 0.845497 | 0.803099 | 0.965137 | 0.057564 |
| 532 | 1,3-dihydroxyacetone | C00184 | HMDB01882 | 0.940856 | 1.054696 | 1.442171 | 0.968040 | 0.782828 | 0.864449 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | C07326 | HMDB02712 | 1.274625 | 1.032870 | 1.243681 | 1.023692 | 0.952805 | 0.975757 |
| 523 | 1,6-anhydroglucose | | HMDB00640 | 1.238380 | 0.881507 | 0.829378 | 1.125241 | 1.036907 | 0.848109 |
| 636 | 10-heptadecenoate (17:1n7) | | | 0.796267 | 1.104475 | 0.800071 | 0.822623 | 1.312559 | 0.741740 |
| 742 | 13-methylmyristic acid | | | 0.522885 | 0.933119 | 1.053420 | 0.981142 | 1.309046 | 0.354055 |
| 744 | 15-methylpalmitate (isobar with 2- | | | 0.507116 | 1.167255 | 1.115206 | 0.996511 | 1.513833 | 0.533293 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | | HMDB11517 | 1.366868 | 1.576872 | 0.975005 | 0.951585 | 1.119687 | 0.889218 |
| 938 | 1-linoleoylglycerophosphocholine | C04100 | | 1.123556 | 1.370209 | 0.865878 | 0.894989 | 1.178065 | 0.933502 |
| 926 | 1-myristoylglycerophosphocholine | | HMDB10379 | 0.416175 | 0.416175 | 0.427186 | 2.096404 | 0.698575 | 0.416175 |
| 936 | 1-oleoylglycerophosphocholine | | | 0.178299 | 0.088629 | 0.185859 | 2.328282 | 1.163134 | 0.065166 |
| 915 | 1-oleoylglycerophosphoethanolamine | | HMDB11506 | 1.128128 | 1.252342 | 0.677501 | 0.738376 | 0.604000 | 0.830202 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | | | 0.440006 | 1.130496 | 1.076263 | 1.079450 | 0.922820 | 0.806115 |
| 929 | 1-palmitoylglycerophosphocholine | | | 0.123750 | 0.125820 | 0.181043 | 2.182270 | 1.378549 | 0.089435 |
| 909 | 1-palmitoylglycerophosphoethanolamine | | HMDB11503 | 1.088055 | 1.385403 | 1.022251 | 1.199668 | 1.166131 | 0.775325 |
| 934 | 1-stearoylglycerophosphocholine | | | 0.193808 | 0.120311 | 0.189197 | 1.838468 | 0.975918 | 0.098363 |
| 533 | 2,3-diphosphoglycerate | C01159 | HMDB01294 | 4.138947 | 1.554595 | 0.311838 | 0.074544 | 0.068895 | 4.676921 |
| 263 | 2-aminobutyrate | C02261 | HMDB00650 | 0.629355 | 0.625711 | 0.769009 | 0.740084 | 0.580321 | 0.496951 |
| 945 | 2-arachidonoylglycerophosphocholine* | | | 0.185345 | 0.191578 | 0.185345 | 1.677087 | 0.185345 | 0.185345 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | | | 0.085869 | 0.067968 | 0.193090 | 1.575407 | 0.558041 | 0.064698 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | | | 0.174717 | 0.095479 | 0.253343 | 1.256097 | 0.748772 | 0.095479 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | | | 0.089145 | 0.134588 | 0.328537 | 0.987333 | 0.648933 | 0.089145 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | | | 0.994715 | 1.127048 | 1.104864 | 0.500813 | 0.500813 | 1.506461 |
| 229 | 2-hydroxybutyrate (AHB) | C05984 | HMDB00008 | 0.962316 | 0.755261 | 0.873506 | 0.941181 | 0.735501 | 0.827288 |
| 714 | 2-hydroxyglutarate | C02630 | HMDB00606 | 0.569776 | 0.439821 | 0.993450 | 0.783255 | 1.070138 | 0.511422 |
| 706 | 2-hydroxypalmitate | | | 0.970627 | 1.168187 | 1.022629 | 0.802534 | 1.235599 | 0.520610 |
| 939 | 2-linoleoylglycerophosphocholine* | | | 0.229996 | 0.229996 | 0.229996 | 1.364130 | 0.769369 | 0.229996 |
| 202 | 2-methylbutyroylcarnitine | | HMDB00378 | 0.854777 | 0.913628 | 0.903239 | 0.726604 | 1.014510 | 1.023880 |
| 937 | 2-oleoylglycerophosphocholine* | | | 0.191712 | 0.191712 | 0.191712 | 1.298431 | 0.666356 | 0.191712 |
| 930 | 2-palmitoylglycerophosphocholine* | | | 0.086420 | 0.086420 | 0.143326 | 2.052493 | 0.832508 | 0.086420 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 935 | 2-stearoylglycerophosphocholine* | | | 0.572527 | 0.142354 | 0.142354 | 1.940494 | 0.940968 | 0.142354 |
| 821 | 3-dehydrocarnitine* | C02636 | HMDB12154 | 1.076919 | 0.924933 | 0.976938 | 1.033407 | 1.013969 | 0.910554 |
| 170 | 3-indoxyl sulfate | | HMDB00682 | 1.712419 | 1.255098 | 1.445637 | 1.530830 | 1.540111 | 1.229409 |
| 172 | 3-methyl-2-oxobutyrate | C00141 | HMDB00019 | 1.075324 | 1.155141 | 1.309651 | 0.984266 | 0.854008 | 0.403093 |
| 173 | 3-methyl-2-oxovalerate | C00671 | HMDB03736 | 1.043241 | 0.978637 | 1.246686 | 1.215393 | 1.035149 | 0.592511 |
| 529 | 3-phosphoglycerate | C00597 | HMDB00807 | 2.374659 | 1.117753 | 0.844108 | 0.429645 | 0.515288 | 3.533836 |
| 193 | 4-methyl-2-oxopentanoate | C00233 | HMDB00695 | 1.156508 | 1.141842 | 1.396480 | 1.094258 | 1.006348 | 0.588241 |
| 266 | 5-methylthioadenosine (MTA) | C00170 | HMDB01173 | 0.449465 | 0.754355 | 1.231740 | 1.271453 | 1.074281 | 0.315499 |
| 282 | 5-oxoproline | C01879 | HMDB00267 | 0.165879 | 0.565747 | 0.968489 | 1.322304 | 1.692893 | 0.157881 |
| 545 | 6-phosphogluconate | C00345 | HMDB01316 | 2.695675 | 1.212385 | 1.018991 | 0.981009 | 0.734737 | 0.598150 |
| 1024 | 7-beta-hydroxycholesterol | C03594 | HMDB06119 | 1.329854 | 1.093651 | 1.080549 | 1.516603 | 1.004637 | 0.363094 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | C14825 | HMDB04701 | 0.113908 | 0.601718 | 0.964045 | 0.972183 | 1.082745 | 0.042011 |
| 672 | 9,10-epoxystearate | | | 0.044171 | 0.773191 | 0.950427 | 0.993213 | 1.196794 | 0.030000 |
| 822 | acetylcarnitine | C02571 | HMDB00201 | 1.126087 | 0.881193 | 0.906692 | 0.820706 | 0.867728 | 0.955412 |
| 601 | acetylphosphate | C00227 | HMDB01494 | 1.029339 | 0.963066 | 1.009106 | 1.075334 | 0.815509 | 0.684729 |
| 1105 | adenine | C00147 | HMDB00034 | 1.395489 | 1.026574 | 0.783973 | 0.632388 | 0.507260 | 1.193781 |
| 1106 | adenosine | C00212 | HMDB00050 | 0.449049 | 0.638120 | 0.679083 | 0.923837 | 1.393348 | 0.984137 |
| 1116 | adenosine 5'-diphosphate (ADP) | C00008 | HMDB01341 | 1.390162 | 1.383267 | 0.897989 | 0.996594 | 1.189003 | 1.444857 |
| 1232 | adenosine 5'diphosphoribose | C00301 | HMDB01178 | 1.267679 | 1.058207 | 1.103961 | 1.020994 | 0.993634 | 1.093751 |
| 1114 | adenosine 5'-monophosphate (AMP) | C00020 | HMDB00045 | 0.715566 | 0.966972 | 0.935805 | 0.904164 | 1.404471 | 1.066409 |
| 665 | adrenate (22:4n6) | C16527 | HMDB02226 | 0.486736 | 1.902288 | 0.889997 | 1.304018 | 1.230291 | 0.369250 |
| 27 | alanine | C00041 | HMDB00161 | 0.912282 | 0.809323 | 1.048377 | 1.073185 | 1.000614 | 0.669428 |
| 1150 | allantoin | C02350 | HMDB00462 | 1.731724 | 1.144911 | 1.216153 | 0.726424 | 1.250808 | 1.063616 |
| 179 | alpha-hydroxyisocaproate | C03264 | HMDB00746 | 0.292412 | 0.292412 | 0.380921 | 0.832896 | 1.423024 | 0.292412 |
| 198 | alpha-hydroxyisovalerate | | HMDB00407 | 0.829316 | 0.644653 | 0.847666 | 0.966061 | 1.251663 | 0.824864 |
| 1266 | alpha-tocopherol | C02477 | HMDB01893 | 1.419880 | 1.212748 | 1.440249 | 1.473337 | 1.096169 | 0.986832 |
| 1034 | androsterone sulfate | C00523 | HMDB02759 | 1.050185 | 0.757073 | 0.922578 | 0.880415 | 0.788449 | 0.847041 |
| 566 | arabinose | C00181 | HMDB00646 | 1.066035 | 0.792435 | 1.187882 | 0.910478 | 0.983765 | 0.851556 |
| 546 | arabitol | C00474 | HMDB01851 | 1.062259 | 0.791483 | 1.076288 | 1.042036 | 0.831019 | 0.870610 |
| 1202 | arabonate | | HMDB00539 | 1.088700 | 0.833567 | 0.776673 | 1.036803 | 1.000331 | 1.008680 |
| 659 | arachidonate (20:4n6) | C00219 | HMDB01043 | 1.089373 | 1.462770 | 0.833837 | 0.994535 | 1.825296 | 0.976271 |
| 241 | arginine | C00062 | HMDB00517 | 1.194589 | 0.559059 | 0.964406 | 0.785271 | 1.480900 | 0.795852 |
| 25 | asparagine | C00152 | HMDB00168 | 1.141829 | 0.913989 | 0.966493 | 0.928296 | 0.674187 | 0.904378 |
| 24 | aspartate | C00049 | HMDB00191 | 1.214478 | 1.001431 | 1.277627 | 1.401880 | 1.213226 | 1.085541 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 721 | azelate (nonanedioate) | C08261 | HMDB00784 | 0.245042 | 0.595599 | 1.073954 | 1.371530 | 1.768580 | 0.230852 |
| 26 | beta-alanine | C00099 | HMDB00056 | 0.900905 | 0.941909 | 0.951472 | 0.931881 | 0.632220 | 0.490479 |
| 7 | beta-hydroxypyruvate | C00168 | HMDB01352 | 1.209736 | 0.795568 | 1.049309 | 0.666684 | 1.002750 | 0.899862 |
| 22 | betaine | | HMDB00043 | 0.794116 | 0.667522 | 0.834714 | 0.823645 | 0.728270 | 0.793730 |
| 1057 | beta-sitosterol | C01753 | HMDB00852 | 0.570500 | 0.349092 | 0.349092 | 0.770647 | 0.357752 | 0.525103 |
| 1216 | biliverdin | C00500 | HMDB01008 | 0.522259 | 0.522259 | 0.522259 | 1.166977 | 0.625312 | 0.551372 |
| 811 | butyrylcarnitine | | | 1.043461 | 0.828255 | 1.079063 | 0.752751 | 0.598389 | 0.999344 |
| 1612 | caffeine | C07481 | HMDB01847 | 0.999314 | 0.822552 | 0.914438 | 0.875849 | 0.830690 | 0.855801 |
| 1059 | campesterol | C01789 | HMDB02869 | 1.094301 | 0.478278 | 1.000000 | 0.776528 | 0.469755 | 1.104270 |
| 622 | caprate (10:0) | C01571 | HMDB00511 | 0.569170 | 0.980594 | 1.284473 | 1.071891 | 0.992421 | 0.430953 |
| 618 | caproate (6:0) | C01585 | HMDB00535 | 1.581021 | 1.065844 | 1.189805 | 0.838839 | 0.788805 | 1.557801 |
| 620 | caprylate (8:0) | C06423 | HMDB00482 | 0.389680 | 0.838546 | 1.716807 | 1.182484 | 1.354962 | 0.814413 |
| 820 | carnitine | | | 1.021174 | 0.823129 | 0.955729 | 0.927607 | 0.920565 | 0.796767 |
| 1300 | catechol sulfate | C00090 | | 1.165133 | 0.995666 | 1.101118 | 1.008261 | 0.969035 | 0.965027 |
| 164 | C-glycosyltryptophan* | | | 1.035688 | 0.857870 | 0.917760 | 0.918208 | 0.924370 | 0.936158 |
| 1020 | cholesterol | C00187 | HMDB00067 | 1.010012 | 0.884618 | 1.005086 | 1.018152 | 0.909531 | 0.831067 |
| 881 | choline | | | 0.457805 | 0.519088 | 0.510624 | 0.566353 | 0.597473 | 0.483461 |
| 582 | cis-aconitate | C00417 | HMDB00072 | 0.647851 | 1.005747 | 1.064489 | 1.053564 | 1.170318 | 0.638058 |
| 641 | cis-vaccenate (18:1n7) | C08367 | | 1.639499 | 1.022769 | 0.551118 | 0.725897 | 1.009816 | 0.563160 |
| 579 | citrate | C00158 | HMDB00094 | 1.455945 | 1.109140 | 1.137108 | 1.011044 | 0.881536 | 1.223980 |
| 248 | citrulline | C00327 | HMDB00904 | 1.152402 | 1.054559 | 1.163516 | 1.053651 | 1.189787 | 1.168537 |
| 259 | creatine | C00300 | HMDB00064 | 0.993535 | 0.891023 | 0.906751 | 0.890437 | 0.862782 | 0.841125 |
| 260 | creatinine | C00791 | HMDB00562 | 0.865685 | 0.968933 | 0.930878 | 0.998699 | 0.767573 | 0.859310 |
| 213 | cysteine | C00097 | HMDB00574 | 0.776267 | 0.747842 | 0.990776 | 1.865414 | 1.711294 | 0.448327 |
| 819 | deoxycarnitine | C01181 | HMDB01161 | 1.040861 | 0.850303 | 0.972640 | 0.851995 | 0.906019 | 0.955015 |
| 655 | dihomo-linoleate (20:2n6) | C16525 | | 0.685223 | 1.012127 | 0.748911 | 0.760888 | 1.377872 | 0.545316 |
| 609 | dihomo-linolenate (20:3n3 or n6) | C03242 | HMDB02925 | 1.113018 | 1.398940 | 0.936092 | 1.103451 | 1.945842 | 0.973365 |
| 531 | dihydroxyacetone phosphate (DHAP) | C00111 | HMDB01473 | 0.385793 | 1.056641 | 0.320859 | 0.622944 | 0.239333 | 44.147339 |
| 3 | dimethylglycine | C01026 | HMDB00092 | 0.993914 | 0.967463 | 0.870135 | 1.538440 | 0.832408 | 0.620077 |
| 613 | docosahexaenoate (DHA; 22:6n3) | C06429 | HMDB02183 | 0.794951 | 1.239805 | 0.934690 | 1.240075 | 2.147000 | 0.747328 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | C16513 | HMDB01976 | 0.658557 | 0.882298 | 0.966259 | 1.000485 | 1.707321 | 0.615944 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | C06428 | HMDB01999 | 1.015692 | 1.335128 | 0.760620 | 1.162985 | 1.596989 | 0.959060 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 1565 | ergothioneine | C05570 | HMDB03045 | 0.835187 | 0.776632 | 0.736140 | 0.680171 | 0.755074 | 0.733015 |
| 735 | erucamide | | | 0.527467 | 0.703786 | 0.741920 | 1.776732 | 0.727185 | 0.427592 |
| 1632 | erythritol | C00503 | HMDB02994 | 0.653841 | 0.720044 | 1.045748 | 1.259075 | 1.305161 | 0.610686 |
| 453 | erythronate* | | HMDB00613 | 0.689475 | 0.775144 | 0.950500 | 1.032711 | 0.960244 | 0.598603 |
| 876 | ethanolamine | C00189 | HMDB00149 | 0.549032 | 1.054160 | 1.158327 | 1.052428 | 0.824532 | 0.585552 |
| 472 | fructose | C00095 | HMDB00660 | 0.919175 | 0.835912 | 1.072641 | 1.142352 | 1.017204 | 0.646730 |
| 524 | fructose-6-phosphate | C05345 | HMDB00124 | 1.048181 | 1.013336 | 1.010773 | 0.788031 | 0.832102 | 0.481086 |
| 594 | fumarate | C00122 | HMDB00134 | 0.699296 | 0.705909 | 0.653853 | 0.714851 | 0.987097 | 0.691151 |
| 404 | gamma-glutamylleucine | | HMDB11171 | 1.263046 | 0.956229 | 0.935706 | 1.260536 | 0.935957 | 0.960392 |
| 521 | glucose | C00293 | HMDB00122 | 1.100613 | 0.894063 | 0.999561 | 0.975802 | 0.956884 | 0.914791 |
| 519 | glucose-6-phosphate (G6P) | C00668 | HMDB01401 | 1.101610 | 0.939321 | 1.137970 | 0.666145 | 0.877208 | 0.075532 |
| 39 | glutamate | C00025 | HMDB03339 | 0.968093 | 0.679776 | 0.890358 | 0.846317 | 0.889278 | 0.957911 |
| 44 | glutamine | C00064 | HMDB00641 | 1.363576 | 1.198844 | 1.033190 | 1.000241 | 0.820056 | 1.274925 |
| 80 | glutaroyl carnitine | | HMDB13130 | 1.225842 | 0.848082 | 0.561030 | 0.561030 | 0.561030 | 0.667386 |
| 283 | glutathione, oxidized (GSSG) | C00127 | HMDB03337 | 1.440573 | 1.002163 | 1.010711 | 0.997837 | 0.719527 | 1.269335 |
| 280 | glutathione, reduced (GSH) | C00051 | HMDB00125 | 1.231496 | 0.756086 | 1.150949 | 1.009302 | 0.735478 | 1.070710 |
| 517 | glycerate | C00258 | HMDB00139 | 0.454046 | 0.579083 | 0.765712 | 0.950256 | 0.917643 | 0.462533 |
| 882 | glycerol 3-phosphate (G3P) | C00093 | HMDB00126 | 1.063160 | 0.882808 | 0.923560 | 0.666260 | 0.866868 | 3.677948 |
| 883 | glycerophosphorylcholine (GPC) | C00670 | HMDB00086 | 1.263060 | 0.997264 | 0.967765 | 0.977253 | 1.072449 | 0.927551 |
| 1 | glycine | C00037 | HMDB00123 | 0.784409 | 0.701784 | 1.029387 | 1.267401 | 1.440536 | 0.613590 |
| 851 | glycochenodeoxycholate | C05466 | HMDB00637 | 0.361362 | 0.333840 | 0.307484 | 0.268684 | 0.332119 | 0.306612 |
| 840 | glycocholate | C01921 | HMDB00138 | 0.132858 | 0.084103 | 0.167936 | 0.151510 | 0.079564 | 0.141719 |
| 849 | glycodeoxycholate | C05464 | HMDB00631 | 0.199279 | 0.199279 | 0.199279 | 0.331379 | 0.293438 | 0.199279 |
| 1318 | glycolate (hydroxyacetate) | C00160 | HMDB00115 | 1.078136 | 0.940027 | 1.117940 | 1.144272 | 0.930150 | 0.838677 |
| 1128 | guanosine | C00387 | HMDB00133 | 1.295695 | 0.984093 | 1.233850 | 1.022857 | 1.131049 | 1.155844 |
| 1212 | heme* | | | 0.954588 | 0.264021 | 0.482578 | 3.174177 | 0.788115 | 0.405137 |
| 619 | heptanoate (7:0) | C17714 | HMDB00666 | 0.800282 | 1.170681 | 1.666856 | 0.736404 | 0.944057 | 1.156421 |
| 823 | hexanoylcarnitine | C01585 | HMDB00705 | 1.978526 | 0.904615 | 1.150736 | 0.889297 | 1.434068 | 1.615980 |
| 1288 | hippurate | C01586 | HMDB00714 | 1.133840 | 0.956417 | 1.012884 | 1.016509 | 1.064161 | 0.921184 |
| 50 | histidine | C00135 | HMDB00177 | 0.898835 | 0.912690 | 0.798434 | 1.230160 | 1.035040 | 1.171108 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | **SAMPLE NAME** | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
| | | | **CLIENT IDENTIFIER** | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | **SAMPLE ID** | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | **PARENT SAMPLE ID** | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | **ACTUAL** | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | **UNIT** | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | **COND DAY** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | **BRADFORD PROTEIN** | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | **KEGG** | **Group HMDB** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 231 | homocysteine | C00155 | HMDB00742 | 0.262199 | 0.375152 | 0.738484 | 1.163485 | 0.992255 | 0.281478 |
| 1585 | homostachydrine* | C08283 | | 1.288188 | 1.026078 | 1.179888 | 1.013992 | 0.950084 | 1.155035 |
| 206 | hydroxyisovaleroyl carnitine | | | 0.724878 | 0.560873 | 0.745301 | 0.673846 | 0.719616 | 0.657910 |
| 1098 | hypoxanthine | C00262 | HMDB00157 | 0.097602 | 0.112866 | 0.430679 | 1.318815 | 2.170569 | 0.121817 |
| 1101 | inosine 5'-monophosphate (IMP) | C00130 | HMDB00175 | 0.377696 | 0.646349 | 0.924064 | 0.598793 | 0.655219 | 0.258697 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | | | 1.302519 | 1.218696 | 1.200162 | 0.988566 | 1.116699 | 5.111154 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | | | 0.995202 | 1.301341 | 0.617255 | 1.004798 | 0.494205 | 4.960977 |
| 496 | Isobar: sorbitol, mannitol | C00392,C0172 | HMDB00247 | 1.054596 | 0.864582 | 1.083342 | 1.049648 | 0.908134 | 0.967651 |
| 200 | isobutyrylcarnitine | | | 1.162361 | 0.961702 | 0.975136 | 0.902758 | 0.844705 | 1.106286 |
| 180 | isoleucine | C00407 | HMDB00172 | 0.987145 | 0.794828 | 0.999866 | 0.997684 | 0.979558 | 0.917794 |
| 478 | isomaltose | C00252 | HMDB02923 | 1.211123 | 0.783606 | 1.193456 | 0.998921 | 0.795175 | 0.705296 |
| 205 | isovalerylcarnitine | | HMDB00688 | 0.957936 | 0.743246 | 0.925570 | 0.903648 | 1.195788 | 0.896412 |
| 144 | kynurenine | C00328 | HMDB00684 | 0.929605 | 0.825327 | 1.077796 | 1.036477 | 0.788213 | 0.979446 |
| 536 | lactate | C00186 | HMDB00190 | 0.184047 | 0.503474 | 0.921057 | 1.116432 | 1.160568 | 0.223943 |
| 1018 | lathosterol | C01189 | HMDB01170 | 1.020373 | 1.053193 | 1.504318 | 0.994947 | 0.965564 | 0.808696 |
| 625 | laurate (12:0) | C02679 | HMDB00638 | 0.924744 | 1.004352 | 1.058769 | 1.097257 | 1.170584 | 0.873382 |
| 181 | leucine | C00123 | HMDB00687 | 0.903947 | 0.780766 | 0.928915 | 0.995498 | 0.979677 | 0.818525 |
| 604 | linoleate (18:2n6) | C01595 | HMDB00673 | 0.661104 | 0.997258 | 0.698140 | 0.785193 | 1.275626 | 0.614669 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | C06427 | HMDB01388 | 0.829378 | 1.153856 | 0.922793 | 0.898516 | 1.253571 | 0.859021 |
| 69 | lysine | C00047 | HMDB00182 | 0.858728 | 0.927582 | 0.968109 | 1.543772 | 0.699000 | 0.692248 |
| 598 | malate | C00149 | HMDB00156 | 0.509580 | 0.674466 | 0.693725 | 0.748274 | 0.831729 | 0.399579 |
| 482 | maltose | C00208 | HMDB00163 | 1.046492 | 0.857338 | 1.018061 | 1.008771 | 0.872358 | 0.833263 |
| 487 | mannose | C00159 | HMDB00169 | 1.205248 | 0.960470 | 1.022661 | 1.056647 | 0.941239 | 0.969336 |
| 489 | mannose-6-phosphate | C00275 | HMDB01078 | 0.974867 | 1.156702 | 1.150395 | 0.925892 | 0.846344 | 0.465820 |
| 635 | margarate (17:0) | | HMDB02259 | 0.676142 | 1.020723 | 1.034499 | 0.813727 | 1.223798 | 0.607831 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 658 | mead acid (20:3n9) | | HMDB10378 | 0.982527 | 1.217503 | 0.593670 | 0.703125 | 2.025167 | 1.028821 |
| 225 | methionine | C00073 | HMDB00696 | 1.507191 | 1.001162 | 0.998838 | 0.745071 | 0.681953 | 1.412109 |
| 890 | myo-inositol | C00137 | HMDB00211 | 0.837540 | 0.810258 | 0.999258 | 0.918080 | 0.721814 | 0.839143 |
| 629 | myristate (14:0) | C06424 | HMDB00806 | 0.566010 | 1.030228 | 1.161382 | 0.963253 | 1.151818 | 0.459958 |
| 630 | myristoleate (14:1n5) | C08322 | HMDB02000 | 0.625324 | 0.658534 | 0.493142 | 0.572631 | 1.380087 | 0.493142 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | C05842 | HMDB04193 | 1.564949 | 1.428541 | 1.499827 | 1.002102 | 1.075192 | 1.136819 |
| 75 | N-6-trimethyllysine | | | 0.660943 | 0.585348 | 0.822405 | 0.705275 | 0.566193 | 0.487751 |
| 4 | N-acetylglycine | | HMDB00532 | 1.175280 | 0.811402 | 1.542740 | 1.046386 | 0.686973 | 0.942530 |
| 227 | N-acetylmethionine | C02712 | HMDB11745 | 0.800527 | 0.903428 | 0.800527 | 0.800527 | 0.832440 | 0.959118 |
| 455 | N-acetylneuraminate | C00270 | HMDB00230 | 0.357287 | 0.538860 | 0.978609 | 1.308516 | 0.936821 | 0.454634 |
| 1221 | nicotinamide | C00153 | HMDB01406 | 0.938633 | 0.969041 | 1.091274 | 1.309828 | 0.970032 | 0.853524 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | C00003 | HMDB00902 | 1.075162 | 0.847859 | 1.002085 | 2.084172 | 0.967308 | 1.302876 |
| 825 | octanoylcarnitine | | | 0.849712 | 0.775525 | 0.952219 | 0.981920 | 0.921344 | 0.653453 |
| 639 | oleate (18:1n9) | C00712 | HMDB00207 | 0.714866 | 0.960577 | 0.673818 | 0.930919 | 0.924696 | 0.621447 |
| 835 | oleoylcarnitine | | HMDB05065 | 0.111343 | 0.103863 | 0.127639 | 1.159799 | 0.495649 | 0.072123 |
| 285 | ophthalmate | | HMDB05765 | 2.351470 | 0.412000 | 0.252181 | 0.252181 | 0.252181 | 2.213700 |
| 244 | ornithine | C00077 | HMDB03374 | 1.044312 | 0.973956 | 1.077857 | 1.075137 | 0.831313 | 0.846538 |
| 632 | palmitate (16:0) | C00249 | HMDB00220 | 0.731859 | 1.097799 | 0.929711 | 0.866888 | 1.214564 | 0.645327 |
| 633 | palmitoleate (16:1n7) | C08362 | HMDB03229 | 0.746184 | 1.082150 | 0.814432 | 0.771888 | 1.206358 | 0.662766 |
| 1004 | palmitoyl sphingomyelin | | | 1.009978 | 0.864505 | 0.988393 | 0.996593 | 0.873151 | 0.810514 |
| 833 | palmitoylcarnitine | | | 0.138978 | 0.059115 | 0.189457 | 1.064403 | 0.519661 | 0.177110 |
| 1243 | pantothenate | C00864 | HMDB00210 | 1.016767 | 0.897232 | 0.956114 | 0.869183 | 0.899775 | 0.885358 |
| 1613 | paraxanthine | C13747 | HMDB01860 | 1.061880 | 0.851574 | 1.126766 | 1.157693 | 0.944562 | 0.920510 |
| 88 | p-cresol sulfate | C01468 | | 1.418439 | 1.199775 | 1.288073 | 1.182466 | 1.271776 | 1.204341 |
| 621 | pelargonate (9:0) | C01601 | HMDB00847 | 0.601400 | 0.968215 | 1.817404 | 1.196536 | 1.274407 | 0.696637 |
| 631 | pentadecanoate (15:0) | C16537 | HMDB00826 | 0.765394 | 1.116842 | 1.018417 | 0.960782 | 1.283807 | 0.646841 |
| 135 | phenol sulfate | C02180 | | 1.194608 | 1.062706 | 1.078474 | 0.990487 | 0.960798 | 1.065396 |
| 128 | phenylacetylglutamine | C05597 | HMDB06344 | 1.447771 | 1.224528 | 1.323932 | 1.434381 | 1.291844 | 1.190817 |
| 83 | phenylalanine | C00079 | HMDB00159 | 0.984373 | 0.855271 | 1.137403 | 1.113927 | 1.009291 | 0.897514 |
| 602 | phosphate | C00009 | HMDB01429 | 0.960793 | 0.920399 | 1.138694 | 1.133536 | 1.040180 | 0.668616 |
| 534 | phosphoenolpyruvate (PEP) | C00074 | HMDB00263 | 4.317937 | 1.447414 | 0.490799 | 0.200344 | 0.336918 | 4.201588 |
| 877 | phosphoethanolamine | C00346 | HMDB00224 | 1.074507 | 0.875807 | 1.225685 | 0.593700 | 0.786465 | 1.080196 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 74 | pipecolate | C00408 | HMDB00070 | 1.102910 | 0.889577 | 0.822084 | 1.139414 | 0.897131 | 0.781710 |
| 1531 | piperine | C03882 | | 1.071879 | 1.101751 | 0.655875 | 0.834467 | 0.708170 | 0.919699 |
| 246 | proline | C00148 | HMDB00162 | 0.915947 | 1.028549 | 0.939995 | 0.915745 | 1.005936 | 0.795303 |
| 809 | propionylcarnitine | C03017 | HMDB00824 | 0.998129 | 0.797025 | 0.812016 | 0.676241 | 0.714173 | 0.811286 |
| 1181 | pseudouridine | C02067 | HMDB00767 | 1.581253 | 1.282899 | 1.098750 | 0.982422 | 1.162511 | 0.761125 |
| 45 | pyroglutamine* | | | 0.737929 | 0.547121 | 0.420202 | 0.448679 | 0.439148 | 0.374612 |
| 603 | pyrophosphate (PPi) | C00013 | HMDB00250 | 1.962899 | 1.222331 | 1.303311 | 1.020032 | 0.385049 | 1.594598 |
| 535 | pyruvate | C00022 | HMDB00243 | 1.118042 | 1.969399 | 2.094208 | 0.810124 | 0.505324 | 0.056113 |
| 1469 | ranitidine | D00422 | HMDB01930 | 1.036527 | 0.947381 | 0.948476 | 0.866407 | 1.039385 | 0.879676 |
| 548 | ribitol | C00474 | HMDB00508 | 0.877273 | 0.711653 | 1.151194 | 0.741076 | 1.118788 | 0.798867 |
| 557 | ribose 5-phosphate | C00117 | HMDB00618 | 1.367338 | 1.252771 | 0.933570 | 0.814745 | 0.672063 | 2.233142 |
| 559 | ribulose | C00309 | HMDB00621,HMDB03371 | 0.838750 | 0.240496 | 0.895948 | 1.227931 | 0.240496 | 1.386884 |
| 224 | S-adenosylhomocysteine (SAH) | C00021 | HMDB00939 | 0.722516 | 0.933287 | 1.079622 | 0.889291 | 1.162824 | 0.618320 |
| 551 | sedoheptulose-7-phosphate | C05382 | HMDB01068 | 1.205791 | 0.370716 | 2.626636 | 1.788112 | 0.461430 | 0.074096 |
| 8 | serine | C00065 | HMDB03406 | 0.897376 | 0.826694 | 0.933398 | 0.972309 | 0.894736 | 0.740037 |
| 216 | S-methylcysteine | | HMDB02108 | 1.546979 | 1.514817 | 1.615735 | 1.747664 | 1.551145 | 1.112397 |
| 281 | S-methylglutathione | C11347 | | 1.405068 | 0.824551 | 0.931198 | 1.286469 | 0.997110 | 1.238279 |
| 270 | spermidine | C00315 | HMDB01257 | 0.779236 | 0.685966 | 0.903530 | 0.851891 | 0.852453 | 0.671940 |
| 1584 | stachydrine | C10172 | HMDB04827 | 0.120808 | 0.078570 | 0.119219 | 0.126803 | 0.132770 | 0.112926 |
| 637 | stearate (18:0) | C01530 | HMDB00827 | 0.713078 | 1.129057 | 0.998799 | 0.875504 | 1.219120 | 0.621096 |
| 1005 | stearoyl sphingomyelin | C00550 | HMDB01348 | 1.277456 | 0.910619 | 0.973538 | 1.056922 | 1.077678 | 0.872663 |
| 834 | stearoylcarnitine | | HMDB00848 | 0.056108 | 0.056108 | 0.217910 | 1.000000 | 0.481530 | 0.056108 |
| 591 | succinylcarnitine | | | 0.711793 | 0.675913 | 0.753938 | 0.736396 | 0.814040 | 0.610032 |
| 1662 | terephthalic acid | C06337 | HMDB02428 | 0.915167 | 0.570385 | 0.624059 | 0.686443 | 0.631354 | 0.559301 |
| 1614 | theobromine | C07480 | HMDB02825 | 1.350359 | 1.111060 | 1.426622 | 1.053549 | 1.151325 | 1.199873 |
| 1615 | theophylline | C07130 | HMDB01889 | 1.171008 | 1.650268 | 1.072864 | 0.617853 | 0.957177 | 1.036258 |
| 549 | threitol | C16884 | HMDB04136 | 0.956725 | 0.969312 | 1.242202 | 1.281014 | 1.140570 | 0.888563 |
| 1199 | threonate | C01620 | HMDB00943 | 1.069841 | 0.883127 | 1.058853 | 0.951108 | 1.015710 | 0.710274 |
| 17 | threonine | C00188 | HMDB00167 | 0.908850 | 0.834363 | 0.872882 | 0.864093 | 0.942662 | 0.772937 |
| 252 | trans-4-hydroxyproline | C01157 | HMDB00725 | 1.248799 | 1.083158 | 1.092664 | 1.275759 | 1.098446 | 1.147332 |

| | | | SAMPLE NAME | DARM-00001 | DARM-00002 | DARM-00003 | DARM-00004 | DARM-00005 | DARM-00006 |
|---|---|---|---|---|---|---|---|---|---|
| | | | CLIENT IDENTIFIER | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 D | NHSCi 2003 T2 I | NHSCi 2003 T2 D | NHSCi 2003 T1 |
| | | | SAMPLE ID | 997731 | 997714 | 997743 | 997745 | 997721 | 997727 |
| | | | PARENT SAMPLE ID | 991346 | 991347 | 991348 | 991349 | 991350 | 991351 |
| | | | | NHSCi 2003 T2 | NHSCi 2003 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 T2 | NHSCi 2003 |
| | | | ACTUAL | D0 | T2 D7 | D14 | D21 | D28 | T1 D0 |
| | | | UNIT | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | | COND DAY | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| | | | BRADFORD PROTEIN | 168.571 | 179.95 | 177.746 | 178.439 | 181.508 | 193.651 |
| PATHWAY SORTORDER | BIOCHEMICAL NAME | KEGG | Group HMDB | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 |
| 501 | trehalose | C01083 | HMDB00975 | 0.108147 | 0.610965 | 1.012624 | 1.338255 | 1.046230 | 0.104490 |
| 1242 | trigonelline (N'-methylnicotinate) | | HMDB00875 | 0.711049 | 0.623862 | 0.645081 | 0.663676 | 0.636632 | 0.647216 |
| 145 | tryptophan | C00078 | HMDB00929 | 1.031677 | 0.788144 | 1.074157 | 1.014829 | 0.943093 | 0.835153 |
| 151 | tryptophan betaine | C09213 | | 0.562156 | 0.508877 | 0.532573 | 0.496551 | 0.519666 | 0.491686 |
| 99 | tyrosine | C00082 | HMDB00158 | 0.869281 | 0.713008 | 0.991781 | 0.926936 | 0.952006 | 0.804564 |
| 1149 | urate | C00366 | HMDB00289 | 1.110170 | 1.013792 | 0.972913 | 0.874034 | 1.018883 | 1.003583 |
| 245 | urea | C00086 | HMDB00294 | 1.147243 | 0.896619 | 1.154535 | 1.091534 | 1.008057 | 0.943828 |
| 1180 | uridine | C00299 | HMDB00296 | 0.424213 | 0.632935 | 0.685118 | 0.767251 | 1.012166 | 0.640234 |
| 190 | valine | C00183 | HMDB00883 | 0.932442 | 0.820464 | 1.000926 | 0.940639 | 0.923756 | 0.870393 |
| 565 | xylitol | C00379 | HMDB00568 | 0.127693 | 0.127693 | 0.127693 | 0.127693 | 0.127693 | 0.127693 |
| 570 | xylonate | C00502,C05411 | | 0.763576 | 0.711723 | 1.095722 | 0.987384 | 1.346684 | 1.242916 |
| 569 | xylose | C00181 | HMDB00098 | 1.034657 | 0.405368 | 0.513480 | 0.708854 | 0.895573 | 0.405368 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 905 | 1,2-propanediol | 0.579393 | 0.881442 | 1.419568 | 1.047499 | 0.071779 | 0.575987 | 1.250987 | 1.276408 | 1.584491 |
| 532 | 1,3-dihydroxyacetone | 1.005572 | 1.295784 | 1.681924 | 1.351797 | 1.032546 | 1.019166 | 1.076962 | 0.931657 | 0.894764 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 1.222268 | 0.995142 | 1.772193 | 0.905907 | 0.939960 | 1.191738 | 1.611112 | 1.080594 | 1.318376 |
| 523 | 1,6-anhydroglucose | 1.307081 | 1.303914 | 1.421176 | 0.985249 | 1.515766 | 0.938190 | 1.525099 | 1.005262 | 1.176818 |
| 636 | 10-heptadecenoate (17:1n7) | 1.011971 | 0.988029 | 1.229869 | 0.837718 | 0.528442 | 0.673333 | 0.775389 | 1.304893 | 1.228168 |
| 742 | 13-methylmyristic acid | 0.956273 | 1.215136 | 1.490650 | 1.156663 | 0.509429 | 0.889129 | 1.082770 | 1.589390 | 1.395014 |
| 744 | 15-methylpalmitate (isobar with 2- | 0.844457 | 1.103403 | 1.382409 | 0.940191 | 0.479921 | 0.760123 | 1.123751 | 1.434375 | 1.459824 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 1.049916 | 1.087377 | 1.555467 | 0.769220 | 1.983977 | 0.986731 | 1.217806 | 0.958717 | 0.771485 |
| 938 | 1-linoleoylglycerophosphocholine | 0.967220 | 0.999949 | 2.227720 | 0.865688 | 1.499100 | 0.934622 | 1.310714 | 1.121451 | 0.950420 |
| 926 | 1-myristoylglycerophosphocholine | 0.417624 | 2.906419 | 2.670861 | 5.384758 | 0.416175 | 0.653119 | 0.789458 | 1.000000 | 1.522096 |
| 936 | 1-oleoylglycerophosphocholine | 0.544009 | 1.726474 | 2.647978 | 4.037094 | 0.065166 | 0.231035 | 0.749125 | 1.000000 | 1.798584 |
| 915 | 1-oleoylglycerophosphoethanolamine | 1.339954 | 0.322900 | 1.875242 | 0.580694 | 1.350258 | 1.229704 | 1.343753 | 1.298771 | 0.879791 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 0.829122 | 1.253203 | 0.977707 | 1.119067 | 0.916368 | 1.889740 | 0.672489 | 0.949738 | 0.829713 |
| 929 | 1-palmitoylglycerophosphocholine | 0.630176 | 1.556422 | 2.942561 | 3.136941 | 0.083969 | 0.250438 | 0.862993 | 1.152353 | 2.071989 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 1.204767 | 0.843694 | 2.424624 | 0.931373 | 2.389639 | 1.260441 | 1.505796 | 1.279065 | 1.265982 |
| 934 | 1-stearoylglycerophosphocholine | 0.473487 | 2.894309 | 2.215544 | 4.321889 | 0.091058 | 0.296757 | 0.689606 | 1.011835 | 1.583255 |
| 533 | 2,3-diphosphoglycerate | 4.972904 | 3.857553 | 2.788181 | 0.746330 | 2.814633 | 1.589136 | 0.482986 | 0.151241 | 0.155468 |
| 263 | 2-aminobutyrate | 0.753116 | 0.750416 | 1.001038 | 0.748359 | 0.659673 | 0.681075 | 0.863260 | 0.683240 | 0.748353 |
| 945 | 2-arachidonoylglycerophosphocholine* | 0.432689 | 2.601587 | 1.158283 | 4.677377 | 0.185345 | 0.359102 | 0.344467 | 0.546725 | 1.114457 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 0.361928 | 2.168727 | 1.141330 | 2.855072 | 0.060242 | 0.424004 | 0.288778 | 0.554670 | 1.112031 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 0.475139 | 2.511314 | 1.644739 | 3.717151 | 0.095479 | 0.257399 | 0.363824 | 0.614259 | 1.123485 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 0.525743 | 2.345279 | 1.100081 | 2.505825 | 0.089145 | 0.178370 | 0.293410 | 0.514275 | 1.054004 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 1.474724 | 1.173821 | 1.084554 | 0.500813 | 1.516810 | 1.212806 | 1.074970 | 1.491817 | 0.909125 |
| 229 | 2-hydroxybutyrate (AHB) | 0.978164 | 0.924134 | 1.223178 | 0.826119 | 0.836621 | 0.844041 | 1.039988 | 0.963358 | 0.906011 |
| 714 | 2-hydroxyglutarate | 1.006550 | 0.980514 | 1.675851 | 1.358799 | 0.423536 | 0.731857 | 0.903798 | 0.905771 | 0.942990 |
| 706 | 2-hydroxypalmitate | 0.898758 | 1.032398 | 2.810047 | 0.972744 | 1.280125 | 0.891865 | 1.796636 | 1.076808 | 0.985628 |
| 939 | 2-linoleoylglycerophosphocholine* | 0.229996 | 1.856319 | 0.855317 | 2.430508 | 0.229996 | 0.229996 | 0.229996 | 0.743047 | 1.114907 |
| 202 | 2-methylbutyroylcarnitine | 0.879397 | 0.547851 | 1.138514 | 0.723311 | 1.025134 | 0.990521 | 1.124479 | 0.883279 | 1.063017 |
| 937 | 2-oleoylglycerophosphocholine* | 0.327408 | 1.306436 | 1.338380 | 2.664556 | 0.191712 | 0.268938 | 0.565977 | 0.692410 | 1.011297 |
| 930 | 2-palmitoylglycerophosphocholine* | 0.368877 | 2.858268 | 1.790289 | 4.241271 | 0.096665 | 0.336862 | 0.531351 | 0.878770 | 1.318114 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 935 | 2-stearoylglycerophosphocholine* | 0.471137 | 1.976910 | 1.093197 | 2.881800 | 0.142354 | 0.299380 | 0.722596 | 0.957433 | 0.948414 |
| 821 | 3-dehydrocarnitine* | 1.055172 | 1.000176 | 1.250741 | 0.997144 | 0.796472 | 0.911967 | 1.030189 | 1.124612 | 1.107199 |
| 170 | 3-indoxyl sulfate | 1.420325 | 1.657545 | 1.671193 | 1.254928 | 1.206457 | 1.458274 | 1.541009 | 1.428152 | 1.320807 |
| 172 | 3-methyl-2-oxobutyrate | 0.293280 | 0.167871 | 0.244905 | 0.346274 | 1.105296 | 0.910051 | 1.327576 | 1.814206 | 1.062547 |
| 173 | 3-methyl-2-oxovalerate | 0.451490 | 0.238624 | 0.300670 | 0.236934 | 0.759330 | 1.084110 | 1.375263 | 1.448203 | 1.193437 |
| 529 | 3-phosphoglycerate | 3.402536 | 2.645908 | 1.485946 | 0.728350 | 2.176234 | 1.217779 | 1.221862 | 0.810977 | 0.737985 |
| 193 | 4-methyl-2-oxopentanoate | 0.460909 | 0.204575 | 0.327624 | 0.237775 | 0.740158 | 1.042256 | 1.272712 | 1.433275 | 1.022380 |
| 266 | 5-methylthioadenosine (MTA) | 1.044263 | 1.367122 | 1.254916 | 1.073550 | 0.289004 | 0.884631 | 0.934973 | 1.010000 | 0.990048 |
| 282 | 5-oxoproline | 0.903885 | 1.130063 | 1.852311 | 1.589864 | 0.153183 | 0.524589 | 0.911681 | 1.281875 | 1.509526 |
| 545 | 6-phosphogluconate | 1.289458 | 1.682037 | 2.413830 | 0.698603 | 2.909097 | 1.828352 | 1.409448 | 1.182087 | 0.613797 |
| 1024 | 7-beta-hydroxycholesterol | 0.908477 | 0.900005 | 1.996547 | 1.666871 | 0.733866 | 0.634096 | 1.241881 | 0.363094 | 0.549513 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 0.620291 | 1.116898 | 1.099395 | 1.044109 | 0.059289 | 0.820655 | 1.167316 | 1.585194 | 1.774989 |
| 672 | 9,10-epoxystearate | 0.817853 | 1.128281 | 1.628748 | 1.142459 | 0.019994 | 0.941708 | 1.716095 | 1.773805 | 1.952782 |
| 822 | acetylcarnitine | 1.091882 | 0.909807 | 0.964254 | 0.724809 | 0.946984 | 0.896049 | 0.929458 | 0.946289 | 0.893631 |
| 601 | acetylphosphate | 1.017109 | 0.933835 | 1.206181 | 0.875451 | 0.973251 | 1.033379 | 1.039707 | 0.884315 | 0.966967 |
| 1105 | adenine | 1.329642 | 1.071167 | 1.069334 | 0.661232 | 1.236276 | 1.089694 | 1.055918 | 1.049744 | 0.983020 |
| 1106 | adenosine | 1.758681 | 2.207580 | 2.464180 | 1.965764 | 1.074284 | 0.449049 | 1.793924 | 1.000000 | 0.958277 |
| 1116 | adenosine 5'-diphosphate (ADP) | 0.990240 | 0.624122 | 1.070870 | 0.621436 | 1.058138 | 0.944544 | 1.303938 | 1.253567 | 1.055236 |
| 1232 | adenosine 5'diphosphoribose | 1.386847 | 1.293181 | 1.343267 | 1.006366 | 0.964464 | 1.119353 | 1.176824 | 1.169441 | 1.089694 |
| 1114 | adenosine 5'-monophosphate (AMP) | 0.831653 | 0.438269 | 1.438381 | 0.813095 | 0.644259 | 0.488595 | 1.187881 | 1.406723 | 1.413759 |
| 665 | adrenate (22:4n6) | 1.927933 | 0.563093 | 0.984966 | 0.739127 | 3.200191 | 0.942035 | 1.083620 | 0.699444 | 0.414703 |
| 27 | alanine | 0.874770 | 0.865188 | 1.228132 | 0.900917 | 0.804196 | 0.921620 | 1.192023 | 1.067891 | 1.089891 |
| 1150 | allantoin | 0.712057 | 0.732183 | 1.734449 | 0.522087 | 0.654238 | 0.967530 | 0.603014 | 2.550497 | 1.724930 |
| 179 | alpha-hydroxyisocaproate | 0.591520 | 0.792749 | 1.336782 | 1.127870 | 0.292412 | 0.292412 | 0.620039 | 1.000000 | 1.270675 |
| 198 | alpha-hydroxyisovalerate | 2.172116 | 2.928365 | 4.530204 | 3.381998 | 0.682432 | 0.723870 | 1.063730 | 1.261846 | 1.557535 |
| 1266 | alpha-tocopherol | 1.030627 | 1.511835 | 2.217995 | 1.259954 | 1.665669 | 1.472035 | 1.655861 | 1.189218 | 1.212788 |
| 1034 | androsterone sulfate | 0.831395 | 0.651221 | 1.000000 | 0.931093 | 0.757549 | 0.737739 | 0.881977 | 0.651221 | 0.734964 |
| 566 | arabinose | 1.413825 | 1.258201 | 1.695844 | 1.021267 | 1.066718 | 0.859743 | 1.447614 | 0.940975 | 0.996570 |
| 546 | arabitol | 1.539209 | 1.391375 | 1.864823 | 1.393495 | 0.974765 | 0.837934 | 1.287182 | 1.001865 | 1.143131 |
| 1202 | arabonate | 1.147734 | 1.072461 | 1.897569 | 0.865369 | 1.037720 | 0.990561 | 1.404891 | 1.117087 | 1.216873 |
| 659 | arachidonate (20:4n6) | 1.078842 | 0.868424 | 1.594571 | 1.230408 | 0.575088 | 0.657857 | 0.789758 | 1.351396 | 1.234454 |
| 241 | arginine | 1.171490 | 0.944364 | 1.266545 | 1.032011 | 0.614042 | 0.726880 | 0.769043 | 1.955988 | 1.330952 |
| 25 | asparagine | 0.946659 | 0.915279 | 1.176999 | 0.845391 | 1.007246 | 0.935787 | 1.024919 | 0.829923 | 0.769433 |
| 24 | aspartate | 1.512632 | 1.584129 | 2.131539 | 1.538915 | 1.155653 | 1.341798 | 1.469940 | 1.375295 | 1.429742 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 C [ | NHSCi 2003 C [ | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 721 | azelate (nonanedioate) | 0.682096 | 1.173113 | 1.756285 | 1.817451 | 0.190083 | 0.717680 | 1.690070 | 1.879211 | 2.461886 |
| 26 | beta-alanine | 0.584413 | 0.726402 | 1.197563 | 0.933910 | 1.128265 | 1.048528 | 1.217643 | 0.504833 | 0.910647 |
| 7 | beta-hydroxypyruvate | 1.180178 | 1.086433 | 1.258438 | 0.896935 | 1.021749 | 0.976858 | 0.997250 | 1.121654 | 1.014890 |
| 22 | betaine | 0.933130 | 0.930214 | 1.009451 | 0.926170 | 0.725891 | 0.814577 | 0.820209 | 0.924074 | 0.915200 |
| 1057 | beta-sitosterol | 0.349092 | 1.164945 | 1.121738 | 0.652741 | 0.349092 | 0.716141 | 1.176649 | 0.754626 | 0.349092 |
| 1216 | biliverdin | 0.782550 | 2.307864 | 1.006988 | 2.029219 | 0.522259 | 0.657488 | 0.522259 | 0.635626 | 0.621075 |
| 811 | butyrylcarnitine | 1.203692 | 0.598389 | 1.228647 | 0.598389 | 0.956265 | 0.598389 | 0.598389 | 0.827407 | 1.000000 |
| 1612 | caffeine | 0.960238 | 0.881993 | 1.128266 | 0.882947 | 0.837952 | 0.822464 | 0.970600 | 0.997440 | 0.808305 |
| 1059 | campesterol | 0.469755 | 0.586117 | 0.906641 | 0.469755 | 0.469755 | 0.744554 | 0.469755 | 0.469755 | 1.265312 |
| 622 | caprate (10:0) | 1.087416 | 1.119543 | 1.400746 | 1.055108 | 0.476975 | 1.014052 | 1.303035 | 1.349362 | 1.262328 |
| 618 | caproate (6:0) | 1.633891 | 1.100260 | 1.165496 | 0.499007 | 1.991645 | 1.327569 | 1.130823 | 0.942546 | 1.104893 |
| 620 | caprylate (8:0) | 1.270852 | 1.623069 | 1.331362 | 0.724652 | 0.995056 | 0.821415 | 1.004944 | 1.265117 | 0.902349 |
| 820 | carnitine | 0.995475 | 0.987856 | 0.962887 | 0.897424 | 0.706026 | 0.879879 | 0.915177 | 0.936674 | 0.768970 |
| 1300 | catechol sulfate | 1.085504 | 1.060961 | 1.227196 | 1.095614 | 0.929375 | 1.004334 | 1.121036 | 1.130126 | 1.033844 |
| 164 | C-glycosyltryptophan* | 1.011477 | 0.789510 | 0.795434 | 0.963034 | 0.843278 | 1.097891 | 0.932025 | 1.096081 | 1.323800 |
| 1020 | cholesterol | 0.978604 | 1.048014 | 1.370470 | 1.082235 | 1.001777 | 0.998223 | 1.247736 | 0.993343 | 0.991372 |
| 881 | choline | 0.691654 | 0.609501 | 0.750462 | 0.608133 | 0.430366 | 0.501531 | 0.601986 | 0.633683 | 0.609711 |
| 582 | cis-aconitate | 1.056201 | 1.058446 | 1.429106 | 1.146542 | 0.581969 | 0.761887 | 1.021169 | 0.963262 | 0.734217 |
| 641 | cis-vaccenate (18:1n7) | 0.457371 | 0.457371 | 1.505220 | 1.198338 | 0.457371 | 0.457371 | 0.921005 | 1.067164 | 0.770131 |
| 579 | citrate | 1.310357 | 1.181393 | 1.364750 | 0.740486 | 1.378132 | 1.256253 | 1.341661 | 1.039516 | 0.965796 |
| 248 | citrulline | 1.207663 | 1.190028 | 1.318900 | 1.331753 | 1.000152 | 1.153451 | 1.195213 | 1.259432 | 1.224716 |
| 259 | creatine | 0.966578 | 0.942507 | 1.038412 | 0.884712 | 0.829310 | 0.879152 | 0.977144 | 0.992343 | 0.947804 |
| 260 | creatinine | 0.738254 | 1.000503 | 1.120363 | 0.989907 | 0.882203 | 0.692257 | 1.007683 | 1.008304 | 0.957200 |
| 213 | cysteine | 0.602932 | 0.935122 | 1.994629 | 1.367534 | 0.733679 | 0.953093 | 1.009224 | 1.500656 | 1.694589 |
| 819 | deoxycarnitine | 0.970031 | 1.021189 | 1.130594 | 0.852577 | 0.803635 | 0.737519 | 0.875669 | 1.129388 | 0.954943 |
| 655 | dihomo-linoleate (20:2n6) | 0.982251 | 0.835159 | 1.341311 | 0.905149 | 0.424406 | 0.557018 | 0.673731 | 0.806718 | 1.011501 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 1.187674 | 0.992377 | 1.763481 | 1.283382 | 0.724500 | 0.557375 | 1.007623 | 1.480575 | 1.276248 |
| 531 | dihydroxyacetone phosphate (DHAP) | 61.998871 | 12.050069 | 2.816575 | 1.000000 | 1.863458 | 0.244270 | 3.489914 | 0.239333 | 0.239333 |
| 3 | dimethylglycine | 0.986748 | 1.110931 | 0.961913 | 0.620077 | 0.801518 | 0.620077 | 0.881063 | 1.138150 | 1.097819 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 1.078151 | 1.029647 | 1.572826 | 1.358235 | 0.388047 | 0.691914 | 0.685331 | 1.267066 | 1.159887 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 0.761750 | 0.892547 | 1.224149 | 1.051463 | 0.319733 | 0.545656 | 0.612659 | 1.247338 | 1.233746 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 1.369553 | 1.123308 | 1.431160 | 1.424403 | 0.545071 | 0.846059 | 0.777166 | 1.513239 | 1.573361 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 T1 I | NHSCi 2003 C [ | NHSCi 2003 C I | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 1565 | ergothioneine | 0.784646 | 0.681988 | 0.930600 | 0.684874 | 0.748471 | 0.634154 | 0.838734 | 0.860915 | 0.792828 |
| 735 | erucamide | 0.412254 | 2.102473 | 0.716545 | 2.860038 | 0.908987 | 0.928090 | 1.490537 | 0.412254 | 1.267889 |
| 1632 | erythritol | 0.984345 | 1.551734 | 3.178189 | 2.935130 | 0.631139 | 0.802128 | 1.114394 | 1.307629 | 1.635783 |
| 453 | erythronate* | 1.007852 | 1.635389 | 3.495116 | 2.871585 | 0.824411 | 0.784139 | 1.217158 | 1.052277 | 1.194033 |
| 876 | ethanolamine | 0.976310 | 1.182276 | 2.139554 | 1.681976 | 0.661163 | 0.973013 | 1.535755 | 0.807254 | 1.055717 |
| 472 | fructose | 0.719437 | 0.779202 | 1.531512 | 1.329779 | 0.894561 | 0.958225 | 1.221530 | 1.144651 | 1.227204 |
| 524 | fructose-6-phosphate | 0.643762 | 1.364401 | 1.464315 | 1.058042 | 0.930426 | 0.980282 | 1.611722 | 1.461723 | 1.224940 |
| 594 | fumarate | 0.965500 | 1.061970 | 2.073842 | 0.999520 | 0.745564 | 0.651111 | 0.989373 | 1.182925 | 1.089384 |
| 404 | gamma-glutamylleucine | 1.218403 | 1.381743 | 1.188831 | 1.027585 | 0.861084 | 1.136177 | 1.043399 | 1.181348 | 0.799874 |
| 521 | glucose | 1.048812 | 1.005284 | 1.222823 | 0.929519 | 0.996624 | 0.987327 | 1.111321 | 1.014258 | 1.000439 |
| 519 | glucose-6-phosphate (G6P) | 0.140622 | 0.562362 | 1.400370 | 0.969094 | 0.837179 | 0.990735 | 1.573977 | 1.398377 | 1.309735 |
| 39 | glutamate | 0.994535 | 0.925599 | 1.150250 | 0.837136 | 1.005465 | 0.785885 | 1.022085 | 0.862060 | 0.841797 |
| 44 | glutamine | 1.062813 | 0.908735 | 0.717282 | 0.661240 | 1.201115 | 1.163193 | 0.999759 | 0.961272 | 0.854713 |
| 80 | glutaroyl carnitine | 0.561030 | 1.301558 | 1.209044 | 0.561030 | 0.561030 | 0.922433 | 0.691707 | 1.329358 | 1.087081 |
| 283 | glutathione, oxidized (GSSG) | 1.210616 | 0.898062 | 0.876079 | 0.715041 | 1.242828 | 1.251761 | 1.035441 | 0.956983 | 0.763271 |
| 280 | glutathione, reduced (GSH) | 1.103042 | 1.039986 | 0.753175 | 0.694965 | 0.895697 | 1.136946 | 1.047623 | 1.055621 | 0.942391 |
| 517 | glycerate | 1.976392 | 3.643052 | 6.423595 | 5.463784 | 0.422712 | 0.776177 | 1.414852 | 1.108956 | 1.519593 |
| 882 | glycerol 3-phosphate (G3P) | 5.540604 | 2.917526 | 1.946988 | 0.946531 | 1.103204 | 0.916270 | 1.210546 | 0.963145 | 0.971072 |
| 883 | glycerophosphorylcholine (GPC) | 0.919466 | 0.969202 | 1.144109 | 1.052735 | 1.002736 | 1.076543 | 0.981281 | 1.007094 | 1.041677 |
| 1 | glycine | 0.865601 | 0.925101 | 1.455365 | 1.246472 | 0.659939 | 0.797561 | 1.123916 | 1.310987 | 1.416995 |
| 851 | glycochenodeoxycholate | 0.352703 | 0.340697 | 0.475566 | 0.337836 | 0.397406 | 0.293892 | 0.355274 | 0.415514 | 0.334810 |
| 840 | glycocholate | 0.104984 | 0.079564 | 0.079564 | 0.132460 | 0.101017 | 0.079564 | 0.161401 | 0.094308 | 0.143415 |
| 849 | glycodeoxycholate | 0.199279 | 0.376987 | 0.516980 | 0.199279 | 0.229346 | 0.199279 | 0.199279 | 0.199279 | 0.241004 |
| 1318 | glycolate (hydroxyacetate) | 1.143183 | 0.932388 | 1.545152 | 1.094163 | 1.017811 | 1.176863 | 1.315408 | 1.107036 | 1.005904 |
| 1128 | guanosine | 1.588398 | 1.145170 | 1.507297 | 0.848515 | 0.930315 | 1.052615 | 1.188748 | 1.185284 | 1.229062 |
| 1212 | heme* | 1.148632 | 6.165361 | 1.599098 | 5.047463 | 0.287670 | 0.917822 | 0.592773 | 0.874613 | 1.271888 |
| 619 | heptanoate (7:0) | 1.422851 | 1.433715 | 1.426777 | 0.665563 | 0.963924 | 1.378515 | 1.445243 | 1.175058 | 1.431199 |
| 823 | hexanoylcarnitine | 0.951152 | 1.008683 | 1.862362 | 1.699812 | 1.812086 | 0.991317 | 0.968976 | 1.276598 | 1.563901 |
| 1288 | hippurate | 1.130380 | 1.090314 | 1.336800 | 1.034929 | 0.886504 | 1.146026 | 1.072708 | 1.272584 | 0.983966 |
| 50 | histidine | 0.891287 | 0.880880 | 1.415637 | 1.104108 | 0.877838 | 0.904200 | 0.869724 | 0.995801 | 0.929091 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 T1 I | NHSCi 2003 C [ | NHSCi 2003 C I | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 231 | homocysteine | 0.531360 | 1.113115 | 2.373456 | 1.230925 | 0.544237 | 0.958724 | 0.870555 | 1.407857 | 1.580528 |
| 1585 | homostachydrine* | 0.892755 | 1.401618 | 1.181822 | 1.244467 | 1.039424 | 1.012518 | 1.063810 | 1.017809 | 1.076011 |
| 206 | hydroxyisovaleroyl carnitine | 0.761654 | 0.751571 | 0.863157 | 0.695321 | 0.569766 | 0.671646 | 0.784426 | 0.781351 | 0.720861 |
| 1098 | hypoxanthine | 8.710523 | 8.865033 | 12.587374 | 9.000891 | 0.118663 | 0.158800 | 0.565500 | 1.116442 | 2.102075 |
| 1101 | inosine 5'-monophosphate (IMP) | 0.585711 | 1.075936 | 1.666630 | 1.269351 | 0.385234 | 0.707626 | 1.197135 | 0.697176 | 0.732847 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 8.921129 | 1.625642 | 0.865789 | 0.634155 | 0.926316 | 0.971366 | 1.139995 | 1.132752 | 1.033888 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 4.962746 | 3.550338 | 1.022636 | 0.473306 | 1.869620 | 0.901465 | 1.651282 | 1.150333 | 1.043849 |
| 496 | Isobar: sorbitol, mannitol | 1.120801 | 1.095420 | 1.038581 | 1.001462 | 0.858118 | 0.967834 | 1.012471 | 1.017625 | 0.955391 |
| 200 | isobutyrylcarnitine | 1.047961 | 0.812636 | 1.089850 | 0.787524 | 1.055922 | 0.946395 | 0.852655 | 1.035817 | 0.980266 |
| 180 | isoleucine | 1.291392 | 1.314360 | 1.440793 | 1.236554 | 0.738711 | 0.942842 | 1.006689 | 1.000134 | 1.042637 |
| 478 | isomaltose | 1.358876 | 1.035678 | 1.427767 | 0.946433 | 0.871907 | 0.708005 | 1.574571 | 1.115136 | 1.133606 |
| 205 | isovalerylcarnitine | 1.011364 | 0.951183 | 1.125490 | 0.983029 | 0.896606 | 0.932978 | 1.153700 | 1.004909 | 1.079103 |
| 144 | kynurenine | 1.231263 | 1.344747 | 1.025897 | 1.031093 | 0.916898 | 0.884145 | 0.938782 | 0.918975 | 0.974600 |
| 536 | lactate | 0.851613 | 1.299007 | 2.068926 | 1.739866 | 0.155290 | 0.509587 | 1.032656 | 1.228308 | 1.408804 |
| 1018 | lathosterol | 1.317971 | 1.082932 | 1.005054 | 1.496966 | 1.357080 | 1.039592 | 1.192467 | 0.907899 | 1.006601 |
| 625 | laurate (12:0) | 1.056739 | 1.093264 | 1.121075 | 1.007549 | 0.741906 | 0.911178 | 0.708836 | 1.100290 | 1.058791 |
| 181 | leucine | 1.126026 | 1.190173 | 1.415574 | 1.111550 | 0.697799 | 0.841679 | 0.969762 | 0.974177 | 0.995073 |
| 604 | linoleate (18:2n6) | 0.875102 | 0.833887 | 1.453063 | 0.949924 | 0.433196 | 0.499054 | 0.711618 | 1.097591 | 1.002742 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 1.027411 | 0.990711 | 1.283112 | 1.160607 | 0.398942 | 0.762193 | 0.712826 | 0.984146 | 1.224040 |
| 69 | lysine | 0.883025 | 1.166988 | 1.472896 | 1.222188 | 0.790392 | 1.019320 | 1.750394 | 0.807935 | 0.465153 |
| 598 | malate | 1.003502 | 1.280109 | 2.074823 | 1.149139 | 0.538331 | 0.655303 | 1.080320 | 0.990412 | 1.110855 |
| 482 | maltose | 1.151323 | 1.047599 | 1.505097 | 0.913686 | 1.244239 | 0.890840 | 1.121392 | 0.991229 | 1.079321 |
| 487 | mannose | 1.000892 | 0.992949 | 1.403258 | 0.957592 | 1.154808 | 1.146123 | 1.222383 | 1.070652 | 1.033415 |
| 489 | mannose-6-phosphate | 0.696962 | 1.172594 | 1.886958 | 0.885715 | 0.909050 | 1.094161 | 1.671348 | 1.544267 | 1.239800 |
| 635 | margarate (17:0) | 0.923266 | 1.135348 | 1.310010 | 0.788685 | 0.548332 | 0.700647 | 1.047673 | 1.081370 | 1.094870 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 658 | mead acid (20:3n9) | 1.333776 | 1.087334 | 1.439768 | 0.932462 | 1.099678 | 0.338017 | 1.068211 | 1.017473 | 1.586494 |
| 225 | methionine | 1.236252 | 0.929883 | 0.811302 | 0.651478 | 1.160123 | 1.180169 | 0.871566 | 0.901873 | 0.687137 |
| 890 | myo-inositol | 0.968812 | 1.005715 | 1.227931 | 0.956508 | 1.021586 | 1.003842 | 1.182792 | 0.867133 | 0.963764 |
| 629 | myristate (14:0) | 0.914252 | 1.098585 | 1.397366 | 0.918903 | 0.504823 | 0.982336 | 1.142496 | 1.422700 | 1.173415 |
| 630 | myristoleate (14:1n5) | 0.493142 | 0.801909 | 1.081880 | 0.943002 | 0.493142 | 0.493142 | 0.493142 | 1.792657 | 0.970121 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 1.383300 | 1.750319 | 1.120382 | 1.061218 | 1.342540 | 1.482435 | 0.997898 | 1.324739 | 1.150634 |
| 75 | N-6-trimethyllysine | 0.836252 | 0.728505 | 0.655402 | 0.783742 | 0.633017 | 0.957624 | 0.823612 | 0.761338 | 0.862918 |
| 4 | N-acetylglycine | 1.610581 | 1.004149 | 1.678312 | 0.949968 | 1.557341 | 1.587705 | 1.364960 | 0.896347 | 0.584292 |
| 227 | N-acetylmethionine | 0.800527 | 0.800527 | 1.080367 | 0.810114 | 0.934350 | 0.800527 | 0.892268 | 1.145774 | 1.130997 |
| 455 | N-acetylneuraminate | 1.046157 | 0.896041 | 1.939640 | 1.942435 | 0.324105 | 0.700931 | 1.405333 | 1.089991 | 1.780015 |
| 1221 | nicotinamide | 1.286544 | 0.957622 | 1.061303 | 1.181597 | 0.875045 | 0.869904 | 1.194063 | 1.526762 | 1.075616 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 1.731941 | 0.997915 | 0.985197 | 0.742747 | 0.722391 | 1.078624 | 0.856726 | 1.029014 | 0.637361 |
| 825 | octanoylcarnitine | 0.783359 | 0.894006 | 1.209520 | 1.028082 | 0.599376 | 0.842428 | 0.880027 | 1.146807 | 1.000816 |
| 639 | oleate (18:1n9) | 0.973637 | 1.482457 | 1.323943 | 0.994752 | 1.219680 | 0.938441 | 1.162406 | 0.979411 | 0.847502 |
| 835 | oleoylcarnitine | 0.268949 | 2.834940 | 1.297484 | 4.715415 | 0.093963 | 0.269900 | 0.344264 | 0.505751 | 0.840201 |
| 285 | ophthalmate | 1.000000 | 0.357655 | 0.252181 | 0.252181 | 1.508191 | 0.421720 | 0.252181 | 0.252181 | 0.252181 |
| 244 | ornithine | 0.979060 | 1.057577 | 1.502068 | 1.109598 | 1.019818 | 1.069739 | 1.261234 | 0.891207 | 0.993771 |
| 632 | palmitate (16:0) | 0.888735 | 1.072139 | 1.569051 | 0.951411 | 0.651755 | 0.773816 | 1.043567 | 1.081979 | 1.063466 |
| 633 | palmitoleate (16:1n7) | 1.026919 | 1.052117 | 2.047386 | 0.979584 | 0.439121 | 0.832635 | 0.728747 | 1.156837 | 1.320546 |
| 1004 | palmitoyl sphingomyelin | 1.005813 | 1.022249 | 1.443170 | 0.999408 | 1.002119 | 0.922277 | 1.278155 | 0.994232 | 1.032554 |
| 833 | palmitoylcarnitine | 0.373139 | 2.170117 | 1.108468 | 4.325253 | 0.059115 | 0.263145 | 0.394131 | 0.597176 | 0.935597 |
| 1243 | pantothenate | 1.002883 | 1.042906 | 1.313703 | 1.255659 | 0.981934 | 0.822225 | 1.198455 | 1.123216 | 1.117671 |
| 1613 | paraxanthine | 1.092740 | 1.281806 | 1.135697 | 1.108726 | 0.775678 | 1.172639 | 1.077312 | 1.018185 | 1.005584 |
| 88 | p-cresol sulfate | 1.329539 | 1.356562 | 1.700649 | 1.269245 | 1.238055 | 1.227651 | 1.449294 | 1.401530 | 1.285396 |
| 621 | pelargonate (9:0) | 1.511461 | 1.540620 | 1.473003 | 0.888205 | 0.696694 | 1.152892 | 1.285336 | 1.031785 | 1.115217 |
| 631 | pentadecanoate (15:0) | 0.955568 | 1.016540 | 1.401995 | 0.890441 | 0.614889 | 0.987654 | 0.988003 | 1.234391 | 0.996066 |
| 135 | phenol sulfate | 1.054251 | 1.118233 | 1.165138 | 1.010064 | 0.952208 | 0.941851 | 1.171854 | 1.335752 | 0.989869 |
| 128 | phenylacetylglutamine | 1.578694 | 1.452507 | 1.623517 | 1.225483 | 1.160408 | 1.250494 | 1.445612 | 1.491337 | 1.335129 |
| 83 | phenylalanine | 1.162565 | 1.148260 | 1.187508 | 1.160993 | 0.751191 | 0.987472 | 1.048000 | 1.127775 | 1.134973 |
| 602 | phosphate | 0.727684 | 0.751826 | 1.234300 | 1.003948 | 0.933507 | 0.996052 | 1.373690 | 1.201725 | 1.200027 |
| 534 | phosphoenolpyruvate (PEP) | 3.894760 | 2.959487 | 2.072928 | 0.821136 | 3.050557 | 2.009289 | 0.720522 | 0.580553 | 0.392959 |
| 877 | phosphoethanolamine | 0.593700 | 0.593700 | 0.996335 | 0.593700 | 0.593700 | 0.831274 | 1.633338 | 0.593700 | 0.819262 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 74 | pipecolate | 1.069883 | 1.134205 | 0.977444 | 1.002204 | 1.013801 | 1.188600 | 1.075593 | 1.137417 | 1.042642 |
| 1531 | piperine | 0.960533 | 0.742917 | 1.179921 | 0.853887 | 1.249044 | 0.728075 | 0.763679 | 0.914611 | 0.966844 |
| 246 | proline | 0.933815 | 0.900005 | 1.248685 | 0.994499 | 0.834910 | 0.829551 | 1.035551 | 1.018197 | 1.014322 |
| 809 | propionylcarnitine | 0.821648 | 0.622675 | 0.778856 | 0.487806 | 0.797352 | 0.723017 | 0.822425 | 0.808531 | 0.730360 |
| 1181 | pseudouridine | 0.788985 | 1.126088 | 1.638792 | 1.000323 | 0.998180 | 0.868874 | 1.197681 | 1.779715 | 1.219948 |
| 45 | pyroglutamine* | 0.597374 | 0.350441 | 0.661227 | 0.699686 | 0.650159 | 0.422165 | 0.651579 | 0.517207 | 0.542282 |
| 603 | pyrophosphate (PPi) | 0.717524 | 0.878915 | 1.009637 | 0.394905 | 1.914621 | 1.822755 | 0.565763 | 0.186096 | 0.385259 |
| 535 | pyruvate | 0.102391 | 0.131934 | 2.234781 | 3.365902 | 1.475749 | 1.639510 | 2.224493 | 0.984990 | 0.820186 |
| 1469 | ranitidine | 1.026638 | 1.000000 | 1.315141 | 0.918342 | 0.929226 | 0.811072 | 1.130570 | 1.097961 | 1.032377 |
| 548 | ribitol | 4.495617 | 5.122583 | 7.448713 | 5.634157 | 0.953701 | 0.705272 | 1.225451 | 0.958717 | 1.127218 |
| 557 | ribose 5-phosphate | 2.712544 | 2.466099 | 1.739737 | 0.865699 | 1.578994 | 1.289816 | 1.277638 | 0.854524 | 1.058120 |
| 559 | ribulose | 3.518619 | 1.756845 | 1.714623 | 0.951284 | 0.240496 | 0.967002 | 0.586343 | 0.838888 | 0.736292 |
| 224 | S-adenosylhomocysteine (SAH) | 0.981614 | 0.874326 | 1.103269 | 0.971546 | 0.549981 | 0.935056 | 1.133643 | 1.321041 | 1.220628 |
| 551 | sedoheptulose-7-phosphate | 0.074096 | 0.074096 | 0.370648 | 1.117716 | 0.288959 | 2.351756 | 0.606188 | 1.196406 | 1.451772 |
| 8 | serine | 0.961262 | 1.021881 | 1.433833 | 1.111375 | 0.827123 | 0.873389 | 1.064693 | 0.967975 | 1.012033 |
| 216 | S-methylcysteine | 1.347967 | 2.027787 | 2.625465 | 1.746811 | 1.542209 | 2.067163 | 2.179524 | 1.810258 | 1.631400 |
| 281 | S-methylglutathione | 1.435206 | 1.234675 | 1.095895 | 0.686720 | 0.964557 | 1.032169 | 1.035304 | 1.032800 | 0.975118 |
| 270 | spermidine | 0.728213 | 0.792122 | 0.977184 | 0.791319 | 0.603725 | 0.745592 | 0.874977 | 1.000993 | 0.999007 |
| 1584 | stachydrine | 0.126761 | 0.113742 | 0.140217 | 0.083990 | 0.110678 | 0.107599 | 0.113977 | 0.160798 | 0.113338 |
| 637 | stearate (18:0) | 1.001200 | 1.113420 | 1.518442 | 0.897809 | 0.614115 | 0.762619 | 1.106370 | 1.094080 | 1.019197 |
| 1005 | stearoyl sphingomyelin | 1.107782 | 1.183502 | 1.470237 | 1.026462 | 1.096071 | 1.059961 | 1.281980 | 1.109648 | 1.155776 |
| 834 | stearoylcarnitine | 0.236361 | 2.549162 | 1.139666 | 4.371011 | 0.101169 | 0.193408 | 0.319916 | 0.412648 | 0.892457 |
| 591 | succinylcarnitine | 0.739038 | 0.699879 | 0.962272 | 0.780915 | 0.640083 | 0.605184 | 0.760776 | 0.870464 | 0.832856 |
| 1662 | terephthalic acid | 0.733730 | 0.795418 | 0.987941 | 0.609384 | 0.814955 | 0.782714 | 0.729966 | 0.751060 | 0.689335 |
| 1614 | theobromine | 1.092207 | 0.995990 | 1.355886 | 0.974437 | 1.222130 | 0.997137 | 1.226037 | 1.301636 | 1.482369 |
| 1615 | theophylline | 1.055476 | 2.037853 | 0.963742 | 0.882810 | 0.593850 | 0.883607 | 1.658663 | 1.290417 | 1.158929 |
| 549 | threitol | 1.227774 | 1.396417 | 2.318889 | 1.486356 | 0.916646 | 1.098222 | 1.454849 | 1.242685 | 1.368344 |
| 1199 | threonate | 1.153959 | 1.073193 | 1.627627 | 1.204023 | 1.030629 | 0.881667 | 1.165691 | 0.998396 | 0.996490 |
| 17 | threonine | 0.918846 | 1.151981 | 1.078225 | 0.891232 | 0.831370 | 0.772558 | 0.850172 | 1.006377 | 0.958014 |
| 252 | trans-4-hydroxyproline | 1.301346 | 1.467660 | 1.254497 | 1.338684 | 1.079311 | 1.322353 | 1.232542 | 1.259168 | 1.324749 |

| | | DARM-00007 | DARM-00008 | DARM-00009 | DARM-00010 | DARM-00011 | DARM-00012 | DARM-00013 | DARM-00014 | DARM-00015 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCi 2003 T1 | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 T1 [ | NHSCi 2003 C [ | NHSCi 2003 C [ | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | 997730 | 997747 | 997713 | 997751 | 997716 | 997752 | 997719 | 997724 | 997729 |
| | | 991352 | 991353 | 991354 | 991355 | 991356 | 991357 | 991358 | 991359 | 991360 |
| | | NHSCi 2003 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 T1 | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C | NHSCi 2003 C |
| | | T1 D7 | D14 | D21 | D28 | D0 | D7 | D14 | D21 | D28 |
| | | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 | 2003 |
| | | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 164.122 | 167.3 | 157.075 | 174.895 | 193.847 | 179.605 | 175.15 | 167.535 | 175.121 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D7 | T1 D14 | T1 D21 | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 501 | trehalose | 0.362640 | 0.987376 | 1.609654 | 1.426670 | 0.113570 | 0.650401 | 1.428155 | 1.125481 | 1.280808 |
| 1242 | trigonelline (N'-methylnicotinate) | 0.715801 | 0.684877 | 0.871114 | 0.585378 | 0.623422 | 0.601493 | 0.693382 | 0.760873 | 0.678253 |
| 145 | tryptophan | 1.078077 | 1.083771 | 1.113171 | 1.070096 | 0.751759 | 0.916593 | 1.010252 | 1.026334 | 1.038789 |
| 151 | tryptophan betaine | 0.563749 | 0.508787 | 0.669942 | 0.503194 | 0.458304 | 0.486344 | 0.559234 | 0.590852 | 0.539042 |
| 99 | tyrosine | 1.001827 | 0.996271 | 0.970865 | 1.064605 | 0.657797 | 0.878995 | 0.919015 | 0.983225 | 0.905808 |
| 1149 | urate | 1.150613 | 0.785304 | 1.132320 | 0.774115 | 0.972108 | 0.898797 | 1.127136 | 1.048037 | 0.910508 |
| 245 | urea | 1.137894 | 1.121389 | 1.516343 | 1.104584 | 1.008742 | 1.027302 | 1.164212 | 1.078467 | 1.153603 |
| 1180 | uridine | 1.008468 | 1.022501 | 1.072821 | 1.092326 | 0.489820 | 0.676550 | 0.646663 | 0.778744 | 0.613988 |
| 190 | valine | 1.015633 | 1.036547 | 1.072693 | 1.005024 | 0.742738 | 0.884658 | 0.936333 | 0.999074 | 0.988365 |
| 565 | xylitol | 1.000000 | 1.100450 | 0.551869 | 0.230551 | 0.127693 | 0.127693 | 0.127693 | 0.127693 | 0.127693 |
| 570 | xylonate | 0.895473 | 1.304235 | 2.210136 | 1.450331 | 0.462607 | 0.657234 | 1.393716 | 1.403347 | 1.195373 |
| 569 | xylose | 0.912174 | 2.319280 | 5.113885 | 3.642480 | 0.628684 | 0.539617 | 0.992577 | 0.902007 | 0.765536 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 905 | 1,2-propanediol | 0.501077 | 1.008225 | 1.193957 | 1.193501 | 1.938786 | 0.508979 | 1.258147 | 0.991775 | 1.268883 |
| 532 | 1,3-dihydroxyacetone | 0.899202 | 1.177730 | 1.244416 | 0.772604 | 1.132467 | 1.168994 | 0.769801 | 1.005678 | 0.959741 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 0.844037 | 1.254906 | 1.004858 | 0.901235 | 0.948845 | 0.907074 | 0.946739 | 0.816629 | 1.175666 |
| 523 | 1,6-anhydroglucose | 1.025619 | 0.956088 | 0.889175 | 0.841386 | 0.962219 | 0.994738 | 1.588749 | 1.606576 | 0.933949 |
| 636 | 10-heptadecenoate (17:1n7) | 0.637262 | 0.970133 | 0.985518 | 1.052469 | 1.538224 | 0.700381 | 1.071490 | 1.082156 | 1.334958 |
| 742 | 13-methylmyristic acid | 0.455073 | 0.815653 | 0.948027 | 0.819492 | 1.621920 | 0.647528 | 0.845897 | 1.066714 | 1.169079 |
| 744 | 15-methylpalmitate (isobar with 2- | 0.597510 | 0.982369 | 1.163702 | 1.024727 | 1.957059 | 0.494582 | 0.861680 | 0.925836 | 1.158560 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 2.419082 | 1.048455 | 0.967015 | 1.023348 | 0.989288 | 0.857216 | 0.782681 | 0.764023 | 0.773242 |
| 938 | 1-linoleoylglycerophosphocholine | 1.855847 | 1.000051 | 0.925648 | 0.931377 | 1.376081 | 0.907058 | 1.006436 | 0.978712 | 0.997585 |
| 926 | 1-myristoylglycerophosphocholine | 0.416175 | 0.988348 | 1.054465 | 0.783463 | 1.151580 | 0.416175 | 1.294287 | 1.441688 | 2.835265 |
| 936 | 1-oleoylglycerophosphocholine | 0.381280 | 1.226697 | 0.980908 | 0.692886 | 2.067848 | 0.266163 | 3.892917 | 3.278638 | 7.683218 |
| 915 | 1-oleoylglycerophosphoethanolamine | 2.621518 | 1.928930 | 0.606206 | 0.805842 | 1.208158 | 0.848328 | 0.546344 | 0.935000 | 0.575729 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 1.023991 | 0.450335 | 0.871233 | 1.022293 | 1.758619 | 0.539628 | 1.299680 | 1.191308 | 1.132647 |
| 929 | 1-palmitoylglycerophosphocholine | 0.361715 | 1.085191 | 0.914809 | 0.696891 | 1.936666 | 0.261963 | 2.979872 | 2.547329 | 4.767351 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 2.224498 | 0.890349 | 0.728149 | 0.739888 | 1.302269 | 0.696349 | 0.859563 | 0.611085 | 0.921061 |
| 934 | 1-stearoylglycerophosphocholine | 0.294113 | 0.988165 | 1.048981 | 1.015904 | 1.690865 | 0.204017 | 2.633812 | 2.394982 | 5.054173 |
| 533 | 2,3-diphosphoglycerate | 3.131756 | 0.966633 | 0.162678 | 0.029859 | 0.029859 | 3.760561 | 4.571819 | 3.055307 | 1.204192 |
| 263 | 2-aminobutyrate | 1.037938 | 1.366085 | 1.276321 | 1.163623 | 1.284605 | 1.086646 | 1.141614 | 1.205569 | 1.178580 |
| 945 | 2-arachidonoylglycerophosphocholine* | 0.204822 | 1.041897 | 1.193644 | 0.911195 | 1.284297 | 0.475697 | 2.489087 | 2.367750 | 4.398900 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 0.248766 | 1.297378 | 1.546375 | 1.140669 | 1.590801 | 0.305701 | 2.801008 | 2.664413 | 4.042665 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 0.366251 | 0.948162 | 1.428324 | 0.924428 | 1.196317 | 0.388730 | 2.868841 | 2.755786 | 4.333425 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 0.236388 | 0.951478 | 1.058894 | 1.157643 | 1.488061 | 0.391367 | 2.983034 | 2.469585 | 4.308172 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 1.241506 | 1.141880 | 0.916301 | 0.710488 | 0.796478 | 0.596475 | 1.130952 | 0.557898 | 0.649441 |
| 229 | 2-hydroxybutyrate (AHB) | 0.963573 | 1.203928 | 1.215463 | 1.044740 | 1.116515 | 1.139958 | 1.171647 | 1.132603 | 1.105859 |
| 714 | 2-hydroxyglutarate | 0.865141 | 1.095801 | 1.443789 | 1.285344 | 2.250042 | 0.686172 | 2.522823 | 2.434008 | 2.650167 |
| 706 | 2-hydroxypalmitate | 1.536941 | 0.870774 | 0.930895 | 0.739916 | 1.158822 | 0.703316 | 1.003106 | 0.996894 | 1.211751 |
| 939 | 2-linoleoylglycerophosphocholine* | 0.229996 | 0.994754 | 0.832122 | 0.822841 | 0.734574 | 0.229996 | 1.696925 | 1.813504 | 3.067099 |
| 202 | 2-methylbutyroylcarnitine | 1.369594 | 1.050483 | 1.001283 | 0.888389 | 1.170955 | 1.005300 | 0.998717 | 0.710477 | 0.831663 |
| 937 | 2-oleoylglycerophosphocholine* | 0.511220 | 1.142690 | 1.000000 | 0.592969 | 1.064918 | 0.446642 | 2.370144 | 1.870782 | 3.969860 |
| 930 | 2-palmitoylglycerophosphocholine* | 0.353213 | 1.039430 | 1.174607 | 1.057279 | 1.514626 | 0.129147 | 2.300603 | 2.070896 | 4.057640 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 935 | 2-stearoylglycerophosphocholine* | 0.142354 | 1.010002 | 0.770604 | 1.000000 | 1.235202 | 0.142354 | 1.503402 | 1.398572 | 3.314417 |
| 821 | 3-dehydrocarnitine* | 0.999833 | 1.072591 | 1.049253 | 0.873041 | 1.188172 | 0.875033 | 1.054565 | 1.000167 | 0.926485 |
| 170 | 3-indoxyl sulfate | 0.627934 | 0.793543 | 0.590916 | 0.630024 | 0.759052 | 0.451256 | 0.569663 | 0.460182 | 0.750213 |
| 172 | 3-methyl-2-oxobutyrate | 1.340545 | 1.640315 | 1.435467 | 1.000000 | 0.980369 | 0.682175 | 0.167871 | 0.167871 | 0.239328 |
| 173 | 3-methyl-2-oxovalerate | 0.873059 | 1.139579 | 1.089805 | 1.017484 | 1.142921 | 0.840581 | 0.563238 | 0.323670 | 0.318889 |
| 529 | 3-phosphoglycerate | 1.238096 | 1.178441 | 0.514662 | 0.310980 | 0.370603 | 3.110964 | 1.987114 | 1.584618 | 0.649989 |
| 193 | 4-methyl-2-oxopentanoate | 1.008235 | 1.345157 | 1.321313 | 0.956152 | 0.993652 | 0.850549 | 0.437402 | 0.239005 | 0.299811 |
| 266 | 5-methylthioadenosine (MTA) | 0.372898 | 0.996410 | 1.157961 | 1.049878 | 0.959408 | 0.451807 | 1.213418 | 1.311506 | 1.104804 |
| 282 | 5-oxoproline | 0.191970 | 0.667539 | 1.022036 | 1.143684 | 1.980196 | 0.200106 | 0.775595 | 1.205515 | 1.344583 |
| 545 | 6-phosphogluconate | 0.644416 | 1.235349 | 0.565711 | 0.467849 | 0.841428 | 0.875263 | 0.723658 | 1.115971 | 0.467849 |
| 1024 | 7-beta-hydroxycholesterol | 1.569456 | 0.476216 | 1.047089 | 0.363094 | 1.138381 | 1.318148 | 0.925294 | 1.004491 | 0.672304 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 0.048331 | 0.802532 | 1.027817 | 1.145545 | 1.713407 | 0.111045 | 0.854273 | 1.105050 | 1.152606 |
| 672 | 9,10-epoxystearate | 0.033463 | 0.809321 | 1.028911 | 1.006787 | 1.547654 | 0.037295 | 0.833233 | 1.227107 | 1.230720 |
| 822 | acetylcarnitine | 1.277266 | 1.241471 | 1.139287 | 0.923100 | 1.099697 | 1.062935 | 1.229760 | 1.029721 | 0.999643 |
| 601 | acetylphosphate | 0.990894 | 1.219679 | 1.245058 | 0.936207 | 1.064480 | 0.978169 | 1.080920 | 1.013816 | 1.010781 |
| 1105 | adenine | 1.206089 | 0.925700 | 0.570488 | 0.358702 | 0.327902 | 1.103432 | 1.211731 | 0.973460 | 0.761106 |
| 1106 | adenosine | 0.744577 | 0.753606 | 0.666923 | 0.982457 | 1.320279 | 0.672741 | 1.458001 | 1.480518 | 1.305395 |
| 1116 | adenosine 5'-diphosphate (ADP) | 1.290323 | 1.033594 | 1.003406 | 0.792081 | 0.989024 | 0.877849 | 0.836119 | 0.722971 | 0.518700 |
| 1232 | adenosine 5'diphosphoribose | 0.881198 | 1.041143 | 0.942067 | 0.721731 | 0.727361 | 0.884578 | 1.174893 | 0.958287 | 0.777991 |
| 1114 | adenosine 5'-monophosphate (AMP) | 0.999976 | 1.000024 | 1.039602 | 1.036467 | 1.855358 | 0.636202 | 0.876975 | 0.658025 | 0.832007 |
| 665 | adrenate (22:4n6) | 1.314933 | 1.583554 | 0.741561 | 1.612064 | 1.808242 | 3.301831 | 0.570350 | 0.930507 | 1.460123 |
| 27 | alanine | 0.925090 | 1.241298 | 1.268784 | 1.069091 | 1.291588 | 0.863901 | 0.980929 | 0.900353 | 0.935163 |
| 1150 | allantoin | 2.172045 | 0.634390 | 0.708213 | 1.222934 | 1.518035 | 0.554513 | 1.000000 | 0.421193 | 1.093115 |
| 179 | alpha-hydroxyisocaproate | 0.292412 | 0.292412 | 0.736097 | 0.903338 | 1.543100 | 0.292412 | 1.047084 | 1.661864 | 1.235539 |
| 198 | alpha-hydroxyisovalerate | 0.603512 | 0.605749 | 0.724186 | 1.033939 | 1.838540 | 0.962598 | 2.580216 | 2.735497 | 2.628104 |
| 1266 | alpha-tocopherol | 0.878454 | 0.925404 | 0.797936 | 0.745309 | 0.803727 | 0.829351 | 0.726907 | 0.645369 | 0.589830 |
| 1034 | androsterone sulfate | 1.375482 | 1.128043 | 1.233316 | 1.069587 | 1.439223 | 1.169557 | 1.403166 | 0.802192 | 1.043725 |
| 566 | arabinose | 0.961928 | 1.006028 | 1.133260 | 0.805106 | 1.072359 | 1.003430 | 1.236761 | 0.852454 | 1.009708 |
| 546 | arabitol | 0.957407 | 0.981489 | 0.854802 | 0.942624 | 1.021827 | 0.809730 | 1.389543 | 1.469408 | 1.373357 |
| 1202 | arabonate | 0.713833 | 1.138744 | 0.917448 | 0.725064 | 1.108036 | 0.862560 | 1.091336 | 0.779331 | 0.721375 |
| 659 | arachidonate (20:4n6) | 0.567370 | 0.749888 | 0.915883 | 1.100946 | 1.845425 | 0.501375 | 0.837303 | 0.868220 | 1.270383 |
| 241 | arginine | 0.419416 | 1.012233 | 0.782343 | 0.781781 | 2.459407 | 0.726401 | 0.987767 | 1.098019 | 1.395338 |
| 25 | asparagine | 1.289194 | 1.350922 | 1.235291 | 0.963008 | 0.885318 | 1.316032 | 1.458511 | 1.100523 | 1.013047 |
| 24 | aspartate | 0.482904 | 0.605235 | 0.664009 | 0.701156 | 0.700856 | 0.901982 | 0.998569 | 0.973182 | 0.880816 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 721 | azelate (nonanedioate) | 0.210289 | 0.662763 | 0.926046 | 1.242125 | 1.738198 | 0.194245 | 0.627354 | 0.838250 | 1.131933 |
| 26 | beta-alanine | 1.800861 | 1.724048 | 2.102594 | 1.327686 | 0.620389 | 1.560572 | 1.641957 | 1.528781 | 1.218936 |
| 7 | beta-hydroxypyruvate | 0.554623 | 1.170740 | 1.065125 | 0.774761 | 1.085895 | 0.851838 | 0.948759 | 0.896470 | 0.672498 |
| 22 | betaine | 1.075655 | 1.201195 | 1.172755 | 0.990549 | 1.182740 | 1.077367 | 1.233125 | 1.200922 | 1.185297 |
| 1057 | beta-sitosterol | 1.378020 | 0.349092 | 0.349092 | 0.991994 | 1.072504 | 1.008006 | 1.095494 | 1.311701 | 1.145349 |
| 1216 | biliverdin | 0.798077 | 0.878080 | 1.794687 | 1.530214 | 1.488774 | 0.526687 | 2.688201 | 2.179164 | 3.642624 |
| 811 | butyrylcarnitine | 0.598389 | 0.958778 | 2.157606 | 0.813252 | 0.871551 | 1.646579 | 1.020169 | 0.598389 | 1.573956 |
| 1612 | caffeine | 1.263467 | 1.205485 | 1.133723 | 1.028486 | 1.065448 | 0.977868 | 1.113836 | 1.089265 | 1.113483 |
| 1059 | campesterol | 0.995934 | 1.087392 | 1.360507 | 0.878240 | 0.469755 | 0.469755 | 0.965511 | 0.932175 | 1.862319 |
| 622 | caprate (10:0) | 0.573585 | 1.046230 | 1.306931 | 0.964397 | 1.267035 | 0.562548 | 0.956619 | 0.989396 | 0.686388 |
| 618 | caproate (6:0) | 1.377155 | 1.529443 | 0.818669 | 0.740630 | 1.057454 | 0.842092 | 1.192223 | 0.436990 | 0.449683 |
| 620 | caprylate (8:0) | 0.632103 | 1.192723 | 1.199343 | 1.473919 | 1.580141 | 0.549565 | 1.849478 | 0.555594 | 1.076247 |
| 820 | carnitine | 1.005071 | 1.243940 | 1.211781 | 0.990124 | 1.252389 | 1.120270 | 1.232238 | 1.269324 | 1.234114 |
| 1300 | catechol sulfate | 0.971109 | 1.042230 | 0.964121 | 0.825281 | 1.012566 | 0.963242 | 1.081185 | 0.957620 | 0.955499 |
| 164 | C-glycosyltryptophan* | 0.964929 | 0.988524 | 1.505223 | 1.076518 | 0.960933 | 0.909000 | 0.903513 | 1.108958 | 1.177757 |
| 1020 | cholesterol | 0.921397 | 1.080995 | 1.136624 | 0.915988 | 1.055749 | 1.021002 | 1.074846 | 0.969248 | 0.933694 |
| 881 | choline | 1.430515 | 1.578485 | 1.370786 | 1.249538 | 1.513476 | 1.427234 | 1.572337 | 1.549981 | 1.470633 |
| 582 | cis-aconitate | 0.723186 | 1.005069 | 1.011291 | 0.909410 | 1.206941 | 0.596630 | 0.994931 | 1.025652 | 1.052424 |
| 641 | cis-vaccenate (18:1n7) | 0.494205 | 1.107788 | 0.457371 | 0.888823 | 0.680862 | 0.824207 | 1.910968 | 0.572285 | 1.190650 |
| 579 | citrate | 0.988956 | 0.973393 | 0.830051 | 0.659026 | 0.670119 | 1.049642 | 1.022152 | 0.712683 | 0.530010 |
| 248 | citrulline | 0.732821 | 0.941961 | 0.786135 | 0.851455 | 0.864658 | 0.802859 | 0.796177 | 0.861970 | 0.857194 |
| 259 | creatine | 1.072934 | 1.166761 | 1.122958 | 0.937071 | 1.135091 | 1.006465 | 1.162302 | 1.106957 | 1.105684 |
| 260 | creatinine | 1.061977 | 1.069059 | 1.025679 | 1.003797 | 1.119094 | 1.022388 | 1.004359 | 1.124995 | 1.052232 |
| 213 | cysteine | 0.470891 | 0.760858 | 1.162170 | 1.491504 | 1.826819 | 0.560433 | 0.521496 | 0.771319 | 1.150021 |
| 819 | deoxycarnitine | 1.094273 | 1.133404 | 1.290251 | 0.893564 | 1.142238 | 0.921844 | 1.122176 | 1.074504 | 1.038118 |
| 655 | dihomo-linoleate (20:2n6) | 0.793124 | 0.988499 | 1.097323 | 1.094015 | 1.870038 | 0.669063 | 1.178471 | 1.411081 | 1.522516 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 0.727908 | 0.798627 | 0.794714 | 0.970348 | 1.443343 | 0.614837 | 0.822653 | 0.945218 | 1.180436 |
| 531 | dihydroxyacetone phosphate (DHAP) | 0.239333 | 0.599793 | 0.239333 | 0.488592 | 0.239333 | 26.246931 | 58.469345 | 11.158892 | 0.239333 |
| 3 | dimethylglycine | 0.688915 | 0.979446 | 1.006086 | 1.513394 | 1.500375 | 0.945475 | 0.888860 | 1.069698 | 0.663023 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 0.443525 | 0.704866 | 1.067516 | 1.027216 | 1.493019 | 0.424190 | 0.972784 | 0.888162 | 1.129717 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 0.412333 | 0.748287 | 1.004777 | 0.999515 | 1.705677 | 0.429058 | 0.799325 | 1.033177 | 1.303055 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 0.321751 | 0.775957 | 0.821262 | 0.908357 | 1.204325 | 0.830439 | 0.845855 | 0.986530 | 1.124767 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 1565 | ergothioneine | 1.452924 | 1.344576 | 1.275889 | 1.069400 | 1.472451 | 1.073396 | 1.291689 | 1.193013 | 1.203446 |
| 735 | erucamide | 3.581430 | 0.412254 | 1.034310 | 1.012411 | 0.771882 | 3.075173 | 1.418402 | 0.954475 | 0.987589 |
| 1632 | erythritol | 0.519126 | 0.792453 | 0.939086 | 0.934951 | 1.221505 | 0.579283 | 1.018653 | 1.407544 | 1.829268 |
| 453 | erythronate* | 0.734372 | 0.917399 | 1.190023 | 0.992148 | 1.384581 | 0.722092 | 1.283408 | 2.038252 | 2.906687 |
| 876 | ethanolamine | 0.904855 | 1.058362 | 1.575824 | 1.160173 | 0.766092 | 0.641429 | 1.070066 | 1.023690 | 0.864240 |
| 472 | fructose | 0.832862 | 1.063905 | 1.090366 | 0.985075 | 1.071791 | 0.808681 | 0.655052 | 0.655034 | 1.014925 |
| 524 | fructose-6-phosphate | 0.842078 | 1.023060 | 0.985739 | 0.610627 | 1.175219 | 0.397472 | 0.989227 | 1.233759 | 0.560529 |
| 594 | fumarate | 0.781422 | 0.947119 | 1.000480 | 0.953925 | 1.715840 | 0.714969 | 1.442458 | 1.524422 | 1.598409 |
| 404 | gamma-glutamylleucine | 1.121323 | 0.725333 | 0.888391 | 0.715255 | 0.671972 | 1.195749 | 1.446832 | 1.080715 | 1.144540 |
| 521 | glucose | 0.966351 | 1.089534 | 1.062043 | 0.860784 | 1.077872 | 1.001462 | 1.073071 | 0.920134 | 0.881752 |
| 519 | glucose-6-phosphate (G6P) | 0.840416 | 1.253397 | 0.936403 | 0.624125 | 1.266786 | 0.232264 | 0.169608 | 0.822482 | 1.058154 |
| 39 | glutamate | 1.199616 | 1.270962 | 1.300098 | 1.005913 | 1.373271 | 1.304027 | 1.469782 | 1.084066 | 0.904710 |
| 44 | glutamine | 1.337271 | 1.179785 | 1.064176 | 0.833892 | 0.794066 | 1.329939 | 1.055028 | 0.793461 | 0.702357 |
| 80 | glutaroyl carnitine | 0.978552 | 1.283623 | 1.034547 | 1.086314 | 1.088812 | 0.798038 | 0.790916 | 0.794879 | 0.820006 |
| 283 | glutathione, oxidized (GSSG) | 1.282356 | 1.172061 | 0.939052 | 0.697792 | 0.846550 | 1.488466 | 1.107346 | 0.891155 | 0.712402 |
| 280 | glutathione, reduced (GSH) | 1.042456 | 0.972324 | 1.127807 | 0.880631 | 0.889339 | 1.072550 | 0.854247 | 1.037525 | 0.990698 |
| 517 | glycerate | 0.363275 | 0.725053 | 0.847936 | 1.003772 | 1.214712 | 0.541739 | 4.288396 | 7.798664 | 8.984795 |
| 882 | glycerol 3-phosphate (G3P) | 1.223840 | 1.023186 | 0.963402 | 0.922959 | 0.970310 | 2.362033 | 3.554280 | 1.810766 | 0.819903 |
| 883 | glycerophosphorylcholine (GPC) | 0.950387 | 1.026028 | 0.960271 | 0.829710 | 0.952660 | 0.988479 | 1.021603 | 1.069304 | 1.057175 |
| 1 | glycine | 0.559408 | 0.959904 | 1.154372 | 1.129173 | 1.751983 | 0.641308 | 0.835534 | 0.828598 | 0.970613 |
| 851 | glycochenodeoxycholate | 3.078268 | 2.166819 | 1.868720 | 1.863959 | 1.998294 | 1.908885 | 2.313250 | 2.062409 | 1.884735 |
| 840 | glycocholate | 1.218197 | 1.110704 | 1.093944 | 1.050813 | 1.312518 | 1.059299 | 1.222289 | 1.061226 | 1.039295 |
| 849 | glycodeoxycholate | 1.281072 | 1.250581 | 1.126701 | 1.183213 | 1.347040 | 0.803958 | 1.031556 | 1.320247 | 1.045791 |
| 1318 | glycolate (hydroxyacetate) | 0.782613 | 1.124610 | 1.104063 | 0.793728 | 0.883599 | 0.873721 | 0.956965 | 0.912868 | 0.848197 |
| 1128 | guanosine | 1.100134 | 1.140500 | 0.903265 | 0.453745 | 0.799816 | 0.863872 | 1.001799 | 0.986811 | 0.998201 |
| 1212 | heme* | 0.687347 | 1.852198 | 2.188751 | 1.072830 | 1.085982 | 1.021296 | 4.959563 | 2.869865 | 5.726540 |
| 619 | heptanoate (7:0) | 0.879660 | 1.467036 | 1.036075 | 1.074240 | 1.385410 | 0.485282 | 1.212419 | 0.426742 | 0.502048 |
| 823 | hexanoylcarnitine | 1.201647 | 0.853883 | 0.819349 | 0.629854 | 1.173287 | 0.870142 | 1.149399 | 0.684310 | 0.856738 |
| 1288 | hippurate | 1.017897 | 0.977590 | 0.943760 | 0.783767 | 0.945345 | 0.854317 | 1.058393 | 0.987116 | 0.970774 |
| 50 | histidine | 1.141519 | 1.147005 | 1.077978 | 0.874496 | 0.985874 | 1.113876 | 1.042943 | 1.004199 | 1.327249 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 I | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 I |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 231 | homocysteine | 0.283300 | 0.475163 | 1.007745 | 1.122871 | 1.114777 | 0.408054 | 0.583348 | 1.610877 | 1.466120 |
| 1585 | homostachydrine* | 0.895599 | 0.913906 | 0.880724 | 0.910255 | 0.671347 | 0.987482 | 0.689098 | 0.792906 | 0.878708 |
| 206 | hydroxyisovaleroyl carnitine | 1.555557 | 1.475419 | 1.338186 | 1.257551 | 1.352897 | 1.136843 | 1.420923 | 1.271762 | 1.239892 |
| 1098 | hypoxanthine | 0.067233 | 0.073749 | 0.376762 | 1.185439 | 2.880014 | 0.078254 | 5.826920 | 5.161455 | 4.634178 |
| 1101 | inosine 5'-monophosphate (IMP) | 0.569606 | 1.262374 | 1.856280 | 1.307858 | 1.828663 | 0.679147 | 0.892558 | 1.424407 | 2.152652 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 1.011434 | 1.150256 | 0.918173 | 0.689814 | 0.842561 | 2.681738 | 8.546598 | 1.371044 | 0.528261 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 0.882393 | 1.017659 | 0.898523 | 0.590153 | 1.049265 | 4.434954 | 6.085914 | 2.878977 | 0.472048 |
| 496 | Isobar: sorbitol, mannitol | 0.983165 | 1.086215 | 0.998538 | 0.908520 | 1.046699 | 1.088187 | 1.105944 | 1.119317 | 1.096617 |
| 200 | isobutyrylcarnitine | 1.285879 | 1.298824 | 1.079126 | 0.912776 | 1.081439 | 1.094675 | 1.065939 | 0.983286 | 0.978169 |
| 180 | isoleucine | 0.904508 | 1.100839 | 1.040173 | 0.921140 | 1.129414 | 0.892762 | 1.307340 | 1.307142 | 1.216562 |
| 478 | isomaltose | 0.786380 | 1.470613 | 1.112872 | 0.903280 | 1.001079 | 1.957774 | 1.071817 | 0.792280 | 0.876707 |
| 205 | isovalerylcarnitine | 1.004065 | 1.102286 | 0.906413 | 0.836451 | 1.000485 | 0.947076 | 1.107538 | 1.012280 | 0.945728 |
| 144 | kynurenine | 0.912488 | 1.340235 | 0.954535 | 1.068438 | 0.991351 | 1.296000 | 1.232886 | 1.155386 | 1.008649 |
| 536 | lactate | 0.219858 | 0.713728 | 0.979672 | 0.987821 | 1.318691 | 0.314322 | 1.010858 | 1.297025 | 1.546916 |
| 1018 | lathosterol | 0.489776 | 0.629410 | 0.658497 | 0.592428 | 0.489776 | 0.489776 | 0.489776 | 0.608806 | 0.696326 |
| 625 | laurate (12:0) | 0.727765 | 0.893438 | 0.973073 | 0.883826 | 1.136358 | 0.847900 | 1.112136 | 1.135608 | 0.914981 |
| 181 | leucine | 0.932373 | 1.154303 | 1.126427 | 0.983899 | 1.282916 | 0.846578 | 1.295956 | 1.243840 | 1.225019 |
| 604 | linoleate (18:2n6) | 0.740226 | 0.943546 | 1.047389 | 1.056420 | 1.532676 | 0.650377 | 1.235684 | 1.224176 | 1.457363 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 0.514370 | 0.992250 | 1.010648 | 0.902997 | 1.476587 | 0.810550 | 1.197361 | 1.016417 | 1.293051 |
| 69 | lysine | 1.071880 | 1.216980 | 1.212152 | 0.945992 | 0.959892 | 1.093781 | 1.223889 | 1.173469 | 1.016303 |
| 598 | malate | 0.719036 | 1.045822 | 0.996498 | 0.974779 | 1.516162 | 0.587334 | 1.575855 | 1.668774 | 1.756515 |
| 482 | maltose | 0.828407 | 1.022714 | 1.042451 | 0.797524 | 0.920378 | 0.974123 | 1.019700 | 0.894867 | 0.951805 |
| 487 | mannose | 0.963028 | 1.086009 | 1.088833 | 0.852053 | 0.964234 | 1.056535 | 0.984285 | 0.854840 | 0.843114 |
| 489 | mannose-6-phosphate | 0.857830 | 0.961492 | 0.918527 | 0.645243 | 1.041229 | 0.446117 | 1.264991 | 1.171008 | 1.030862 |
| 635 | margarate (17:0) | 0.751814 | 0.979277 | 1.057576 | 0.978154 | 1.787250 | 0.646236 | 1.032539 | 0.932111 | 1.116143 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 658 | mead acid (20:3n9) | 1.023907 | 0.846368 | 0.429630 | 1.190257 | 0.598479 | 0.379121 | 0.684029 | 0.967622 | 0.849523 |
| 225 | methionine | 1.484732 | 1.556007 | 1.093167 | 0.767968 | 0.785262 | 1.482286 | 1.429376 | 1.110052 | 0.844176 |
| 890 | myo-inositol | 1.072864 | 1.183885 | 1.243195 | 1.018537 | 0.993139 | 1.270321 | 1.270127 | 1.000742 | 0.907486 |
| 629 | myristate (14:0) | 0.632412 | 0.997450 | 1.040445 | 1.061978 | 1.389486 | 0.521104 | 1.087679 | 0.943317 | 0.982699 |
| 630 | myristoleate (14:1n5) | 0.743900 | 0.493142 | 1.060393 | 1.029879 | 1.508858 | 0.639250 | 1.075540 | 1.430668 | 0.493142 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 0.650682 | 0.609814 | 0.677527 | 0.989965 | 0.738252 | 1.031610 | 0.579258 | 0.536434 | 0.725869 |
| 75 | N-6-trimethyllysine | 1.368356 | 1.410117 | 1.042377 | 1.165226 | 1.206613 | 1.455469 | 1.235048 | 1.103404 | 1.239353 |
| 4 | N-acetylglycine | 0.703126 | 1.015153 | 1.076402 | 0.584292 | 0.995851 | 0.943287 | 0.830171 | 0.820991 | 0.584292 |
| 227 | N-acetylmethionine | 1.574492 | 0.950742 | 0.800527 | 1.350351 | 1.256783 | 0.843524 | 1.421345 | 0.800527 | 1.185046 |
| 455 | N-acetylneuraminate | 0.497311 | 1.056485 | 1.021391 | 0.940026 | 1.107883 | 0.371034 | 1.073767 | 0.725931 | 1.412426 |
| 1221 | nicotinamide | 0.814811 | 1.011838 | 0.898458 | 0.765642 | 1.170664 | 0.795070 | 1.157654 | 0.970815 | 1.156090 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 0.956705 | 1.272578 | 2.370546 | 1.934508 | 1.123941 | 2.371158 | 2.876988 | 0.880158 | 0.742219 |
| 825 | octanoylcarnitine | 1.213300 | 1.314767 | 1.210047 | 1.106624 | 1.139082 | 0.836387 | 1.070222 | 1.119745 | 1.260096 |
| 639 | oleate (18:1n9) | 0.986547 | 1.005248 | 1.308166 | 1.188103 | 1.170810 | 1.211565 | 1.315366 | 1.203807 | 1.278957 |
| 835 | oleoylcarnitine | 0.489242 | 1.528689 | 2.466769 | 1.901271 | 2.201156 | 0.438430 | 4.465172 | 4.405629 | 10.564249 |
| 285 | ophthalmate | 3.551742 | 1.265355 | 0.442083 | 0.317707 | 0.252181 | 4.305184 | 1.997412 | 1.021023 | 0.470232 |
| 244 | ornithine | 0.939261 | 1.143336 | 1.192263 | 0.931368 | 0.814906 | 0.869352 | 1.104434 | 1.057265 | 0.910761 |
| 632 | palmitate (16:0) | 0.913437 | 0.969764 | 1.017147 | 0.903961 | 1.471748 | 0.676940 | 1.002933 | 0.999613 | 1.101544 |
| 633 | palmitoleate (16:1n7) | 0.513091 | 0.815732 | 0.793765 | 1.124851 | 1.185019 | 0.732571 | 1.036071 | 1.231488 | 1.073138 |
| 1004 | palmitoyl sphingomyelin | 0.961134 | 1.115795 | 1.186349 | 0.929576 | 1.078754 | 0.898686 | 1.139961 | 1.000592 | 0.874015 |
| 833 | palmitoylcarnitine | 0.478760 | 1.196707 | 1.940597 | 1.450066 | 1.780151 | 0.407763 | 3.175823 | 2.972802 | 6.705207 |
| 1243 | pantothenate | 0.945577 | 1.082141 | 1.026898 | 0.997117 | 1.059047 | 0.979483 | 1.114799 | 1.046370 | 0.905345 |
| 1613 | paraxanthine | 0.758178 | 1.100879 | 1.023721 | 0.871267 | 0.959727 | 0.842121 | 1.043439 | 0.994415 | 0.898474 |
| 88 | p-cresol sulfate | 0.759756 | 0.817534 | 0.774604 | 0.710700 | 0.748159 | 0.667677 | 0.813802 | 0.675227 | 0.695812 |
| 621 | pelargonate (9:0) | 0.583328 | 1.344405 | 1.071773 | 1.040874 | 1.402575 | 0.410839 | 1.092199 | 0.658950 | 0.603910 |
| 631 | pentadecanoate (15:0) | 0.739352 | 0.956042 | 1.038052 | 0.947417 | 1.428828 | 0.765198 | 1.088934 | 0.967923 | 1.196280 |
| 135 | phenol sulfate | 0.974653 | 1.009513 | 0.907712 | 0.795517 | 0.979679 | 0.963932 | 1.153787 | 0.951593 | 0.898472 |
| 128 | phenylacetylglutamine | 0.695259 | 0.726709 | 0.755868 | 0.584470 | 0.839592 | 0.707988 | 0.761715 | 0.664343 | 0.735338 |
| 83 | phenylalanine | 0.727383 | 1.011808 | 0.990709 | 0.871037 | 1.030560 | 0.744195 | 1.023801 | 1.009952 | 0.959216 |
| 602 | phosphate | 0.892017 | 1.168188 | 1.181990 | 1.011836 | 1.172479 | 0.768304 | 0.703605 | 0.610242 | 0.773958 |
| 534 | phosphoenolpyruvate (PEP) | 2.126739 | 1.031623 | 0.291297 | 0.193772 | 0.155305 | 4.071632 | 2.866429 | 1.887392 | 0.647512 |
| 877 | phosphoethanolamine | 0.923308 | 1.072515 | 1.405192 | 1.003665 | 1.173373 | 1.634368 | 0.815893 | 1.129493 | 0.868065 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 74 | pipecolate | 0.795467 | 1.110439 | 0.866838 | 0.747487 | 1.142169 | 0.935262 | 1.097380 | 0.972062 | 1.037049 |
| 1531 | piperine | 1.794483 | 1.780262 | 1.038199 | 1.033156 | 0.917698 | 1.041107 | 1.759989 | 1.271048 | 1.495063 |
| 246 | proline | 1.013856 | 1.046929 | 0.983892 | 0.909081 | 1.180662 | 0.879096 | 1.020036 | 1.005501 | 1.005694 |
| 809 | propionylcarnitine | 1.652190 | 1.517885 | 1.303306 | 1.078465 | 1.254020 | 1.376766 | 1.343697 | 1.097893 | 1.001871 |
| 1181 | pseudouridine | 0.918881 | 1.108099 | 0.880978 | 0.734292 | 1.010960 | 0.570276 | 0.967920 | 1.152684 | 0.804972 |
| 45 | pyroglutamine* | 1.505178 | 1.739141 | 1.525632 | 1.340829 | 1.820351 | 1.569546 | 1.742140 | 1.800413 | 1.531138 |
| 603 | pyrophosphate (PPi) | 1.619585 | 2.014208 | 0.944148 | 0.725752 | 0.421184 | 2.803005 | 1.259798 | 1.055006 | 0.657354 |
| 535 | pyruvate | 2.169760 | 2.358569 | 1.015010 | 0.542479 | 0.747050 | 0.065020 | 0.039915 | 0.108379 | 2.064760 |
| 1469 | ranitidine | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 |
| 548 | ribitol | 0.746264 | 1.290269 | 0.602225 | 0.875069 | 1.077702 | 0.777809 | 4.827632 | 6.291121 | 5.674953 |
| 557 | ribose 5-phosphate | 0.941880 | 0.887955 | 0.857664 | 0.877680 | 0.767096 | 2.235521 | 3.494890 | 1.843313 | 0.662457 |
| 559 | ribulose | 1.233137 | 0.777685 | 0.776057 | 0.705694 | 1.603587 | 1.000000 | 6.182086 | 4.766923 | 1.423436 |
| 224 | S-adenosylhomocysteine (SAH) | 0.670923 | 1.173121 | 0.990527 | 0.908534 | 1.327612 | 0.585667 | 1.009473 | 1.159935 | 0.868522 |
| 551 | sedoheptulose-7-phosphate | 0.312007 | 1.297012 | 1.479980 | 0.603954 | 1.226593 | 0.074096 | 0.093846 | 0.074096 | 0.594090 |
| 8 | serine | 0.961744 | 1.266789 | 1.218023 | 1.025300 | 1.216261 | 0.987967 | 1.253440 | 1.178263 | 1.160987 |
| 216 | S-methylcysteine | 0.562773 | 0.607159 | 0.428310 | 0.887603 | 0.734662 | 0.539099 | 0.677550 | 0.470051 | 0.581260 |
| 281 | S-methylglutathione | 0.690237 | 1.587726 | 0.966433 | 0.923935 | 0.742056 | 0.810818 | 1.399870 | 1.538145 | 0.995664 |
| 270 | spermidine | 1.062502 | 1.289947 | 1.218212 | 1.044024 | 1.280570 | 0.922495 | 1.182150 | 1.071928 | 1.063963 |
| 1584 | stachydrine | 2.095102 | 2.330842 | 2.110076 | 1.839202 | 2.319102 | 1.922350 | 2.249901 | 2.111208 | 2.184161 |
| 637 | stearate (18:0) | 0.843957 | 1.055444 | 1.084165 | 0.975553 | 1.556442 | 0.642299 | 1.004454 | 0.976885 | 1.077237 |
| 1005 | stearoyl sphingomyelin | 0.865486 | 0.911076 | 1.080005 | 0.786180 | 0.917909 | 0.922069 | 1.172109 | 0.914078 | 0.903442 |
| 834 | stearoylcarnitine | 0.406720 | 1.136923 | 2.020013 | 1.656963 | 1.843958 | 0.310522 | 3.205297 | 2.808168 | 6.886410 |
| 591 | succinylcarnitine | 1.183375 | 1.337074 | 1.301392 | 1.084051 | 1.445426 | 1.037728 | 1.223270 | 1.260462 | 1.322879 |
| 1662 | terephthalic acid | 1.182466 | 1.144063 | 1.345530 | 1.147011 | 1.371383 | 1.214571 | 1.404467 | 1.103014 | 1.189349 |
| 1614 | theobromine | 0.686930 | 0.607131 | 1.420081 | 0.695816 | 1.002863 | 0.642601 | 0.744874 | 0.658977 | 0.784564 |
| 1615 | theophylline | 0.857493 | 0.841441 | 0.852026 | 1.044626 | 1.110884 | 0.661419 | 0.868306 | 0.828888 | 0.440691 |
| 549 | threitol | 0.605065 | 0.800077 | 0.887474 | 0.757795 | 0.899228 | 0.740354 | 1.046007 | 1.065307 | 1.030688 |
| 1199 | threonate | 0.884623 | 1.056487 | 1.001604 | 0.909616 | 1.062214 | 0.921414 | 0.909397 | 1.018455 | 1.052177 |
| 17 | threonine | 0.993623 | 1.330512 | 1.399478 | 1.081520 | 1.268171 | 1.056761 | 1.242720 | 1.244335 | 1.182913 |
| 252 | trans-4-hydroxyproline | 0.814001 | 0.774311 | 0.829652 | 0.849252 | 0.805627 | 0.572124 | 0.905691 | 0.920689 | 0.768722 |

| | | DARM-00016 | DARM-00017 | DARM-00018 | DARM-00019 | DARM-00020 | DARM-00021 | DARM-00022 | DARM-00023 | DARM-00024 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T2 D | NHSCI 1866 T1 | NHSCI 1866 T1 | NHSCI 1866 T1 D | NHSCI 1866 T1 D |
| | | 997715 | 997736 | 997748 | 997740 | 997720 | 997746 | 997738 | 997739 | 997737 |
| | | 991361 | 991362 | 991363 | 991364 | 991365 | 991366 | 991367 | 991368 | 991369 |
| | | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 T2 | NHSCI 1866 | NHSCI 1866 | NHSCI 1866 T1 | NHSCI 1866 T1 |
| | | T2 D0 | T2 D7 | D14 | D21 | D28 | T1 D0 | T1 D7 | D14 | D21 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| | | 176.276 | 164.34 | 172.339 | 203.125 | 169.237 | 179.08 | 165.545 | 173.574 | 171.422 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T2 D0 | T2 D7 | T2 D14 | T2 D21 | T2 D28 | T1 D0 | T1 D7 | T1 D14 | T1 D21 |
| 501 | trehalose | 0.201019 | 0.850848 | 1.406976 | 1.468295 | 1.387215 | 0.238892 | 0.629188 | 0.817213 | 1.234079 |
| 1242 | trigonelline (N'-methylnicotinate) | 1.272694 | 1.372181 | 1.291222 | 1.128886 | 1.249649 | 1.237602 | 1.396669 | 1.306094 | 1.279538 |
| 145 | tryptophan | 0.817334 | 1.095493 | 1.015031 | 0.924403 | 0.989748 | 0.804220 | 1.055440 | 1.011476 | 0.975269 |
| 151 | tryptophan betaine | 1.603943 | 1.661904 | 1.530906 | 1.330058 | 1.623229 | 1.330451 | 1.600966 | 1.481023 | 1.493108 |
| 99 | tyrosine | 0.968936 | 1.194225 | 1.180995 | 1.056896 | 1.208565 | 0.998173 | 1.229578 | 1.191890 | 1.152029 |
| 1149 | urate | 1.265110 | 1.161604 | 0.988206 | 0.854142 | 1.073201 | 1.089558 | 1.119075 | 0.882419 | 0.904778 |
| 245 | urea | 0.800316 | 1.026784 | 0.987892 | 0.812787 | 0.956288 | 0.823694 | 0.991944 | 0.845993 | 0.855559 |
| 1180 | uridine | 0.831653 | 0.991532 | 1.096638 | 1.024148 | 1.473673 | 0.814876 | 1.395201 | 1.248259 | 1.136566 |
| 190 | valine | 0.972327 | 1.166725 | 1.181283 | 0.977507 | 1.158445 | 0.943391 | 1.185855 | 1.083818 | 1.099776 |
| 565 | xylitol | 0.127693 | 0.127693 | 0.127693 | 0.176147 | 0.127693 | 0.127693 | 3.035000 | 3.016489 | 1.694447 |
| 570 | xylonate | 0.859141 | 0.700778 | 1.047475 | 0.881897 | 0.844633 | 0.663354 | 1.184012 | 1.286874 | 1.494055 |
| 569 | xylose | 0.405368 | 1.222699 | 0.857077 | 0.405368 | 1.423885 | 0.779886 | 1.196334 | 2.876936 | 3.427724 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 905 | 1,2-propanediol | 1.962303 | 0.563461 | 0.773673 | 1.188689 | 1.091823 | 1.385370 |
| 532 | 1,3-dihydroxyacetone | 0.936173 | 0.879981 | 0.749898 | 0.994428 | 0.706877 | 1.082746 |
| 515 | 1,5-anhydroglucitol (1,5-AG) | 1.009787 | 1.012087 | 0.746767 | 0.869682 | 0.821318 | 0.777494 |
| 523 | 1,6-anhydroglucose | 1.364420 | 1.297502 | 0.891604 | 0.915285 | 0.763173 | 0.988839 |
| 636 | 10-heptadecenoate (17:1n7) | 1.403745 | 0.828227 | 1.043206 | 1.049363 | 1.261397 | 0.927437 |
| 742 | 13-methylmyristic acid | 1.530483 | 0.603959 | 1.018858 | 1.136946 | 1.039832 | 0.979638 |
| 744 | 15-methylpalmitate (isobar with 2- | 1.495298 | 0.533960 | 0.933209 | 0.938384 | 1.364927 | 1.003488 |
| 919 | 1-arachidonoylglycerophosphoethanolamine* | 0.818711 | 1.309575 | 1.237829 | 1.010712 | 1.061398 | 0.783981 |
| 938 | 1-linoleoylglycerophosphocholine | 1.056072 | 0.968415 | 1.238837 | 1.016508 | 1.211700 | 0.809547 |
| 926 | 1-myristoylglycerophosphocholine | 0.936136 | 0.416175 | 0.416175 | 0.923876 | 0.678494 | 3.272995 |
| 936 | 1-oleoylglycerophosphocholine | 1.791263 | 0.077483 | 0.290619 | 0.924987 | 1.459732 | 5.534157 |
| 915 | 1-oleoylglycerophosphoethanolamine | 1.366971 | 1.344172 | 1.065000 | 0.798952 | 1.261417 | 0.814458 |
| 970 | 1-palmitoylglycerol (1-monopalmitin) | 0.861226 | 0.719199 | 0.876449 | 1.356011 | 1.035025 | 1.231294 |
| 929 | 1-palmitoylglycerophosphocholine | 1.718517 | 0.043437 | 0.315703 | 0.885723 | 1.491287 | 3.485666 |
| 909 | 1-palmitoylglycerophosphoethanolamine | 0.561704 | 0.957055 | 0.992772 | 1.007228 | 0.741135 | 0.624214 |
| 934 | 1-stearoylglycerophosphocholine | 1.557930 | 0.038298 | 0.255335 | 0.766923 | 1.059703 | 4.757974 |
| 533 | 2,3-diphosphoglycerate | 0.260365 | 2.813990 | 1.000000 | 0.192421 | 0.036846 | 0.034709 |
| 263 | 2-aminobutyrate | 1.440552 | 1.146852 | 1.057026 | 1.246625 | 0.998962 | 1.096195 |
| 945 | 2-arachidonoylglycerophosphocholine* | 1.000000 | 0.185345 | 0.301695 | 0.661601 | 0.866965 | 3.947168 |
| 920 | 2-arachidonoylglycerophosphoethanolamine* | 1.490698 | 0.067699 | 0.312859 | 0.887969 | 1.189819 | 3.367121 |
| 923 | 2-docosahexaenoylglycerophosphoethanolamine* | 1.305922 | 0.136031 | 0.529947 | 1.146430 | 1.051838 | 3.821691 |
| 922 | 2-docosapentaenoylglycerophosphoethanolamine* | 1.294222 | 0.089145 | 0.328395 | 1.000000 | 1.111352 | 3.272113 |
| 1360 | 2-ethylhexanoate (isobar with 2-propylpentanoate) | 0.580689 | 0.854823 | 1.005285 | 0.956193 | 0.542068 | 0.568130 |
| 229 | 2-hydroxybutyrate (AHB) | 1.160729 | 1.040493 | 1.021836 | 1.108594 | 0.868716 | 1.077310 |
| 714 | 2-hydroxyglutarate | 3.238803 | 0.844283 | 0.759518 | 1.171081 | 1.299516 | 1.817171 |
| 706 | 2-hydroxypalmitate | 1.355718 | 0.759887 | 1.030246 | 0.884788 | 1.132533 | 0.823016 |
| 939 | 2-linoleoylglycerophosphocholine* | 1.221832 | 0.229996 | 0.528060 | 0.694372 | 1.005246 | 3.306186 |
| 202 | 2-methylbutyroylcarnitine | 0.994122 | 1.280913 | 1.280844 | 1.029904 | 1.430659 | 0.715979 |
| 937 | 2-oleoylglycerophosphocholine* | 1.015496 | 0.191712 | 0.351808 | 0.683406 | 0.837879 | 3.361709 |
| 930 | 2-palmitoylglycerophosphocholine* | 1.189122 | 0.108070 | 0.343618 | 0.804478 | 0.960570 | 4.302079 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 935 | 2-stearoylglycerophosphocholine* | 1.071904 | 0.142354 | 0.142354 | 0.503256 | 0.579957 | 3.726528 |
| 821 | 3-dehydrocarnitine* | 1.112274 | 0.902835 | 0.999223 | 0.985691 | 0.960373 | 0.956818 |
| 170 | 3-indoxyl sulfate | 0.666928 | 0.604031 | 0.615128 | 0.532224 | 0.389686 | 0.720274 |
| 172 | 3-methyl-2-oxobutyrate | 0.167871 | 1.492745 | 1.369522 | 1.331473 | 0.963997 | 0.869145 |
| 173 | 3-methyl-2-oxovalerate | 0.486341 | 0.996945 | 1.003055 | 1.166572 | 1.063349 | 0.910344 |
| 529 | 3-phosphoglycerate | 0.647234 | 1.177113 | 0.882247 | 0.807327 | 0.436468 | 0.391823 |
| 193 | 4-methyl-2-oxopentanoate | 0.449847 | 1.070740 | 1.090726 | 1.196609 | 0.894189 | 0.765792 |
| 266 | 5-methylthioadenosine (MTA) | 1.135995 | 0.433355 | 0.631642 | 1.003590 | 0.854859 | 0.941843 |
| 282 | 5-oxoproline | 1.600759 | 0.187985 | 0.602352 | 0.977964 | 1.194557 | 1.410001 |
| 545 | 6-phosphogluconate | 0.487973 | 1.565474 | 0.794300 | 0.467849 | 0.467849 | 0.467849 |
| 1024 | 7-beta-hydroxycholesterol | 0.866651 | 0.666341 | 0.728016 | 1.146114 | 0.995509 | 0.459523 |
| 712.5 | 9,10-epoxyoctadec-12(Z)-enoic acid | 1.720280 | 0.097580 | 0.679865 | 0.867279 | 1.228049 | 1.272163 |
| 672 | 9,10-epoxystearate | 1.820843 | 0.057486 | 0.753563 | 0.940167 | 1.264035 | 1.214890 |
| 822 | acetylcarnitine | 1.080696 | 1.169595 | 1.123487 | 1.071160 | 1.080324 | 1.000358 |
| 601 | acetylphosphate | 1.118297 | 0.885714 | 0.898878 | 1.057195 | 0.821014 | 0.939531 |
| 1105 | adenine | 0.538223 | 1.228781 | 1.016980 | 0.744226 | 0.637906 | 0.576433 |
| 1106 | adenosine | 1.484763 | 1.519858 | 0.977006 | 0.997186 | 1.758229 | 0.934218 |
| 1116 | adenosine 5'-diphosphate (ADP) | 0.561842 | 1.144367 | 1.183384 | 1.041595 | 0.821974 | 0.580406 |
| 1232 | adenosine 5'diphosphoribose | 0.708303 | 0.862716 | 0.900600 | 0.803150 | 0.797305 | 0.643408 |
| 1114 | adenosine 5'-monophosphate (AMP) | 1.416475 | 0.782735 | 1.014159 | 1.210037 | 1.393270 | 1.260668 |
| 665 | adrenate (22:4n6) | 1.653082 | 0.472529 | 0.964801 | 0.866192 | 1.015034 | 1.199391 |
| 27 | alanine | 1.205319 | 0.999386 | 1.011664 | 1.222115 | 0.967846 | 1.076178 |
| 1150 | allantoin | 1.338042 | 1.943129 | 0.966256 | 0.421193 | 0.614564 | 0.949476 |
| 179 | alpha-hydroxyisocaproate | 1.767613 | 0.292412 | 0.292412 | 0.497329 | 0.810051 | 1.156211 |
| 198 | alpha-hydroxyisovalerate | 3.656355 | 0.558210 | 0.529065 | 0.758533 | 0.929130 | 1.172533 |
| 1266 | alpha-tocopherol | 1.013168 | 0.904921 | 0.692161 | 0.981713 | 0.568316 | 0.646692 |
| 1034 | androsterone sulfate | 1.383558 | 0.854975 | 1.245888 | 1.097636 | 1.010608 | 1.409117 |
| 566 | arabinose | 1.238260 | 0.836238 | 0.991687 | 0.973576 | 0.760419 | 0.742416 |
| 546 | arabitol | 1.807193 | 0.971075 | 0.772679 | 0.834015 | 0.734172 | 0.998135 |
| 1202 | arabonate | 0.825139 | 0.639898 | 1.012679 | 0.964548 | 0.658951 | 0.999669 |
| 659 | arachidonate (20:4n6) | 2.044924 | 0.846104 | 0.978080 | 1.005465 | 1.371726 | 1.095372 |
| 241 | arginine | 1.696769 | 0.576222 | 1.317440 | 1.745899 | 1.514322 | 0.569095 |
| 25 | asparagine | 1.289376 | 1.143792 | 0.995290 | 1.119770 | 0.782254 | 1.004710 |
| 24 | aspartate | 0.830984 | 0.667982 | 0.474023 | 0.627891 | 0.587960 | 0.753229 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 721 | azelate (nonanedioate) | 1.838439 | 0.145765 | 0.453006 | 0.814958 | 1.152765 | 1.340694 |
| 26 | beta-alanine | 1.923831 | 1.530797 | 0.767572 | 0.839805 | 0.717139 | 1.777530 |
| 7 | beta-hydroxypyruvate | 1.016385 | 1.021221 | 0.827159 | 1.119480 | 0.499616 | 0.767661 |
| 22 | betaine | 1.333675 | 1.118360 | 1.082670 | 1.161894 | 1.093691 | 1.098355 |
| 1057 | beta-sitosterol | 1.139472 | 0.686697 | 1.093839 | 1.275950 | 0.861017 | 0.741912 |
| 1216 | biliverdin | 1.070354 | 0.565964 | 0.741221 | 0.522259 | 1.000000 | 1.436399 |
| 811 | butyrylcarnitine | 0.841708 | 0.952815 | 1.455763 | 0.598389 | 1.058027 | 1.090460 |
| 1612 | caffeine | 1.196775 | 1.125601 | 1.108164 | 1.014405 | 1.000686 | 1.007368 |
| 1059 | campesterol | 1.872022 | 1.052831 | 0.725153 | 1.483716 | 1.394295 | 1.055198 |
| 622 | caprate (10:0) | 1.007579 | 0.532248 | 0.757435 | 1.097380 | 0.830727 | 0.736372 |
| 618 | caproate (6:0) | 0.462978 | 0.836562 | 0.844482 | 0.588986 | 0.537642 | 0.495527 |
| 620 | caprylate (8:0) | 0.760430 | 0.765345 | 0.888824 | 1.284749 | 0.905589 | 0.791654 |
| 820 | carnitine | 1.334424 | 1.089571 | 1.004525 | 1.132457 | 1.009443 | 1.127019 |
| 1300 | catechol sulfate | 1.037193 | 0.960727 | 0.968757 | 0.912922 | 0.931018 | 0.871487 |
| 164 | C-glycosyltryptophan* | 1.073840 | 1.083510 | 1.135640 | 1.101687 | 1.063441 | 1.089226 |
| 1020 | cholesterol | 1.155205 | 0.970677 | 0.898323 | 1.093240 | 0.794897 | 0.919676 |
| 881 | choline | 1.642235 | 1.430865 | 1.401498 | 1.467480 | 1.407785 | 1.347892 |
| 582 | cis-aconitate | 1.152070 | 0.682573 | 0.846721 | 0.908149 | 0.917629 | 0.814284 |
| 641 | cis-vaccenate (18:1n7) | 2.198575 | 1.211049 | 1.057250 | 0.986304 | 0.990184 | 1.301888 |
| 579 | citrate | 0.481910 | 1.038135 | 0.818767 | 0.805495 | 0.588418 | 0.503089 |
| 248 | citrulline | 0.999848 | 0.734952 | 0.696646 | 0.838719 | 0.752438 | 0.817569 |
| 259 | creatine | 1.221663 | 1.046839 | 1.065430 | 1.044015 | 1.031773 | 1.020537 |
| 260 | creatinine | 1.293007 | 1.043565 | 0.737654 | 0.820706 | 0.999497 | 0.998604 |
| 213 | cysteine | 1.407057 | 0.543762 | 0.749065 | 1.340087 | 1.105029 | 1.471856 |
| 819 | deoxycarnitine | 1.208492 | 1.025422 | 1.039724 | 1.022425 | 0.978811 | 0.943533 |
| 655 | dihomo-linoleate (20:2n6) | 1.946395 | 0.837818 | 1.410214 | 1.217187 | 1.747208 | 1.218597 |
| 609 | dihomo-linolenate (20:3n3 or n6) | 1.732804 | 0.894730 | 0.966922 | 1.041964 | 1.290825 | 0.828665 |
| 531 | dihydroxyacetone phosphate (DHAP) | 0.239333 | 0.507248 | 0.511241 | 0.239333 | 0.239333 | 0.337648 |
| 3 | dimethylglycine | 1.406961 | 1.287437 | 1.597749 | 1.231047 | 1.062675 | 1.477251 |
| 613 | docosahexaenoate (DHA; 22:6n3) | 1.558157 | 0.699621 | 0.968683 | 0.936022 | 1.329143 | 0.871083 |
| 611 | docosapentaenoate (n3 DPA; 22:5n3) | 1.829772 | 0.598146 | 1.089808 | 1.069857 | 1.579700 | 1.256369 |
| 610 | eicosapentaenoate (EPA; 20:5n3) | 1.318244 | 0.846667 | 0.794184 | 0.856813 | 1.031976 | 1.013470 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 1565 | ergothioneine | 1.386868 | 1.331635 | 1.263646 | 1.209918 | 1.218306 | 1.096833 |
| 735 | erucamide | 0.412254 | 2.048367 | 0.864038 | 1.366639 | 0.412254 | 1.679250 |
| 1632 | erythritol | 2.824399 | 0.565976 | 0.617972 | 0.946709 | 0.833464 | 1.015656 |
| 453 | erythronate* | 3.332240 | 0.811976 | 0.813199 | 0.965586 | 0.962365 | 1.306343 |
| 876 | ethanolamine | 1.369070 | 0.730151 | 0.515675 | 0.723090 | 0.566198 | 1.485089 |
| 472 | fructose | 1.499154 | 0.831481 | 0.887200 | 1.069168 | 0.904015 | 1.068746 |
| 524 | fructose-6-phosphate | 0.910504 | 1.110631 | 1.081938 | 1.276781 | 0.973879 | 0.908795 |
| 594 | fumarate | 1.659439 | 1.003627 | 1.230403 | 1.366010 | 1.243402 | 1.153230 |
| 404 | gamma-glutamylleucine | 0.671972 | 0.972415 | 0.861748 | 0.671972 | 0.941181 | 0.723008 |
| 521 | glucose | 1.073864 | 1.062467 | 0.963776 | 1.020154 | 0.865520 | 0.903436 |
| 519 | glucose-6-phosphate (G6P) | 1.078075 | 1.016150 | 1.054900 | 1.179862 | 1.009265 | 1.039973 |
| 39 | glutamate | 1.172528 | 1.135226 | 1.018940 | 1.149158 | 0.864379 | 0.955808 |
| 44 | glutamine | 0.708525 | 1.373010 | 1.189218 | 0.964980 | 0.821338 | 0.798523 |
| 80 | glutaroyl carnitine | 0.814561 | 1.073446 | 0.899838 | 1.049391 | 1.000000 | 1.261064 |
| 283 | glutathione, oxidized (GSSG) | 0.694916 | 1.302133 | 1.094876 | 0.887813 | 0.783689 | 1.011041 |
| 280 | glutathione, reduced (GSH) | 0.980108 | 1.150578 | 0.778673 | 1.077067 | 0.898670 | 0.864791 |
| 517 | glycerate | 11.667626 | 0.405735 | 0.793935 | 0.996228 | 1.143282 | 1.410938 |
| 882 | glycerol 3-phosphate (G3P) | 0.976814 | 1.240466 | 1.087626 | 1.075427 | 0.859943 | 0.605443 |
| 883 | glycerophosphorylcholine (GPC) | 1.235262 | 1.118117 | 0.941748 | 1.079808 | 0.982553 | 0.995264 |
| 1 | glycine | 1.437647 | 0.644370 | 0.776633 | 1.143726 | 1.050041 | 1.170692 |
| 851 | glycochenodeoxycholate | 2.172812 | 2.433296 | 2.047159 | 1.991974 | 1.813181 | 1.524434 |
| 840 | glycocholate | 1.326063 | 1.208381 | 1.218318 | 1.000000 | 1.043352 | 0.878028 |
| 849 | glycodeoxycholate | 1.388473 | 0.949834 | 0.751288 | 1.203790 | 0.968444 | 1.177614 |
| 1318 | glycolate (hydroxyacetate) | 1.119927 | 0.946077 | 0.890375 | 1.098857 | 0.819823 | 0.994096 |
| 1128 | guanosine | 0.673816 | 0.755494 | 0.774575 | 0.822097 | 0.746231 | 0.716737 |
| 1212 | heme* | 0.653546 | 0.095646 | 0.317162 | 0.958180 | 0.978704 | 4.653585 |
| 619 | heptanoate (7:0) | 0.595348 | 0.623683 | 0.693780 | 0.587462 | 0.609394 | 0.662417 |
| 823 | hexanoylcarnitine | 0.809135 | 1.645624 | 1.131565 | 0.690039 | 0.810615 | 0.840919 |
| 1288 | hippurate | 1.050381 | 0.898740 | 1.057115 | 0.934900 | 0.852371 | 0.889626 |
| 50 | histidine | 1.195045 | 0.866347 | 1.015573 | 1.047351 | 0.930853 | 0.873263 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 231 | homocysteine | 2.202654 | 0.399736 | 0.490051 | 1.324761 | 1.078158 | 1.169184 |
| 1585 | homostachydrine* | 1.025057 | 1.027667 | 0.676588 | 0.897241 | 0.659175 | 0.772919 |
| 206 | hydroxyisovaleroyl carnitine | 1.394634 | 1.289270 | 1.381048 | 1.288663 | 1.243729 | 1.205365 |
| 1098 | hypoxanthine | 6.127630 | 0.101341 | 0.083798 | 0.280312 | 0.883558 | 2.099629 |
| 1101 | inosine 5'-monophosphate (IMP) | 2.658472 | 0.463627 | 1.102380 | 1.971251 | 1.092462 | 1.112853 |
| 527 | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | 0.494691 | 0.902267 | 0.909041 | 0.844247 | 0.861112 | 0.577429 |
| 561 | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | 0.535723 | 0.876557 | 0.812388 | 0.909738 | 0.577133 | 0.670054 |
| 496 | Isobar: sorbitol, mannitol | 0.996924 | 0.951858 | 0.969587 | 0.931073 | 0.942483 | 0.960446 |
| 200 | isobutyrylcarnitine | 1.057582 | 1.016714 | 1.130305 | 0.959998 | 0.942708 | 0.884175 |
| 180 | isoleucine | 1.428627 | 0.967821 | 1.004091 | 0.958783 | 0.925595 | 0.977112 |
| 478 | isomaltose | 1.227936 | 1.012143 | 0.950239 | 0.959263 | 0.751023 | 0.865603 |
| 205 | isovalerylcarnitine | 1.106746 | 1.088225 | 0.999515 | 1.112517 | 1.100029 | 0.861429 |
| 144 | kynurenine | 0.976332 | 1.061583 | 1.020485 | 0.916273 | 1.159457 | 0.933957 |
| 536 | lactate | 2.094846 | 0.218916 | 0.559940 | 0.989142 | 1.014542 | 1.206432 |
| 1018 | lathosterol | 0.489776 | 0.489776 | 0.489776 | 0.627744 | 0.489776 | 0.489776 |
| 625 | laurate (12:0) | 0.995648 | 0.862836 | 0.993126 | 1.121053 | 1.092028 | 0.922148 |
| 181 | leucine | 1.455482 | 1.004502 | 1.013630 | 1.029515 | 0.979941 | 1.089607 |
| 604 | linoleate (18:2n6) | 1.784699 | 0.934485 | 1.194274 | 1.172507 | 1.429780 | 1.029350 |
| 608 | linolenate [alpha or gamma; (18:3n3 or 6)] | 1.402727 | 1.007750 | 0.937029 | 1.139813 | 1.144420 | 0.943566 |
| 69 | lysine | 1.449671 | 0.983697 | 0.766798 | 0.955336 | 0.613590 | 1.257529 |
| 598 | malate | 1.626989 | 0.670175 | 0.887241 | 1.181244 | 1.063635 | 1.451410 |
| 482 | maltose | 1.215619 | 1.109761 | 0.921452 | 1.109842 | 0.878572 | 0.819446 |
| 487 | mannose | 0.999108 | 1.042200 | 0.955978 | 1.081089 | 0.814603 | 0.861041 |
| 489 | mannose-6-phosphate | 1.203799 | 0.908216 | 0.804798 | 1.025133 | 0.927659 | 1.043882 |
| 635 | margarate (17:0) | 1.352060 | 0.672355 | 1.072389 | 0.969226 | 1.266985 | 0.905158 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 658 | mead acid (20:3n9) | 1.218585 | 1.172672 | 0.726815 | 1.091334 | 0.676024 | 0.425026 |
| 225 | methionine | 0.873652 | 1.491814 | 1.427271 | 1.016848 | 0.720229 | 0.655113 |
| 890 | myo-inositol | 1.215006 | 1.138390 | 0.941009 | 1.061353 | 0.841823 | 0.911860 |
| 629 | myristate (14:0) | 1.233155 | 0.551269 | 0.893466 | 1.002550 | 1.187990 | 0.929182 |
| 630 | myristoleate (14:1n5) | 0.493142 | 1.802446 | 0.705813 | 1.055310 | 1.180227 | 0.860889 |
| 1242.1 | N1-Methyl-2-pyridone-5-carboxamide | 0.919549 | 0.565019 | 0.827482 | 0.847894 | 0.367389 | 0.703122 |
| 75 | N-6-trimethyllysine | 1.276546 | 1.181597 | 1.756851 | 1.180948 | 1.400720 | 1.112876 |
| 4 | N-acetylglycine | 1.119319 | 0.929361 | 0.756931 | 0.745083 | 1.107049 | 1.113820 |
| 227 | N-acetylmethionine | 1.198684 | 1.151241 | 0.934098 | 1.216606 | 0.989625 | 1.000000 |
| 455 | N-acetylneuraminate | 1.937645 | 0.364520 | 0.452407 | 1.131994 | 1.036507 | 0.923535 |
| 1221 | nicotinamide | 1.128037 | 1.019320 | 0.946052 | 0.988162 | 1.015114 | 0.922631 |
| 1224 | nicotinamide adenine dinucleotide (NAD+) | 0.868102 | 0.997339 | 0.981609 | 1.035125 | 0.951168 | 1.944172 |
| 825 | octanoylcarnitine | 1.051807 | 1.065294 | 0.932738 | 0.977123 | 1.008875 | 0.999185 |
| 639 | oleate (18:1n9) | 1.528451 | 0.805042 | 0.887890 | 1.026755 | 0.951155 | 1.059180 |
| 835 | oleoylcarnitine | 2.779433 | 0.056114 | 0.407851 | 1.164793 | 1.584396 | 9.073618 |
| 285 | ophthalmate | 0.252181 | 3.902869 | 0.946024 | 0.535167 | 0.252181 | 0.252181 |
| 244 | ornithine | 1.196890 | 0.932498 | 0.797281 | 0.871167 | 0.661629 | 1.006229 |
| 632 | palmitate (16:0) | 1.301430 | 0.766287 | 1.007077 | 1.000387 | 1.152141 | 0.949563 |
| 633 | palmitoleate (16:1n7) | 1.278836 | 0.956717 | 1.146023 | 0.841215 | 1.020416 | 0.718337 |
| 1004 | palmitoyl sphingomyelin | 1.133156 | 1.008461 | 0.935966 | 1.066178 | 0.751650 | 0.901174 |
| 833 | palmitoylcarnitine | 2.010902 | 0.059115 | 0.524652 | 0.915916 | 1.110798 | 8.697425 |
| 1243 | pantothenate | 1.069212 | 0.907531 | 0.920280 | 0.920629 | 1.398636 | 0.942652 |
| 1613 | paraxanthine | 1.085177 | 0.948751 | 0.837932 | 0.881288 | 0.864666 | 0.852477 |
| 88 | p-cresol sulfate | 0.789020 | 0.770020 | 0.769045 | 0.725472 | 0.715997 | 0.667300 |
| 621 | pelargonate (9:0) | 0.837061 | 0.360075 | 0.700338 | 0.768938 | 0.741228 | 0.599953 |
| 631 | pentadecanoate (15:0) | 1.419314 | 0.712829 | 1.024571 | 1.086036 | 1.357093 | 1.003934 |
| 135 | phenol sulfate | 1.080150 | 1.039700 | 0.860615 | 1.076993 | 0.978846 | 0.785161 |
| 128 | phenylacetylglutamine | 0.680346 | 0.604740 | 0.665487 | 0.688121 | 0.667230 | 0.693889 |
| 83 | phenylalanine | 1.132419 | 0.804835 | 0.876091 | 0.877652 | 0.881666 | 0.938853 |
| 602 | phosphate | 1.110857 | 0.946588 | 0.949372 | 1.190405 | 0.944489 | 1.020523 |
| 534 | phosphoenolpyruvate (PEP) | 0.279542 | 2.330041 | 1.000000 | 0.575670 | 0.181336 | 0.155305 |
| 877 | phosphoethanolamine | 0.712319 | 0.593700 | 0.593700 | 0.593700 | 0.593700 | 0.593700 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 74 | pipecolate | 1.009720 | 0.898390 | 0.815539 | 0.821096 | 0.873731 | 0.997796 |
| 1531 | piperine | 0.958771 | 1.319098 | 1.470407 | 1.615822 | 0.782269 | 0.825044 |
| 246 | proline | 1.195957 | 0.942258 | 1.033618 | 0.983038 | 1.045444 | 0.978514 |
| 809 | propionylcarnitine | 1.063614 | 1.457202 | 1.446774 | 1.233793 | 1.105600 | 1.125514 |
| 1181 | pseudouridine | 1.128058 | 1.095967 | 0.810404 | 0.638275 | 0.790413 | 0.999677 |
| 45 | pyroglutamine* | 1.601902 | 1.262071 | 1.827425 | 1.304051 | 1.359677 | 1.632543 |
| 603 | pyrophosphate (PPi) | 0.761614 | 1.243354 | 1.085167 | 0.990363 | 0.285513 | 0.794945 |
| 535 | pyruvate | 4.683874 | 2.276982 | 1.490731 | 0.710654 | 0.596456 | 0.493004 |
| 1469 | ranitidine | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 | 0.811072 |
| 548 | ribitol | 8.146637 | 0.742077 | 0.821356 | 0.652676 | 0.652824 | 1.041283 |
| 557 | ribose 5-phosphate | 0.609062 | 0.758696 | 0.754124 | 1.146996 | 1.109373 | 0.461602 |
| 559 | ribulose | 2.586649 | 0.240496 | 0.824892 | 1.085540 | 0.912667 | 1.285401 |
| 224 | S-adenosylhomocysteine (SAH) | 1.306917 | 0.665980 | 1.038199 | 1.065144 | 1.192103 | 1.081832 |
| 551 | sedoheptulose-7-phosphate | 1.663972 | 0.882284 | 0.561685 | 0.753922 | 1.195141 | 2.407375 |
| 8 | serine | 1.464692 | 0.968525 | 0.965250 | 1.198912 | 0.926531 | 1.074484 |
| 216 | S-methylcysteine | 0.731956 | 0.453662 | 0.457515 | 0.823196 | 0.438733 | 0.633290 |
| 281 | S-methylglutathione | 0.811779 | 0.856518 | 1.097021 | 0.837567 | 1.002890 | 1.572077 |
| 270 | spermidine | 1.260416 | 1.050133 | 1.067759 | 1.135426 | 1.152412 | 1.121663 |
| 1584 | stachydrine | 2.395504 | 2.159253 | 2.096279 | 2.038510 | 1.981464 | 2.006947 |
| 637 | stearate (18:0) | 1.289608 | 0.685765 | 0.988116 | 0.976713 | 1.131377 | 0.956837 |
| 1005 | stearoyl sphingomyelin | 1.077618 | 0.861948 | 0.762315 | 0.861358 | 0.889997 | 0.750174 |
| 834 | stearoylcarnitine | 1.762390 | 0.056108 | 0.283844 | 0.924164 | 1.141065 | 6.515597 |
| 591 | succinylcarnitine | 1.623486 | 1.094559 | 1.165168 | 1.233136 | 1.269955 | 1.269939 |
| 1662 | terephthalic acid | 1.158495 | 1.296798 | 1.150642 | 1.012059 | 1.056469 | 1.091768 |
| 1614 | theobromine | 1.074257 | 0.671401 | 0.864160 | 0.825930 | 0.888004 | 0.649509 |
| 1615 | theophylline | 1.151086 | 1.300377 | 1.238272 | 0.774866 | 1.379035 | 0.624518 |
| 549 | threitol | 1.245565 | 0.590636 | 0.676204 | 0.890473 | 0.657034 | 0.823696 |
| 1199 | threonate | 1.293257 | 0.923661 | 0.782371 | 0.869069 | 0.804530 | 0.717342 |
| 17 | threonine | 1.551739 | 0.972354 | 0.912796 | 1.029784 | 1.131052 | 1.200651 |
| 252 | trans-4-hydroxyproline | 0.773043 | 0.683168 | 0.753799 | 0.801991 | 0.796526 | 0.663000 |

| | | DARM-00025 | DARM-00026 | DARM-00027 | DARM-00028 | DARM-00029 | DARM-00030 |
|---|---|---|---|---|---|---|---|
| | | NHSCI 1866 T1 [ | NHSCI 1866 CC | NHSCI 1866 C [ | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 C |
| | | 997732 | 997735 | 997723 | 997728 | 997722 | 997744 |
| | | 991370 | 991371 | 991372 | 991373 | 991374 | 991375 |
| | | NHSCI 1866 T1 | NHSCI 1866 C | NHSCI 1866 C | NHSCI 1866 | NHSCI 1866 C | NHSCI 1866 C |
| | | D28 | D0 | D7 | C D14 | D21 | D28 |
| | | 1866 | 1866 | 1866 | 1866 | 1866 | 1866 |
| | | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| | | 155.949 | 177.522 | 181.946 | 180.175 | 185.286 | 186.197 |
| **PATHWAY SORTORDER** | **BIOCHEMICAL NAME** | T1 D28 | C D0 | C D7 | C D14 | C D21 | C D28 |
| 501 | trehalose | 1.534496 | 0.202847 | 0.589175 | 1.247912 | 0.961607 | 1.668020 |
| 1242 | trigonelline (N'-methylnicotinate) | 1.405095 | 1.311146 | 1.197020 | 1.208728 | 1.239240 | 1.197533 |
| 145 | tryptophan | 1.112154 | 0.904279 | 0.839975 | 0.924663 | 0.888689 | 0.905762 |
| 151 | tryptophan betaine | 1.763188 | 1.536409 | 1.481729 | 1.504200 | 1.433442 | 1.418162 |
| 99 | tyrosine | 1.238953 | 1.068877 | 1.011654 | 1.067225 | 1.012833 | 1.136778 |
| 1149 | urate | 0.925810 | 1.211955 | 1.081120 | 0.996417 | 0.958618 | 0.770822 |
| 245 | urea | 1.080118 | 0.904948 | 0.786405 | 0.905784 | 0.770561 | 0.826782 |
| 1180 | uridine | 1.462895 | 0.770914 | 0.875236 | 1.017241 | 1.177429 | 1.186555 |
| 190 | valine | 1.224885 | 0.998034 | 0.979434 | 1.049638 | 1.002854 | 1.053645 |
| 565 | xylitol | 1.069224 | 0.127693 | 0.127693 | 0.136454 | 0.127693 | 0.127693 |
| 570 | xylonate | 1.012615 | 0.764882 | 0.768001 | 1.025344 | 0.723918 | 0.911486 |
| 569 | xylose | 4.831216 | 1.249813 | 1.338657 | 1.007424 | 0.405368 | 0.755134 |

Shaded cells indicate p≤0.05 (red=higher green=lower blue-bold 0.05<p<0.10)

T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 1 | Amino acid | Glycine, serine and threonine metabolism | glycine | C00037 | HMDB00123 | 0.96 |
| 3 | | | dimethylglycine | C01026 | HMDB00092 | 0.75 |
| 4 | | | N-acetylglycine | | HMDB00532 | 0.76 |
| 7 | | | beta-hydroxypyruvate | C00168 | HMDB01352 | 0.86 |
| 8 | | | serine | C00065 | HMDB03406 | 0.96 |
| 17 | | | threonine | C00188 | HMDB00167 | 1.01 |
| 22 | | | betaine | | HMDB00043 | 1.01 |
| 24 | | Alanine and aspartate metabolism | aspartate | C00049 | HMDB00191 | 1.09 |
| 25 | | | asparagine | C00152 | HMDB00168 | 1.03 |
| 26 | | | beta-alanine | C00099 | HMDB00056 | 0.77 |
| 27 | | | alanine | C00041 | HMDB00161 | 0.85 |
| 39 | | Glutamate metabolism | glutamate | C00025 | HMDB03339 | 1.06 |
| 44 | | | glutamine | C00064 | HMDB00641 | 1.01 |
| 45 | | | pyroglutamine* | | | 1.02 |
| 50 | | Histidine metabolism | histidine | C00135 | HMDB00177 | 1.31 |
| 69 | | Lysine metabolism | lysine | C00047 | HMDB00182 | 1.01 |
| 74 | | | pipecolate | C00408 | HMDB00070 | 0.90 |
| 75 | | | N-6-trimethyllysine | C03793 | HMDB01325 | 1.07 |
| 80 | | | glutaroyl carnitine | | HMDB13130 | 0.90 |
| 83 | | Phenylalanine & tyrosine metabolism | phenylalanine | C00079 | HMDB00159 | 1.06 |
| 88 | | | p-cresol sulfate | C01468 | | 0.93 |
| 99 | | | tyrosine | C00082 | HMDB00158 | 1.04 |
| 128 | | | phenylacetylglutamine | C05597 | HMDB06344 | 1.08 |
| 135 | | | phenol sulfate | C02180 | | 1.02 |
| 144 | | Tryptophan metabolism | kynurenine | C00328 | HMDB00684 | 1.15 |
| 145 | | | tryptophan | C00078 | HMDB00929 | 0.99 |
| 151 | | | tryptophan betaine | C09213 | | 0.91 |
| 164 | | | C-glycosyltryptophan* | | | 0.96 |
| 170 | | | 3-indoxyl sulfate | | HMDB00682 | 0.93 |
| 172 | | Valine, leucine and isoleucine metabolism | 3-methyl-2-oxobutyrate | C00141 | HMDB00019 | 0.42 |
| 173 | | | 3-methyl-2-oxovalerate | C00671 | HMDB03736 | 0.82 |
| 179 | | | alpha-hydroxyisocaproate | C03264 | HMDB00746 | 1.00 |
| 180 | | | isoleucine | C00407 | HMDB00172 | 1.06 |
| 181 | | | leucine | C00123 | HMDB00687 | 0.98 |
| 190 | | | valine | C00183 | HMDB00883 | 1.04 |
| 193 | | | 4-methyl-2-oxopentanoate | C00233 | HMDB00695 | 0.79 |
| 198 | | | alpha-hydroxyisovalerate | | HMDB00407 | **1.44** |
| 200 | | | isobutyrylcarnitine | | | 1.06 |
| 202 | | | 2-methylbutyroylcarnitine | | HMDB00378 | 0.88 |
| 205 | | | isovalerylcarnitine | | HMDB00688 | 0.93 |
| 206 | | | hydroxyisovaleroyl carnitine | | | 0.97 |

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T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 213 | | Cysteine, methionine, SAM, taurine metabolism | cysteine | C00097 | HMDB00574 | 0.79 |
| 216 | | | S-methylcysteine | | HMDB02108 | 0.83 |
| 224 | | | S-adenosylhomocysteine (SAH) | C00021 | HMDB00939 | 0.99 |
| 225 | | | methionine | C00073 | HMDB00696 | 1.09 |
| 227 | | | N-acetylmethionine | C02712 | HMDB11745 | 0.86 |
| 229 | | | 2-hydroxybutyrate (AHB) | C05984 | HMDB00008 | 1.05 |
| 231 | | | homocysteine | C00155 | HMDB00742 | 0.73 |
| 241 | | Urea cycle; arginine-, proline-, metabolism | arginine | C00062 | HMDB00517 | 1.28 |
| 244 | | | ornithine | C00077 | HMDB03374 | 0.88 |
| 245 | | | urea | C00086 | HMDB00294 | 0.92 |
| 246 | | | proline | C00148 | HMDB00162 | 0.94 |
| 248 | | | citrulline | C00327 | HMDB00904 | 1.14 |
| 252 | | | trans-4-hydroxyproline | C01157 | HMDB00725 | 0.98 |
| 259 | | Creatine metabolism | creatine | C00300 | HMDB00064 | 0.98 |
| 260 | | | creatinine | C00791 | HMDB00562 | 0.98 |
| 263 | | Butanoate metabolism | 2-aminobutyrate | C02261 | HMDB00650 | 0.88 |
| 266 | | Polyamine metabolism | 5-methylthioadenosine (MTA) | C00170 | HMDB01173 | 1.06 |
| 270 | | | spermidine | C00315 | HMDB01257 | 0.96 |
| 280 | | Glutathione metabolism | glutathione, reduced (GSH) | C00051 | HMDB00125 | 1.05 |
| 281 | | | S-methylglutathione | C11347 | | 1.13 |
| 282 | | | 5-oxoproline | C01879 | HMDB00267 | 1.05 |
| 283 | | | glutathione, oxidized (GSSG) | C00127 | HMDB03337 | 1.08 |
| 285 | | | ophthalmate | | HMDB05765 | 1.20 |
| 404 | Peptide | gamma-glutamyl | gamma-glutamylleucine | | HMDB11171 | 1.18 |
| 453 | | Aminosugars metabolism | erythronate* | | HMDB00613 | **0.81** |
| 455 | | | N-acetylneuraminate | C00270 | HMDB00230 | 1.20 |
| 472 | | Fructose, mannose, galactose, starch, and sucrose metabolism | fructose | C00095 | HMDB00660 | 0.84 |
| 478 | | | isomaltose | C00252 | HMDB02923 | 1.41 |
| 482 | | | maltose | C00208 | HMDB00163 | **0.77** |
| 487 | | | mannose | C00159 | HMDB00169 | 0.92 |
| 489 | | | mannose-6-phosphate | C00275 | HMDB01078 | 0.50 |
| 496 | | | Isobar: sorbitol, mannitol | C00392,C01722,C01697,C01489,C00794,C01507 | HMDB00247 | **1.14** |
| 501 | | | trehalose | C01083 | HMDB00975 | 1.09 |

Shaded cells indicate p≤0.05 (red=higher green=lower blue-bold 0.05<p<0.10)

T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 515 | Carbohydrate | Glycolysis, gluconeogenesis, pyruvate metabolism | 1,5-anhydroglucitol (1,5-AG) | C07326 | HMDB02712 | 0.96 |
| 517 | | | glycerate | C00258 | HMDB00139 | 1.21 |
| 519 | | | glucose-6-phosphate (G6P) | C00668 | HMDB01401 | 0.17 |
| 521 | | | glucose | C00293 | HMDB00122 | 0.93 |
| 523 | | | 1,6-anhydroglucose | | HMDB00640 | 0.66 |
| 524 | | | fructose-6-phosphate | C05345 | HMDB00124 | 0.43 |
| 527 | | | Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate | | | 4.26 |
| 529 | | | 3-phosphoglycerate | C00597 | HMDB00807 | 1.98 |
| 531 | | | dihydroxyacetone phosphate (DHAP) | C00111 | HMDB01473 | 29.69 |
| 532 | | | 1,3-dihydroxyacetone | C00184 | HMDB01882 | 1.06 |
| 533 | | | 2,3-diphosphoglycerate | C01159 | HMDB01294 | 1.50 |
| 534 | | | phosphoenolpyruvate (PEP) | C00074 | HMDB00263 | 1.54 |
| 535 | | | pyruvate | C00022 | HMDB00243 | 0.03 |
| 536 | | | lactate | C00186 | HMDB00190 | 1.44 |
| 545 | | Nucleotide sugars, pentose metabolism | 6-phosphogluconate | C00345 | HMDB01316 | 0.33 |
| 546 | | | arabitol | C00474 | HMDB01851 | 0.86 |
| 548 | | | ribitol | C00474 | HMDB00508 | 0.93 |
| 549 | | | threitol | C16884 | HMDB04136 | 1.08 |
| 551 | | | sedoheptulose-7-phosphate | C05382 | HMDB01068 | 0.13 |
| 557 | | | ribose 5-phosphate | C00117 | HMDB00618 | 1.91 |
| 559 | | | ribulose | C00309 | HMDB00621,HMDB02374 | 4.96 |
| 561 | | | Isobar: ribulose 5-phosphate, xylulose 5-phosphate | | | 3.42 |
| 565 | | | xylitol | C00379 | HMDB00568 | 1.00 |
| 566 | | | arabinose | C00181 | HMDB00646 | 0.97 |
| 569 | | | xylose | C00181 | HMDB00098 | 0.63 |

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T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 570 | | | xylonate | C00502,C05411 | | **1.55** |
| 579 | Energy | Krebs cycle | citrate | C00158 | HMDB00094 | 0.94 |
| 582 | | | cis-aconitate | C00417 | HMDB00072 | 0.98 |
| 591 | | | succinylcarnitine | | | 0.95 |
| 594 | | | fumarate | C00122 | HMDB00134 | 0.80 |
| 598 | | | malate | C00149 | HMDB00156 | 0.82 |
| 601 | | Oxidative phosphorylation | acetylphosphate | C00227 | HMDB01494 | 0.89 |
| 602 | | | phosphate | C00009 | HMDB01429 | 0.76 |
| 603 | | | pyrophosphate (PPi) | C00013 | HMDB00250 | 1.39 |
| 604 | | Essential fatty acid | linoleate (18:2n6) | C01595 | HMDB00673 | 0.92 |
| 608 | | | linolenate [alpha or gamma; (18:3n3 or 6)] | C06427 | HMDB01388 | 1.19 |
| 609 | | | dihomo-linolenate (20:3n3 or n6) | C03242 | HMDB02925 | 0.98 |
| 610 | | | eicosapentaenoate (EPA; 20:5n3) | C06428 | HMDB01999 | 1.29 |
| 611 | | | docosapentaenoate (n3 DPA; 22:5n3) | C16513 | HMDB01976 | 1.14 |
| 613 | | | docosahexaenoate (DHA; 22:6n3) | C06429 | HMDB02183 | 1.08 |
| 618 | | Medium chain fatty acid | caproate (6:0) | C01585 | HMDB00535 | 0.85 |
| 619 | | | heptanoate (7:0) | C17714 | HMDB00666 | 1.03 |
| 620 | | | caprylate (8:0) | C06423 | HMDB00482 | 0.77 |
| 621 | | | pelargonate (9:0) | C01601 | HMDB00847 | 1.05 |
| 622 | | | caprate (10:0) | C01571 | HMDB00511 | 0.98 |
| 625 | | | laurate (12:0) | C02679 | HMDB00638 | 1.07 |
| 629 | | Long chain fatty acid | myristate (14:0) | C06424 | HMDB00806 | 0.93 |
| 630 | | | myristoleate (14:1n5) | C08322 | HMDB02000 | 0.49 |
| 631 | | | pentadecanoate (15:0) | C16537 | HMDB00826 | 1.06 |
| 632 | | | palmitate (16:0) | C00249 | HMDB00220 | 0.93 |
| 633 | | | palmitoleate (16:1n7) | C08362 | HMDB03229 | 1.00 |
| 635 | | | margarate (17:0) | | HMDB02259 | 1.03 |
| 636 | | | 10-heptadecenoate (17:1n7) | | | 1.06 |
| 637 | | | stearate (18:0) | C01530 | HMDB00827 | 0.97 |
| 639 | | | oleate (18:1n9) | C00712 | HMDB00207 | 0.91 |
| 641 | | | cis-vaccenate (18:1n7) | C08367 | | 0.83 |
| 655 | | | dihomo-linoleate (20:2n6) | C16525 | | 0.96 |
| 658 | | | mead acid (20:3n9) | | HMDB10378 | 0.62 |
| 659 | | | arachidonate (20:4n6) | C00219 | HMDB01043 | 1.04 |
| 665 | | | adrenate (22:4n6) | C16527 | HMDB02226 | 1.00 |
| 670.01 | | | 9,10-epoxyoctadec-12(Z)-enoic acid | C14825 | HMDB04701 | 0.98 |
| 672 | | Fatty acid, oxidized | 9,10-epoxystearate | | | 0.87 |
| 706 | | Fatty acid, monohydroxy | 2-hydroxypalmitate | | | **0.60** |
| 714 | | Fatty acid, dicarboxylate | 2-hydroxyglutarate | C02630 | HMDB00606 | 0.94 |
| 721 | | | azelate (nonanedioate) | C08261 | HMDB00784 | 1.27 |
| 735 | | Fatty acid, amide | erucamide | | | 1.18 |

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T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 742 | Lipid | Fatty acid, branched | 13-methylmyristic acid | | | 0.90 |
| 744 | | | 15-methylpalmitate (isobar with 2-methylpalmitate) | | | 1.01 |
| 809 | | Fatty acid metabolism (also BCAA metabolism) | propionylcarnitine | C03017 | HMDB00824 | 0.97 |
| 811 | | | butyrylcarnitine | | | 1.39 |
| 819 | | Carnitine metabolism | deoxycarnitine | C01181 | HMDB01161 | 1.03 |
| 820 | | | carnitine | | | 1.07 |
| 821 | | | 3-dehydrocarnitine* | C02636 | HMDB12154 | 1.05 |
| 822 | | | acetylcarnitine | C02571 | HMDB00201 | 0.95 |
| 823 | | | hexanoylcarnitine | C01585 | HMDB00705 | **0.72** |
| 825 | | | octanoylcarnitine | | | 0.89 |
| 833 | | | palmitoylcarnitine | | | **4.95** |
| 834 | | | stearoylcarnitine | | HMDB00848 | 2.33 |
| 835 | | | oleoylcarnitine | | HMDB05065 | 3.40 |
| 840 | | Bile acid metabolism | glycocholate | C01921 | HMDB00138 | 0.92 |
| 849 | | | glycodeoxycholate | C05464 | HMDB00631 | 0.85 |
| 851 | | | glycochenodeoxycholate | C05466 | HMDB00637 | **0.78** |
| 876 | | Glycerolipid metabolism | ethanolamine | C00189 | HMDB00149 | 0.88 |
| 877 | | | phosphoethanolamine | C00346 | HMDB00224 | 2.29 |
| 881 | | | choline | | | 1.03 |
| 882 | | | glycerol 3-phosphate (G3P) | C00093 | HMDB00126 | 2.58 |
| 883 | | | glycerophosphorylcholine (GPC) | C00670 | HMDB00086 | 0.90 |
| 890 | | Inositol metabolism | myo-inositol | C00137 | HMDB00211 | 0.98 |
| 905 | | Ketone bodies | 1,2-propanediol | C00717,C02912,C00583,C01506,C02917 | HMDB01881 | 0.89 |
| 909 | | Lysolipid | 1-palmitoylglycerophosphoethanolamine | | HMDB11503 | 0.44 |
| 915 | | | 1-oleoylglycerophosphoethanolamine | | HMDB11506 | 0.62 |
| 919 | | | 1-arachidonoylglycerophosphoethanolamine* | | HMDB11517 | 0.53 |
| 920 | | | 2-arachidonoylglycerophosphoethanolamine* | | | 2.90 |
| 922 | | | 2-docosapentaenoylglycerophosphoethanolamine* | | | 2.70 |
| 923 | | | 2-docosahexaenoylglycerophosphoethanolamine* | | | 2.09 |
| 926 | | | 1-myristoylglycerophosphocholine | | HMDB10379 | 1.00 |
| 929 | | | 1-palmitoylglycerophosphocholine | | | 2.76 |
| 930 | | | 2-palmitoylglycerophosphocholine* | | | 1.05 |
| 934 | | | 1-stearoylglycerophosphocholine | | | 2.34 |
| 935 | | | 2-stearoylglycerophosphocholine* | | | 1.00 |
| 936 | | | 1-oleoylglycerophosphocholine | | | 2.32 |
| 937 | | | 2-oleoylglycerophosphocholine* | | | 1.66 |
| 938 | | | 1-linoleoylglycerophosphocholine | C04100 | | 0.75 |
| 939 | | | 2-linoleoylglycerophosphocholine* | | | 1.00 |

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T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 945 | | | 2-arachidonoylglycerophosphocholine* | | | 1.78 |
| 970 | | Monoacylglycerol | 1-palmitoylglycerol (1-monopalmitin) | | | 0.82 |
| 1004 | | Sphingolipid | palmitoyl sphingomyelin | | | 0.85 |
| 1005 | | | stearoyl sphingomyelin | C00550 | HMDB01348 | 0.92 |
| 1018 | | Sterol/Steroid | lathosterol | C01189 | HMDB01170 | 0.70 |
| 1020 | | | cholesterol | C00187 | HMDB00067 | 0.94 |
| 1024 | | | 7-beta-hydroxycholesterol | C03594 | HMDB06119 | 1.20 |
| 1034 | | | androsterone sulfate | C00523 | HMDB02759 | 1.25 |
| 1057 | | | beta-sitosterol | C01753 | HMDB00852 | 1.48 |
| 1059 | | | campesterol | C01789 | HMDB02869 | 1.03 |
| 1098 | Nucleotide | Purine metabolism, (hypo)xanthine/inosine containing | hypoxanthine | C00262 | HMDB00157 | 0.91 |
| 1101 | | | inosine 5'-monophosphate (IMP) | C00130 | HMDB00175 | 1.10 |
| 1105 | | Purine metabolism, adenine containing | adenine | C00147 | HMDB00034 | 0.93 |
| 1106 | | | adenosine | C00212 | HMDB00050 | 0.64 |
| 1114 | | | adenosine 5'-monophosphate (AMP) | C00020 | HMDB00045 | 1.19 |
| 1116 | | | adenosine 5'-diphosphate (ADP) | C00008 | HMDB01341 | 1.05 |
| 1128 | | Purine metabolism, guanine containing | guanosine | C00387 | HMDB00133 | 1.20 |
| 1149 | | Purine metabolism, urate metabolism | urate | C00366 | HMDB00289 | 0.96 |
| 1150 | | | allantoin | C02350 | HMDB00462 | 0.62 |
| 1180 | | Pyrimidine metabolism, uracil containing | uridine | C00299 | HMDB00296 | 1.15 |
| 1181 | | | pseudouridine | C02067 | HMDB00767 | **0.64** |
| 1199 | Cofactors and vitamins | Ascorbate and aldarate metabolism | threonate | C01620 | HMDB00943 | 0.83 |
| 1202 | | | arabonate | | HMDB00539 | 1.12 |
| 1212 | | Hemoglobin and porphyrin metabolism | heme* | | | 3.72 |
| 1216 | | | biliverdin | C00500 | HMDB01008 | 0.99 |
| 1221 | | Nicotinate and nicotinamide metabolism | nicotinamide | C00153 | HMDB01406 | 0.87 |
| 1224 | | | nicotinamide adenine dinucleotide (NAD+) | C00003 | HMDB00902 | 2.14 |
| 1232 | | | adenosine 5'diphosphoribose | C00301 | HMDB01178 | 1.08 |
| 1242 | | | trigonelline (N'-methylnicotinate) | | HMDB00875 | 0.97 |

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T1: anaerobic T2: +CO2

| PATHWAY SORT | SUPER PATHWAY | SUB PATHWAY | BIOCHEMICAL NAME | Kegg | HMDB | T1-0 C-0 |
|---|---|---|---|---|---|---|
| 1242.1 | | | N1-Methyl-2-pyridone-5-carboxamide | C05842 | HMDB04193 | 1.14 |
| 1243 | | Pantothenate and CoA metabolism | pantothenate | C00864 | HMDB00210 | 0.99 |
| 1266 | | Tocopherol metabolism | alpha-tocopherol | C02477 | HMDB01893 | 0.71 |
| 1288 | Xenobiotics | Benzoate metabolism | hippurate | C01586 | HMDB00714 | 0.99 |
| 1300 | | | catechol sulfate | C00090 | | 1.02 |
| 1318 | | Chemical | glycolate (hydroxyacetate) | C00160 | HMDB00115 | 0.87 |
| 1360 | | | 2-ethylhexanoate (isobar with 2-propylpentanoate) | | | 0.89 |
| 1469 | | Drug | ranitidine | 422 | HMDB01930 | 0.97 |
| 1531 | | Food component/Plant | piperine | C03882 | | 0.76 |
| 1565 | | | ergothioneine | C05570 | HMDB03045 | 0.87 |
| 1584 | | | stachydrine | C10172 | HMDB04827 | 0.90 |
| 1585 | | | homostachydrine* | C08283 | | 1.04 |
| 1612 | | Xanthine metabolism | caffeine | C07481 | HMDB01847 | 0.93 |
| 1613 | | | paraxanthine | C13747 | HMDB01860 | 1.02 |
| 1614 | | | theobromine | C07480 | HMDB02825 | 0.97 |
| 1615 | | | theophylline | C07130 | HMDB01889 | 0.90 |
| 1632 | | Sugar, sugar substitute, starch | erythritol | C00503 | HMDB02994 | 0.99 |
| 1662 | | Phthalate | terephthalic acid | C06337 | HMDB02428 | 0.84 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| 1 | 1.08 | **0.77** | 1.03 | 1.04 | 1.03 | 1.06 | 0.96 | 1.02 | 1.23 | 1.07 | 0.98 | 1.25 | 0.99 |
| 3 | 0.85 | 1.03 | 0.74 | 0.79 | 0.81 | 0.88 | 0.89 | 1.39 | 0.91 | 1.07 | 1.04 | 0.86 | 1.88 |
| 4 | 1.04 | 0.86 | 1.13 | 1.22 | 0.76 | 0.78 | 1.24 | 0.81 | 0.99 | 1.00 | 0.75 | 1.44 | 0.72 |
| 7 | 1.18 | 0.94 | 1.19 | 1.07 | 0.86 | 1.09 | 1.00 | 0.89 | 1.17 | 1.01 | 0.92 | 1.07 | 0.75 |
| 8 | 1.20 | 0.97 | 1.37 | **1.23** | 1.04 | 1.14 | 0.95 | 1.05 | 1.01 | 1.08 | 0.95 | 0.98 | 0.77 |
| 17 | 1.28 | 1.27 | 1.06 | 1.13 | 1.05 | **1.28** | 1.21 | 0.91 | 1.02 | 1.04 | 1.00 | 0.95 | 0.86 |
| 22 | 1.14 | 1.08 | 1.09 | 1.12 | 1.01 | 0.98 | 1.01 | 0.90 | 0.95 | 1.00 | **0.86** | 0.94 | 0.83 |
| 24 | 1.38 | 1.22 | 1.53 | 1.09 | 0.93 | 0.88 | 0.93 | 1.07 | 0.88 | 0.85 | 0.64 | **0.76** | **0.70** |
| 25 | 1.25 | 0.94 | 1.36 | 1.20 | 1.13 | 1.17 | 1.03 | 1.17 | 0.88 | 1.09 | 0.94 | 1.09 | 0.86 |
| 26 | 1.23 | 1.10 | 1.98 | 1.06 | 1.02 | 1.47 | 1.48 | **1.85** | 0.47 | 1.32 | 1.20 | 1.35 | 0.94 |
| 27 | 0.96 | 0.73 | 1.06 | 0.97 | 1.02 | 1.06 | 0.96 | 1.05 | 1.06 | 1.20 | 1.11 | 1.31 | 0.99 |
| 39 | **1.37** | 0.93 | 1.19 | 1.12 | 1.01 | 1.08 | 1.01 | 1.07 | 1.26 | 0.96 | **0.79** | 1.09 | 0.90 |
| 44 | 0.90 | 0.87 | 0.80 | 0.83 | 1.05 | 1.01 | 1.07 | 1.03 | 0.98 | 1.04 | **1.12** | 1.23 | 1.29 |
| 45 | 1.04 | 1.10 | 1.17 | 1.06 | 1.17 | 1.02 | 0.99 | 0.95 | 1.04 | 1.15 | 0.98 | 0.90 | 0.82 |
| 50 | 1.01 | 0.98 | 1.42 | **1.28** | 1.17 | 1.07 | 0.98 | 1.09 | 1.12 | 0.89 | 1.06 | 1.00 | 0.77 |
| 69 | 1.18 | 0.86 | **1.75** | **1.55** | 1.09 | 1.20 | 0.81 | **1.75** | 0.96 | 1.08 | 1.02 | 0.93 | 1.00 |
| 74 | 1.08 | 1.11 | 1.00 | 0.99 | 0.99 | 1.00 | 0.89 | 0.94 | 1.00 | 1.11 | 0.92 | 0.80 | 0.94 |
| 75 | 0.76 | 0.91 | 0.88 | 1.04 | 1.12 | 0.74 | 0.93 | 0.87 | 0.90 | 1.04 | 0.96 | 1.02 | 0.99 |
| 80 | 0.74 | 1.20 | 0.87 | **0.59** | 1.35 | 1.17 | 0.92 | 0.71 | 0.70 | 1.50 | 1.58 | 0.76 | 0.81 |
| 83 | 1.17 | 1.12 | 1.07 | 1.11 | 1.10 | 1.00 | 1.11 | 0.99 | 0.98 | 1.04 | 0.85 | 0.99 | 0.92 |
| 88 | 1.07 | 0.93 | 1.13 | 1.05 | 1.08 | 1.01 | 0.95 | 0.89 | 1.03 | 1.16 | 0.94 | 1.02 | **0.79** |
| 99 | **1.18** | 1.10 | 1.06 | 1.13 | 1.06 | 1.01 | 1.09 | 0.99 | 1.06 | 1.02 | **0.85** | 0.99 | 0.93 |
| 128 | **1.22** | 0.99 | 1.09 | 0.94 | **1.21** | 1.02 | 0.97 | 0.94 | 1.05 | 1.13 | 0.83 | 0.98 | **0.86** |
| 135 | 1.23 | 0.92 | 0.89 | **1.18** | 1.09 | 1.15 | 0.88 | 0.77 | 1.09 | 1.07 | 0.94 | 0.96 | 0.87 |
| 144 | **1.29** | 1.35 | 0.98 | 1.05 | 0.93 | 1.14 | 1.10 | 1.01 | 0.93 | 0.81 | 0.88 | 0.81 | 1.03 |
| 145 | **1.21** | 1.08 | 1.09 | 1.12 | 1.12 | 1.07 | 1.08 | 1.01 | 0.99 | 1.13 | 0.88 | 1.00 | 0.93 |
| 151 | 1.10 | 0.96 | 1.07 | 1.16 | 1.09 | 1.10 | 1.00 | 0.90 | 1.09 | **1.19** | 1.00 | 1.04 | 0.84 |
| 164 | 0.86 | 0.93 | 0.91 | 0.84 | 1.04 | 0.83 | 1.19 | 0.92 | 0.78 | 1.08 | 0.96 | 1.28 | 1.01 |
| 170 | 0.96 | 1.02 | 1.33 | 0.94 | 1.29 | 0.99 | 0.98 | 1.19 | 1.13 | **1.39** | 1.03 | 0.96 | 0.89 |
| 172 | 0.20 | 0.13 | 0.17 | 0.27 | 0.93 | 1.23 | 1.03 | 0.71 | 0.95 | 2.23 | 6.06 | 8.18 | 4.10 |
| 173 | 0.49 | 0.22 | 0.25 | 0.34 | 1.09 | 1.01 | 0.92 | 0.89 | 1.04 | 1.34 | 2.09 | 4.16 | 3.60 |
| 179 | 2.80 | 2.20 | 1.42 | 1.19 | 1.00 | 1.00 | 1.00 | 0.96 | 1.22 | 1.00 | 0.36 | 0.46 | **0.67** |
| 180 | 1.33 | 1.33 | 1.38 | 1.32 | 1.11 | 0.97 | 1.04 | 1.00 | 1.04 | 1.04 | 0.73 | 0.78 | 0.72 |
| 181 | 1.31 | **1.22** | 1.35 | **1.23** | 1.08 | 1.04 | 1.03 | 1.01 | 1.09 | 1.10 | 0.80 | 0.84 | 0.75 |
| 190 | 1.18 | 1.07 | 1.09 | 1.09 | 1.09 | 1.07 | 1.10 | 0.96 | 1.02 | 1.05 | 0.90 | 1.03 | 0.88 |
| 193 | 0.42 | 0.18 | 0.27 | 0.38 | 1.20 | 1.17 | 1.10 | 0.88 | 1.12 | 1.50 | 2.77 | 6.13 | 3.27 |
| 198 | 3.79 | 3.11 | 3.27 | 2.58 | 1.15 | 1.00 | 0.86 | 0.91 | 1.13 | 0.80 | 0.26 | 0.28 | 0.28 |
| 200 | 1.02 | 0.99 | 1.05 | 0.99 | 1.18 | 1.09 | 1.13 | 0.92 | 1.03 | 1.11 | 1.07 | 1.14 | 0.88 |
| 202 | 0.83 | 0.58 | 0.85 | 0.97 | 0.96 | 0.86 | 0.88 | **0.70** | 1.23 | 1.10 | 1.05 | 1.51 | 0.82 |
| 205 | 1.10 | 0.87 | 0.98 | 1.08 | 0.99 | 0.96 | **0.81** | 0.83 | 1.13 | 1.06 | 0.87 | 0.93 | 0.84 |
| 206 | 1.06 | 0.98 | 1.04 | 1.09 | **1.23** | 0.99 | 1.01 | 0.95 | 1.08 | **1.27** | 0.93 | 1.03 | 0.92 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| 213 | 0.66 | **0.73** | 1.21 | 0.88 | 0.98 | 0.89 | 0.92 | 1.29 | 1.12 | 1.24 | 1.34 | 1.26 | 1.07 |
| 216 | 0.80 | 0.83 | 1.43 | 1.09 | 1.06 | 0.84 | 0.68 | 1.17 | 1.01 | 1.28 | 1.05 | 0.82 | 0.82 |
| 224 | 1.01 | 0.93 | 0.78 | 0.99 | 1.15 | 1.07 | 0.94 | 0.72 | 1.08 | 1.16 | 1.06 | 1.02 | 0.91 |
| 225 | 1.02 | 1.08 | 1.02 | 1.14 | 1.13 | 0.98 | 1.11 | 0.93 | 1.09 | 1.03 | 0.96 | 1.03 | 0.91 |
| 227 | 1.28 | 0.76 | 1.06 | 0.94 | 1.14 | 1.07 | 0.76 | 1.01 | 0.98 | 1.32 | 0.83 | 1.00 | 0.95 |
| 229 | 1.15 | 0.96 | **1.27** | 1.00 | 1.03 | 1.05 | 0.97 | 1.08 | 0.93 | 0.98 | 0.91 | 1.02 | 0.85 |
| 231 | 0.77 | 1.24 | 1.54 | 1.25 | **0.58** | **0.59** | 0.80 | 0.92 | 0.77 | 0.79 | 0.76 | 0.64 | **0.60** |
| 241 | 1.06 | 0.81 | 0.77 | 1.44 | 1.36 | 0.77 | 0.69 | **0.45** | **2.07** | 1.06 | 0.73 | 0.86 | 0.59 |
| 244 | 1.12 | 0.99 | 1.55 | 1.15 | 1.02 | 1.13 | 1.06 | **1.29** | 0.82 | 1.16 | 1.02 | 1.07 | 0.83 |
| 245 | 1.17 | 0.95 | **1.28** | 1.10 | 1.02 | 1.06 | 1.03 | 1.03 | 0.99 | 1.10 | 0.90 | 1.09 | 0.80 |
| 246 | 1.05 | 0.94 | 1.09 | 1.10 | 1.09 | 1.11 | 0.95 | 0.88 | 1.10 | **1.15** | 1.06 | 1.01 | 0.81 |
| 248 | 1.08 | 1.01 | 1.08 | **1.14** | 1.09 | 1.08 | 0.96 | 0.95 | 1.01 | 0.96 | 1.00 | 0.95 | 0.88 |
| 252 | 1.06 | **1.17** | 0.98 | 1.06 | **1.17** | 0.89 | 0.94 | 1.03 | 0.96 | 1.20 | **0.84** | 0.80 | 1.05 |
| 259 | 1.09 | 1.01 | 1.06 | 1.07 | 1.10 | 1.06 | 1.00 | 0.90 | 1.02 | 1.12 | 0.97 | 0.99 | 0.85 |
| 260 | **1.22** | 1.16 | 1.08 | 1.17 | 1.00 | 1.43 | 1.07 | 1.00 | 0.96 | 1.02 | 1.17 | 0.92 | 0.92 |
| 263 | 1.09 | 0.93 | 1.30 | 1.19 | 0.92 | 1.15 | 0.97 | 1.13 | 1.01 | 1.05 | 1.05 | 1.05 | 0.87 |
| 266 | 1.49 | **1.38** | 1.27 | 1.14 | 1.14 | 1.15 | 1.23 | 1.24 | 1.05 | 1.07 | 0.78 | 0.89 | 0.98 |
| 270 | 1.05 | 0.93 | 0.95 | 0.97 | 1.11 | 1.09 | 1.06 | 0.88 | 1.01 | 1.16 | 1.03 | 1.14 | 0.93 |
| 280 | 1.02 | 0.98 | 0.89 | 0.93 | 1.11 | 0.90 | 1.07 | 0.97 | 0.90 | 1.06 | 0.88 | 1.10 | 1.08 |
| 281 | 1.33 | 1.48 | 1.03 | **0.59** | 1.15 | 1.13 | 1.01 | 1.09 | 0.68 | 1.02 | 0.85 | 0.68 | 1.06 |
| 282 | 1.49 | **1.24** | 1.29 | 1.09 | 1.05 | 1.09 | 1.05 | 1.00 | **1.26** | 1.00 | 0.73 | 0.85 | 0.77 |
| 283 | 0.99 | 0.93 | 0.91 | **0.79** | 1.07 | 0.93 | 1.01 | 0.97 | 0.88 | 0.99 | 0.94 | 1.09 | 1.07 |
| 285 | 2.19 | **1.75** | 1.43 | 1.00 | 1.09 | 1.23 | 0.88 | 1.13 | 1.00 | 0.91 | 0.56 | **0.50** | 0.79 |
| 404 | **1.33** | 1.44 | 1.10 | 1.12 | 1.30 | 0.84 | 1.06 | 0.93 | 1.06 | 1.11 | 0.63 | **0.74** | 0.85 |
| 453 | 1.43 | 1.68 | 3.18 | 2.48 | 0.87 | 1.06 | 0.98 | 1.01 | 0.94 | 1.08 | 0.74 | 0.58 | 0.32 |
| 455 | 1.84 | **0.64** | **1.58** | **1.44** | 1.24 | 1.38 | 0.79 | 1.06 | 0.76 | 1.04 | 0.75 | 1.23 | 0.67 |
| 472 | 0.74 | 0.63 | 1.24 | 1.23 | 1.02 | 1.03 | 0.94 | 1.04 | 0.91 | 1.20 | 1.38 | 1.51 | 0.84 |
| 478 | 1.47 | 0.72 | 1.23 | 1.09 | 1.06 | 1.36 | 0.91 | 1.02 | 0.90 | 0.75 | 0.93 | 1.26 | 0.83 |
| 482 | 1.20 | 0.87 | **1.31** | 1.12 | 0.80 | 1.04 | 0.92 | 0.97 | 0.94 | 1.04 | 0.87 | 1.06 | **0.74** |
| 487 | 0.94 | **0.80** | 1.19 | 1.03 | 0.99 | 0.97 | 0.92 | 1.01 | 1.01 | 1.07 | 1.03 | 1.14 | 0.85 |
| 489 | 1.03 | 0.87 | 1.18 | 0.91 | 1.01 | 1.12 | 0.77 | **0.64** | 0.83 | 2.01 | 1.08 | 0.88 | 0.54 |
| 496 | **1.15** | **1.14** | 1.09 | 1.04 | 1.13 | 1.01 | 1.07 | 1.00 | 1.02 | 0.99 | **0.88** | 0.94 | 0.92 |
| 501 | 0.80 | 0.67 | 1.36 | 1.00 | 0.98 | 1.18 | 0.90 | 1.34 | 0.83 | 0.90 | 1.47 | 1.34 | 0.99 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| ~~515~~ | 1.12 | 0.73 | 1.55 | 0.91 | 1.09 | 1.18 | 0.91 | 1.01 | 0.91 | 1.13 | 1.05 | 1.24 | 0.65 |
| 517 | 3.99 | 4.75 | 6.84 | 5.85 | 0.99 | 0.83 | 0.67 | 0.87 | 0.73 | 0.81 | 0.21 | 0.14 | 0.13 |
| 519 | 0.15 | 0.50 | 1.02 | 0.87 | 1.05 | 1.07 | 0.75 | 0.54 | 0.91 | 6.31 | 7.07 | 1.50 | 0.52 |
| 521 | 1.09 | 0.90 | 1.12 | 1.05 | 1.00 | 1.02 | 0.97 | 0.98 | 1.07 | 1.08 | 0.93 | 1.07 | 0.87 |
| 523 | 1.58 | 1.19 | 1.33 | 1.08 | 0.80 | 1.00 | **0.70** | 1.11 | 0.92 | 1.23 | 0.63 | 0.59 | 0.84 |
| 524 | 0.79 | 0.90 | 0.83 | 0.92 | 0.93 | 0.99 | 0.69 | 0.57 | 0.94 | 2.15 | 1.25 | 0.77 | 0.69 |
| 527 | 9.29 | 1.51 | 0.70 | 0.70 | 1.27 | 1.26 | 1.07 | 0.84 | 1.22 | 0.30 | 0.14 | 0.71 | 1.20 |
| 529 | 2.57 | 2.08 | 1.71 | 1.22 | 1.08 | 1.09 | 0.67 | 0.59 | 0.78 | 0.54 | 0.43 | 0.32 | 0.35 |
| 531 | 159.45 | 6.22 | **6.38** | 2.15 | 0.26 | 2.19 | 0.15 | 2.32 | 0.83 | 0.01 | 0.01 | 0.02 | 0.36 |
| 532 | 1.00 | 1.11 | 1.61 | 1.16 | 0.96 | 1.26 | 1.30 | 1.06 | 0.97 | 0.90 | 1.26 | 1.17 | **0.66** |
| 533 | 3.69 | 10.24 | 21.23 | 5.29 | 1.29 | 0.97 | 0.70 | 0.56 | 0.52 | 0.86 | 0.26 | 0.07 | 0.03 |
| 534 | 2.25 | 3.74 | 3.57 | 2.01 | 1.20 | 0.82 | **0.60** | **0.52** | 0.90 | 0.78 | 0.37 | 0.16 | 0.14 |
| 535 | 0.05 | 0.08 | 2.72 | 6.13 | 0.88 | 1.38 | 1.06 | 0.86 | 0.95 | 27.14 | 30.41 | 12.94 | 0.31 |
| 536 | 1.74 | 1.28 | 1.61 | 1.47 | 1.08 | 1.14 | 0.94 | 0.94 | 0.95 | **0.75** | 0.65 | 0.73 | 0.58 |
| 545 | 0.77 | 1.49 | 1.75 | 1.10 | 0.75 | 0.93 | 0.84 | 0.88 | 1.46 | 2.27 | 1.22 | 0.57 | 0.50 |
| 546 | 1.82 | 1.35 | 1.87 | 1.49 | 1.04 | 1.10 | 0.91 | 1.14 | 0.87 | 1.20 | 0.61 | 0.68 | 0.61 |
| 548 | 6.11 | 6.08 | 8.14 | 6.35 | 0.96 | 1.31 | 0.93 | 1.00 | 1.01 | 1.03 | 0.21 | 0.15 | 0.12 |
| 549 | **1.28** | 1.05 | 1.76 | **1.25** | 1.04 | 1.00 | 0.91 | 1.07 | 0.93 | 0.96 | **0.78** | 0.87 | 0.61 |
| 551 | 0.06 | 0.11 | 0.40 | 0.72 | 1.30 | 0.57 | **3.02** | 1.00 | 0.44 | 10.24 | 9.93 | 27.71 | 2.48 |
| 557 | 3.04 | **1.78** | 1.22 | 0.97 | 0.99 | 1.05 | 0.74 | 0.86 | 0.95 | 0.52 | 0.34 | 0.42 | 0.70 |
| 559 | 5.41 | 3.90 | 1.79 | 1.75 | 4.31 | 0.57 | 1.00 | 1.10 | 0.91 | 0.87 | 0.10 | 0.26 | 0.62 |
| 561 | 6.45 | 2.51 | 0.87 | 0.59 | 0.68 | 1.35 | 0.59 | 0.92 | 0.90 | 0.20 | 0.21 | 0.24 | 1.07 |
| 565 | 15.80 | 15.59 | 8.80 | 5.09 | 1.00 | 1.00 | 0.97 | 1.19 | 1.00 | 1.00 | 0.06 | 0.06 | 0.14 |
| 566 | 1.43 | 0.87 | 1.59 | 1.30 | 1.07 | 0.97 | 0.96 | 1.01 | 1.18 | 1.09 | 0.68 | 1.10 | 0.63 |
| 569 | 1.12 | 2.60 | 6.53 | 5.57 | 0.77 | 0.87 | 0.69 | 0.85 | 1.53 | 1.21 | 0.77 | 0.26 | 0.13 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| 570 | 1.46 | 1.07 | 1.74 | 1.17 | 1.32 | 0.99 | 0.89 | 0.88 | 1.04 | 0.85 | 0.68 | 0.83 | 0.50 |
| 579 | 1.12 | 0.88 | 1.16 | 0.83 | 1.01 | 1.00 | 0.92 | 1.03 | 1.06 | 1.08 | 0.89 | 1.04 | 0.88 |
| 582 | 1.28 | 1.08 | 1.32 | 1.48 | 1.08 | 1.25 | 1.08 | 1.04 | 1.54 | 1.11 | 0.98 | 1.00 | 0.79 |
| 591 | 1.11 | 0.98 | 1.07 | 1.14 | 1.09 | 1.14 | 1.03 | 0.85 | 1.07 | 1.15 | 1.03 | 1.05 | 0.80 |
| 594 | 1.28 | 1.10 | 1.51 | 1.19 | 0.85 | 0.88 | 0.70 | 0.69 | 1.21 | 1.05 | 0.69 | 0.64 | 0.45 |
| 598 | 1.67 | 1.30 | 1.87 | 1.08 | 1.02 | 1.12 | 0.75 | 0.84 | 0.92 | 1.24 | 0.67 | 0.57 | 0.45 |
| 601 | 1.09 | 0.93 | 1.30 | 1.05 | 1.09 | 1.13 | 1.07 | 1.18 | 0.99 | 1.21 | 1.04 | 1.16 | 0.91 |
| 602 | 0.74 | 0.53 | 0.94 | 0.95 | 0.99 | 1.07 | 0.91 | 1.00 | 1.00 | 1.29 | 1.46 | 1.70 | 1.07 |
| 603 | 0.68 | 1.24 | 3.53 | 0.98 | 1.13 | 1.11 | 1.44 | 3.70 | 0.68 | 0.81 | 1.64 | 1.16 | 1.05 |
| 604 | 1.25 | 1.09 | 1.15 | 1.35 | 1.02 | 1.15 | 0.93 | 0.73 | 1.38 | 1.11 | 0.92 | 0.85 | 0.63 |
| 608 | 1.31 | 1.08 | 1.21 | 1.18 | 0.96 | 1.26 | 1.04 | 0.85 | 1.26 | 0.80 | 0.96 | 0.96 | 0.70 |
| 609 | 1.32 | 0.95 | 1.06 | 1.43 | 1.14 | 1.44 | 0.84 | 0.75 | 1.61 | 1.16 | 1.09 | 0.89 | 0.70 |
| 610 | 1.35 | 1.29 | 1.00 | 1.06 | 0.96 | 1.29 | 0.97 | 0.81 | 1.08 | 0.75 | 0.95 | 0.75 | 0.81 |
| 611 | 0.95 | 1.14 | 0.89 | 1.16 | 1.17 | 1.00 | 1.17 | 0.71 | 1.37 | 1.02 | 1.04 | 1.02 | 0.79 |
| 613 | 1.24 | 1.18 | 1.04 | 1.44 | 1.14 | 1.17 | 1.23 | 0.87 | 1.79 | 1.06 | 0.95 | 1.04 | 0.84 |
| 618 | 1.30 | 0.89 | 1.09 | 0.60 | 1.05 | 1.19 | 1.17 | 1.07 | 1.15 | 1.23 | 0.92 | 1.31 | 0.98 |
| 619 | 1.27 | 0.92 | 1.08 | 0.60 | 1.06 | 1.27 | 1.33 | 1.01 | 1.11 | 1.02 | 1.00 | 1.45 | 0.94 |
| 620 | 1.82 | 0.95 | 1.11 | 0.88 | 0.58 | 1.19 | 1.27 | 1.22 | 1.73 | 0.75 | 0.65 | 1.34 | 1.10 |
| 621 | 1.40 | 1.07 | 1.17 | 1.01 | 1.12 | 1.25 | 1.41 | 1.26 | 1.56 | 1.07 | 0.89 | 1.31 | 1.08 |
| 622 | 1.15 | 0.88 | 0.96 | 1.03 | 1.13 | 1.14 | 1.08 | 0.93 | 1.13 | 1.15 | 0.99 | 1.23 | 0.98 |
| 625 | 1.14 | 1.22 | 0.93 | 1.01 | 1.03 | 1.00 | 1.11 | 0.90 | 1.16 | 0.96 | 0.88 | 0.91 | 0.97 |
| 629 | 1.07 | 0.95 | 0.91 | 1.02 | 1.13 | 1.08 | 1.03 | 0.78 | 1.21 | 1.22 | 1.01 | 1.08 | 0.85 |
| 630 | 1.31 | 1.44 | 0.53 | 0.78 | 0.60 | 0.96 | 1.00 | 0.54 | 1.58 | 1.21 | 0.73 | 0.70 | 1.02 |
| 631 | 1.02 | 0.96 | 1.00 | 1.15 | 1.13 | 1.03 | 0.99 | 0.74 | 1.36 | 1.07 | 1.01 | 1.04 | 0.73 |
| 632 | 1.06 | 1.01 | 1.20 | 1.12 | 1.16 | 1.16 | 0.95 | 0.79 | 1.33 | 1.24 | 1.09 | 0.94 | 0.66 |
| 633 | 1.04 | 1.45 | 1.43 | 1.11 | 0.90 | 0.96 | 1.02 | 0.87 | 1.17 | 0.90 | 0.92 | 0.70 | 0.61 |
| 635 | 1.10 | 1.03 | 1.03 | 1.07 | 1.17 | 1.13 | 1.04 | 0.76 | 1.51 | 1.14 | 1.02 | 1.01 | 0.74 |
| 636 | 1.21 | 1.13 | 1.00 | 1.04 | 1.06 | 1.21 | 0.98 | 0.73 | 1.32 | 0.99 | 1.00 | 0.86 | 0.73 |
| 637 | 1.15 | 1.00 | 1.17 | 1.11 | 1.20 | 1.25 | 1.00 | 0.83 | 1.40 | 1.23 | 1.09 | 1.00 | 0.71 |
| 639 | 1.25 | 1.23 | 1.35 | 1.32 | 0.84 | 1.08 | 0.91 | 1.10 | 1.10 | 0.93 | 0.86 | 0.74 | 0.81 |
| 641 | 1.56 | 0.54 | 1.31 | 1.64 | 1.28 | 1.41 | 0.53 | 0.78 | 0.82 | 1.54 | 0.90 | 0.98 | 0.60 |
| 655 | 1.10 | 1.19 | 1.12 | 1.28 | 1.17 | 1.02 | 0.98 | 0.73 | 1.46 | 1.22 | 0.93 | 0.82 | 0.65 |
| 658 | 1.89 | 0.95 | 1.35 | 1.07 | 0.88 | 1.94 | 0.47 | 1.12 | 1.30 | 1.43 | 1.02 | 0.50 | 0.83 |
| 659 | 1.17 | 0.97 | 1.05 | 1.41 | 1.17 | 1.35 | 0.97 | 0.77 | 1.58 | 1.12 | 1.15 | 1.01 | 0.73 |
| 665 | 1.31 | 0.77 | 1.43 | 1.48 | 0.49 | 1.83 | 0.84 | 1.70 | 1.88 | 0.49 | 1.40 | 1.09 | 1.19 |
| 670.01 | 0.98 | 1.09 | 0.80 | 0.91 | 1.03 | 0.94 | 0.98 | 0.75 | 0.92 | 1.06 | 0.95 | 0.90 | 0.94 |
| 672 | 0.97 | 0.89 | 0.94 | 0.94 | 1.00 | 0.93 | 0.75 | 0.66 | 0.87 | 1.15 | 0.96 | 0.84 | 0.70 |
| 706 | 0.99 | 0.76 | 1.82 | 1.29 | 1.23 | 1.06 | 0.73 | 0.70 | 1.32 | 2.05 | 1.07 | 0.96 | 0.38 |
| 714 | 2.37 | 1.65 | 1.96 | 1.67 | 1.13 | 1.03 | 1.17 | 0.94 | 1.20 | 1.20 | 0.44 | 0.71 | 0.48 |
| 721 | 1.12 | 0.80 | 0.95 | 0.96 | 1.36 | 1.07 | 0.80 | 0.86 | 0.92 | 1.07 | 0.96 | 0.99 | 0.90 |
| 735 | 1.02 | 1.07 | 2.07 | 1.11 | 1.39 | 0.62 | 0.62 | 3.38 | 0.51 | 1.17 | 0.61 | 0.58 | 1.64 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| 742 | 0.94 | 1.03 | 1.01 | 1.13 | 0.88 | 0.92 | 0.90 | **0.68** | 1.23 | 0.98 | 0.97 | 0.88 | **0.68** |
| 744 | 1.01 | 0.98 | 0.91 | 0.99 | 1.09 | 1.27 | 1.11 | 0.72 | 1.41 | 1.07 | 1.26 | 1.12 | 0.80 |
| 809 | 1.00 | **0.84** | 0.93 | 0.84 | **1.18** | 1.07 | 1.03 | 0.92 | 1.06 | **1.21** | 1.07 | 1.23 | 0.99 |
| 811 | 1.08 | 1.00 | 1.49 | 0.69 | 0.86 | 0.87 | 2.70 | 0.83 | 0.70 | **0.62** | 0.80 | 2.70 | 0.56 |
| 819 | 1.18 | 1.10 | 1.03 | 1.09 | 1.17 | 1.12 | 1.19 | 0.83 | 1.08 | 1.14 | 0.95 | 1.08 | **0.80** |
| 820 | 1.18 | 1.10 | 1.13 | 1.18 | 1.13 | 1.10 | 1.06 | 0.99 | 1.15 | 1.06 | 0.93 | 0.96 | 0.87 |
| 821 | 1.10 | 0.99 | 1.04 | 1.02 | **1.22** | 1.05 | 1.01 | 0.91 | 1.07 | 1.16 | 0.95 | 1.01 | 0.88 |
| 822 | **1.15** | 0.97 | 0.97 | 0.95 | **1.14** | 1.05 | 1.02 | 0.86 | 1.04 | 1.19 | 0.91 | 1.05 | 0.89 |
| 823 | 0.99 | 1.02 | 1.30 | 1.04 | 0.92 | 0.83 | 1.19 | 0.73 | 1.08 | 1.28 | 0.84 | 1.16 | 0.56 |
| 825 | 1.04 | 1.08 | 1.15 | 1.04 | 1.24 | 1.18 | 1.16 | 0.97 | 1.03 | 1.38 | 1.13 | 1.07 | 0.85 |
| 833 | 4.50 | **3.93** | 4.57 | 0.66 | **5.22** | 1.59 | 1.63 | 1.47 | 0.24 | 1.06 | **0.35** | **0.41** | 0.32 |
| 834 | 7.21 | **4.31** | 5.17 | 0.83 | 2.94 | 2.50 | 1.80 | 1.71 | 0.31 | 1.26 | 0.35 | 0.42 | 0.33 |
| 835 | 6.99 | 4.80 | **5.68** | 0.76 | 4.00 | 2.41 | 1.72 | 1.46 | 0.27 | 1.18 | 0.34 | 0.36 | 0.26 |
| 840 | 1.02 | 0.98 | 0.98 | 1.43 | 1.03 | 0.92 | 1.09 | 1.06 | 1.36 | 1.12 | 0.90 | 1.11 | 1.07 |
| 849 | 1.29 | 1.21 | 1.34 | 1.12 | 1.26 | 1.53 | 0.95 | 1.30 | 1.16 | 1.48 | 1.18 | **0.78** | 0.97 |
| 851 | 1.14 | 1.02 | 1.06 | 1.35 | 1.22 | 1.07 | 0.93 | 0.96 | 1.25 | 1.55 | 0.94 | 0.91 | **0.90** |
| 876 | 1.37 | 0.98 | 2.19 | 1.20 | 1.04 | 1.42 | 1.21 | 1.61 | 0.63 | 1.18 | 1.03 | 1.24 | 0.74 |
| 877 | 0.99 | 0.77 | 1.57 | 0.92 | 1.68 | 1.37 | 1.18 | 1.35 | 1.39 | 0.74 | 1.38 | 1.53 | 0.86 |
| 881 | **1.19** | 1.04 | 1.09 | 1.15 | 1.01 | 1.10 | 0.91 | 0.89 | 1.08 | 0.99 | 0.93 | 0.87 | **0.82** |
| 882 | 4.54 | 2.07 | 1.52 | 1.22 | 0.98 | 0.95 | 0.83 | 0.87 | 1.17 | 0.38 | 0.21 | 0.40 | **0.57** |
| 883 | 0.96 | 0.99 | 1.11 | 1.12 | 1.04 | 1.00 | 0.94 | 0.91 | 0.99 | 1.16 | 1.04 | 0.95 | 0.82 |
| 890 | 1.15 | 0.89 | 1.25 | 1.16 | 0.88 | 1.03 | 1.00 | 1.13 | 0.91 | 0.91 | 0.89 | 1.12 | 0.91 |
| 905 | 1.36 | 0.77 | 1.14 | 1.01 | 0.94 | 1.04 | 0.84 | 0.84 | 0.98 | 1.05 | 0.77 | 1.09 | 0.74 |
| 909 | 0.92 | **0.58** | 1.66 | 0.79 | 0.99 | 1.01 | 0.70 | 0.96 | 1.31 | 2.25 | 1.10 | 1.20 | 0.58 |
| 915 | 0.82 | 0.59 | 0.96 | 1.15 | 1.39 | 1.39 | 0.60 | 0.60 | 1.07 | 2.23 | 1.69 | 1.02 | 0.63 |
| 919 | 0.82 | 0.83 | 1.15 | 1.02 | 1.15 | 1.18 | 0.87 | 0.98 | 1.36 | 2.17 | 1.43 | 1.05 | 0.85 |
| 920 | 4.29 | 4.11 | 2.97 | 0.97 | 2.62 | 1.85 | 1.48 | 1.56 | 0.48 | 0.90 | 0.43 | **0.36** | 0.52 |
| 922 | 6.92 | 3.72 | **3.33** | 0.88 | 1.83 | 2.14 | 1.07 | 1.32 | 0.49 | 0.68 | 0.31 | 0.29 | 0.40 |
| 923 | **4.25** | 3.49 | **3.59** | 1.02 | 2.34 | 1.33 | 1.11 | 1.31 | 0.39 | 1.12 | 0.31 | 0.32 | 0.36 |
| 926 | 1.60 | 2.54 | 3.28 | 1.32 | 1.00 | 1.31 | 0.86 | 1.72 | 0.39 | 1.00 | 0.82 | **0.34** | 0.52 |
| 929 | 6.38 | 2.35 | 2.92 | 0.87 | **3.81** | 2.14 | 0.63 | 1.09 | 0.60 | 1.38 | **0.34** | 0.27 | 0.37 |
| 930 | 3.92 | **3.69** | 3.18 | 0.97 | 2.15 | 1.65 | 0.99 | 1.69 | 0.42 | 2.04 | 0.42 | 0.27 | 0.53 |
| 934 | **5.63** | **3.63** | 3.51 | 0.93 | **3.77** | 2.01 | 0.85 | 1.38 | 0.42 | 1.61 | 0.36 | 0.23 | 0.39 |
| 935 | **4.47** | 2.75 | 2.87 | 0.85 | 2.51 | 2.61 | 0.74 | 1.91 | 0.47 | 2.51 | 0.58 | 0.27 | 0.67 |
| 936 | 8.51 | 2.99 | **4.20** | 0.79 | **3.92** | 2.52 | 0.70 | 1.23 | 0.44 | 1.69 | **0.30** | 0.23 | **0.29** |
| 937 | 4.35 | 2.54 | **3.47** | 0.84 | 1.83 | 2.15 | 0.95 | 1.24 | 0.40 | 1.10 | 0.49 | **0.38** | 0.36 |
| 938 | 0.91 | 0.85 | 1.38 | 1.09 | 1.21 | 1.09 | 0.77 | 0.78 | 1.45 | **1.62** | 1.20 | 0.91 | 0.57 |
| 939 | 2.54 | 3.97 | 2.24 | 0.83 | 1.00 | 1.62 | 1.15 | 1.25 | 0.34 | 1.00 | 0.64 | 0.29 | 0.56 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| 945 | 4.42 | 4.94 | 3.93 | 1.12 | 1.05 | 1.87 | 1.37 | 1.83 | **0.29** | 0.59 | 0.42 | 0.28 | 0.47 |
| 970 | 0.77 | 1.21 | 1.06 | 0.96 | 0.90 | 0.57 | 0.96 | 1.06 | 1.30 | 1.09 | 0.74 | 0.80 | 1.00 |
| 1004 | 1.15 | 0.86 | **1.33** | 1.10 | 0.98 | 1.07 | 0.93 | 1.10 | 1.01 | 1.15 | 0.92 | 1.08 | 0.83 |
| 1005 | 1.25 | 0.98 | 1.19 | 1.10 | 1.09 | 1.00 | 0.96 | 0.92 | 1.05 | 1.19 | 0.80 | 0.98 | 0.78 |
| 1018 | 1.18 | 0.93 | 1.22 | 1.33 | 0.82 | 1.10 | 1.19 | 1.14 | 0.97 | 1.16 | 0.93 | 1.28 | 0.93 |
| 1020 | 1.08 | 0.86 | **1.29** | 1.17 | 0.98 | 1.04 | 0.91 | 1.08 | 1.03 | 1.04 | 0.96 | 1.06 | 0.84 |
| 1024 | 1.35 | 0.80 | 1.96 | 2.51 | 2.07 | 1.15 | 0.89 | 1.38 | 2.12 | 1.72 | 0.86 | 1.12 | 0.70 |
| 1034 | 1.13 | 0.73 | **1.23** | 1.08 | 1.50 | 0.95 | 1.09 | 1.17 | 1.04 | 1.20 | 0.84 | 1.48 | 0.95 |
| 1057 | 0.80 | 1.01 | 1.40 | **1.64** | **1.88** | 0.39 | 0.28 | 1.09 | 1.31 | 1.27 | **0.48** | 0.28 | 0.78 |
| 1059 | 0.98 | 0.78 | 1.49 | 1.01 | 1.37 | 1.07 | 1.21 | 0.89 | **0.40** | 1.33 | 1.09 | 1.55 | 0.60 |
| 1098 | 59.92 | 16.58 | 8.61 | 3.60 | 0.75 | 0.77 | 0.95 | 1.25 | 1.20 | 0.82 | 0.01 | 0.06 | 0.15 |
| 1101 | 0.82 | 0.79 | 2.13 | 2.13 | 1.12 | 1.05 | 0.88 | 1.07 | 1.35 | 1.01 | 1.29 | 1.11 | 0.50 |
| 1105 | 1.21 | 1.14 | 1.08 | 0.77 | 1.06 | 0.93 | **0.75** | 0.59 | 0.54 | 1.13 | **0.77** | 0.66 | 0.54 |
| 1106 | 2.26 | 1.32 | 1.37 | **1.82** | 0.46 | 0.98 | 0.48 | 0.69 | 1.43 | 0.72 | 0.43 | 0.36 | **0.51** |
| 1114 | 1.14 | 0.46 | 0.81 | 0.83 | 1.20 | 1.31 | 0.82 | 0.69 | 1.22 | 1.01 | 1.15 | 1.80 | 0.85 |
| 1116 | 0.86 | 0.57 | 0.77 | 0.72 | 1.22 | 1.14 | 0.81 | 0.86 | 1.33 | 1.15 | 1.32 | 1.41 | 1.13 |
| 1128 | 1.42 | 1.06 | **1.30** | 0.78 | 1.42 | 1.16 | 1.06 | **0.76** | 0.99 | 1.19 | 0.82 | 1.00 | 0.59 |
| 1149 | 1.15 | 0.79 | 1.02 | 1.01 | 1.09 | 1.10 | 0.92 | 0.86 | 1.24 | 1.13 | 0.96 | 1.18 | 0.85 |
| 1150 | 0.89 | 1.13 | 0.89 | 0.70 | 1.50 | 0.92 | 1.88 | 0.62 | 1.04 | **2.41** | 1.04 | 1.67 | 0.69 |
| 1180 | 1.55 | 1.36 | 1.13 | 1.42 | 1.00 | 1.05 | 1.07 | 0.92 | 1.38 | 0.86 | 0.68 | 0.78 | **0.81** |
| 1181 | 1.05 | 1.24 | 0.95 | 0.96 | 1.19 | 1.42 | 1.08 | 0.67 | 0.98 | 1.88 | 1.36 | 0.87 | 0.70 |
| 1199 | 1.24 | 1.03 | 1.49 | 1.46 | 1.00 | 1.17 | 1.01 | 1.03 | 1.21 | 1.20 | 0.94 | 0.99 | 0.69 |
| 1202 | 1.12 | 0.78 | 1.47 | 0.76 | 1.07 | 0.98 | 0.71 | 0.99 | 0.95 | 0.96 | 0.88 | 0.91 | 0.67 |
| 1212 | 4.95 | **5.83** | 3.95 | 0.96 | **4.28** | 1.71 | 1.72 | 2.29 | 0.32 | 1.15 | 0.35 | 0.30 | 0.58 |
| 1216 | **2.48** | 4.30 | 2.84 | 1.51 | 1.21 | 1.00 | 2.22 | 1.65 | 1.03 | 1.22 | **0.40** | **0.52** | 0.58 |
| 1221 | **1.35** | 0.88 | 0.87 | 1.16 | 0.93 | 1.09 | 0.91 | 0.82 | 1.07 | 1.06 | 0.81 | 1.03 | 0.94 |
| 1224 | 2.24 | 0.99 | 0.87 | 0.62 | 1.18 | 1.03 | 1.78 | 2.03 | 0.81 | **0.55** | 0.46 | 1.80 | 2.33 |
| 1232 | 1.27 | 1.14 | 1.08 | 0.99 | 1.18 | 1.04 | 1.03 | 0.89 | 0.99 | 1.09 | **0.82** | 0.91 | 0.82 |
| 1242 | **1.17** | 1.05 | 1.08 | 1.06 | 1.03 | 1.11 | 1.02 | 0.90 | 1.01 | 1.05 | 0.94 | 0.97 | 0.83 |

| | ANVOA Contrasts | | | | ANVOA Contrasts | | | | | ANVOA Contrasts | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-7 C-7 | T1-14 C-14 | T1-21 C-21 | T1-28 C-28 | T2-0 C-0 | T2-7 C-7 | T2-14 C-14 | T2-21 C-21 | T2-28 C-28 | T2-0 T1-0 | T2-7 T1-7 | T2-14 T1-14 | T2-21 T1-21 |
| ~~1242.1~~ | 0.85 | 1.24 | 1.09 | 1.07 | 1.16 | 0.88 | 1.18 | 1.18 | 0.98 | 1.02 | 1.04 | 0.95 | 1.08 |
| 1243 | 1.22 | 0.99 | 0.88 | 1.13 | 1.04 | 1.14 | 0.94 | 0.74 | 0.95 | 1.05 | 0.93 | 0.95 | 0.84 |
| 1266 | 0.81 | 0.82 | 1.60 | 1.22 | 0.89 | 0.99 | 0.85 | 1.26 | 1.02 | 1.27 | 1.22 | 1.04 | 0.79 |
| 1288 | 0.99 | 1.03 | 1.09 | 1.11 | 1.21 | 0.88 | 0.97 | **0.85** | 1.07 | 1.21 | 0.88 | 0.94 | 0.78 |
| 1300 | 1.10 | 0.99 | 1.06 | 1.12 | 1.13 | 1.03 | 1.02 | 0.89 | 1.04 | 1.11 | 0.94 | 1.02 | 0.84 |
| 1318 | 1.02 | **0.76** | 1.24 | 1.11 | 0.95 | 1.00 | 0.92 | 1.01 | 0.91 | 1.09 | 0.98 | 1.20 | 0.81 |
| 1360 | 1.17 | 0.85 | 0.85 | 0.73 | 0.94 | 1.02 | 1.00 | 0.60 | 0.88 | 1.06 | 0.87 | 1.17 | 0.70 |
| 1469 | 1.13 | 0.93 | 1.11 | 0.94 | 1.06 | 1.08 | 0.91 | 0.88 | 1.00 | 1.09 | 0.96 | 0.97 | 0.79 |
| 1531 | 1.24 | 0.85 | 1.58 | 1.01 | 1.12 | 1.31 | 0.71 | 1.10 | 0.91 | 1.46 | 1.06 | 0.84 | 0.70 |
| 1565 | 1.09 | 0.92 | 1.03 | 1.10 | 1.10 | 1.12 | 0.98 | **0.84** | 1.18 | 1.27 | 1.02 | 1.07 | 0.82 |
| 1584 | 1.08 | 1.03 | 1.09 | 1.17 | 0.98 | 1.09 | 1.04 | 0.92 | 1.16 | 1.09 | 1.01 | 1.00 | 0.85 |
| 1585 | 0.94 | 1.12 | **1.23** | **1.23** | 1.06 | 1.15 | 1.05 | 1.15 | 0.88 | 1.02 | **1.23** | 0.94 | 0.93 |
| 1612 | 1.07 | 0.99 | 1.12 | 1.15 | **1.15** | 1.05 | 1.03 | 0.95 | 1.04 | 1.23 | 0.98 | 1.04 | **0.85** |
| 1613 | 1.06 | 1.16 | 1.08 | 1.18 | 1.06 | 0.97 | 1.10 | 1.08 | 1.02 | 1.03 | 0.91 | 0.94 | 1.00 |
| 1614 | 0.99 | 0.81 | 0.98 | 0.96 | 1.08 | 0.92 | **1.39** | 0.80 | 1.01 | 1.11 | 0.94 | 1.72 | 0.82 |
| 1615 | 0.91 | 1.18 | **0.53** | 1.14 | 1.07 | 1.17 | 0.79 | 0.62 | 1.16 | 1.19 | 1.30 | 0.67 | 1.18 |
| 1632 | 1.41 | 1.44 | 2.34 | 2.17 | 0.98 | 1.07 | 0.96 | 1.02 | 0.95 | 0.99 | **0.76** | 0.67 | 0.44 |
| 1662 | 1.11 | 1.09 | 1.20 | 0.99 | 0.99 | 0.89 | 1.13 | 1.01 | 1.12 | 1.18 | 0.80 | 1.04 | 0.84 |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| 1 | 1.19 | 1.21 | 1.74 | 1.81 | 1.98 | 1.44 | 1.04 | 1.10 | 1.36 | 1.40 | 1.93 | 2.14 | 1.03 |
| 3 | 1.15 | 1.06 | 1.01 | 1.05 | 1.23 | 0.95 | 1.04 | 1.17 | 1.20 | 1.39 | 1.04 | 1.29 | 1.16 |
| 4 | 0.81 | 0.94 | 0.85 | 0.81 | 0.68 | 0.90 | 0.95 | 0.85 | 1.29 | 0.97 | 1.20 | 1.10 | 0.75 |
| 7 | 1.09 | 0.88 | 1.04 | 0.79 | 0.87 | 1.17 | 0.77 | 1.10 | 1.22 | 1.13 | 1.10 | 1.09 | 0.93 |
| 8 | 0.82 | 1.02 | 1.26 | 1.06 | 1.16 | 1.23 | 0.84 | 1.10 | 1.28 | 1.27 | 1.50 | 1.49 | 0.99 |
| 17 | 0.90 | 0.93 | 1.04 | 1.19 | 1.20 | 1.12 | 1.14 | 1.01 | 1.18 | 1.31 | 1.24 | 1.34 | 1.11 |
| 22 | 0.85 | 1.03 | 1.07 | 1.09 | 1.09 | 1.04 | 1.02 | 1.00 | 1.16 | 1.14 | 1.17 | 1.21 | 0.98 |
| 24 | 0.81 | 1.00 | 1.15 | 1.08 | 1.20 | 1.16 | 0.94 | 1.11 | 1.26 | 1.29 | 1.52 | 1.19 | 1.02 |
| 25 | 0.73 | 0.90 | 1.00 | 0.75 | 0.82 | 1.11 | 0.75 | 1.10 | 1.08 | 0.91 | 0.99 | 0.96 | 0.84 |
| 26 | 0.44 | 0.68 | 0.77 | 0.46 | 1.01 | 1.13 | 0.59 | 2.20 | 1.09 | 1.10 | 1.18 | 1.39 | 1.01 |
| 27 | 1.09 | 1.07 | 1.34 | 1.13 | 1.20 | 1.25 | 0.84 | 1.06 | 1.21 | 1.15 | 1.41 | 1.37 | 0.95 |
| 39 | 1.13 | 0.84 | 1.01 | 0.81 | 0.84 | 1.20 | 0.80 | 1.04 | 1.09 | 0.89 | 0.91 | 0.89 | 0.82 |
| 44 | 1.18 | 0.91 | 0.76 | 0.69 | 0.64 | 0.84 | 0.91 | 0.93 | 0.81 | 0.65 | 0.54 | 0.53 | 0.80 |
| 45 | 0.98 | 1.18 | 1.02 | 0.98 | 1.14 | 0.87 | 0.96 | 1.16 | 1.20 | 1.11 | 1.13 | 1.18 | 0.92 |
| 50 | 0.88 | 1.10 | 1.10 | 1.10 | 1.03 | 1.00 | 1.00 | 0.94 | 0.85 | 0.82 | 1.20 | 1.01 | 0.97 |
| 69 | 0.62 | 1.01 | 1.53 | 0.80 | 0.97 | 1.51 | 0.53 | 1.21 | 1.18 | 1.31 | 1.39 | 1.50 | 1.11 |
| 74 | 1.01 | 1.05 | 0.99 | 1.05 | 1.07 | 0.95 | 1.06 | 1.01 | 1.26 | 1.23 | 1.17 | 1.17 | 0.97 |
| 75 | 0.86 | 1.50 | 1.10 | 1.19 | 1.09 | 0.74 | 1.08 | 0.91 | 1.07 | 0.94 | 0.98 | 1.06 | 0.88 |
| 80 | 1.20 | 1.11 | 1.07 | 1.43 | 1.44 | 0.96 | 1.34 | 1.01 | 0.92 | 1.43 | 1.38 | 0.94 | 1.55 |
| 83 | 0.89 | 1.20 | 1.24 | 1.29 | 1.33 | 1.03 | 1.04 | 1.03 | 1.33 | 1.31 | 1.31 | 1.40 | 0.99 |
| 88 | 0.98 | 0.99 | 1.08 | 1.05 | 0.97 | 1.09 | 0.97 | 0.92 | 1.14 | 1.09 | 1.28 | 1.10 | 0.95 |
| 99 | 0.94 | 1.09 | 1.15 | 1.16 | 1.18 | 1.05 | 1.00 | 1.02 | 1.24 | 1.21 | 1.18 | 1.28 | 0.98 |
| 128 | 1.12 | 1.09 | 1.21 | 1.22 | 1.15 | 1.11 | 1.01 | 0.94 | 1.23 | 1.11 | 1.24 | 1.00 | 0.90 |
| 135 | 0.93 | 0.90 | 1.13 | 1.16 | 0.89 | 1.25 | 1.03 | 0.77 | 1.09 | 1.02 | 1.02 | 1.03 | 0.94 |
| 144 | 0.89 | 0.96 | 0.94 | 1.05 | 0.96 | 0.97 | 1.12 | 0.92 | 1.08 | 1.10 | 0.89 | 0.88 | 1.01 |
| 145 | 0.89 | 1.06 | 1.17 | 1.16 | 1.17 | 1.10 | 0.99 | 1.02 | 1.30 | 1.28 | 1.27 | 1.33 | 0.98 |
| 151 | 0.95 | 0.99 | 1.03 | 1.01 | 0.98 | 1.05 | 0.98 | 0.97 | 1.19 | 1.09 | 1.19 | 1.24 | 0.92 |
| 164 | 0.93 | 1.16 | 1.06 | 1.12 | 1.25 | 0.91 | 1.06 | 1.12 | 1.04 | 1.03 | 1.07 | 1.10 | 0.99 |
| 170 | 1.20 | 1.15 | 1.15 | 1.00 | 1.13 | 1.00 | 0.88 | 1.12 | 1.18 | 1.26 | 1.44 | 1.14 | 1.06 |
| 172 | 3.57 | 0.88 | 1.02 | 1.07 | 0.74 | 1.17 | 1.04 | 0.70 | 0.42 | 0.31 | 0.45 | 0.47 | 0.73 |
| 173 | 3.01 | 1.19 | 1.45 | 1.43 | 1.20 | 1.22 | 0.99 | 0.84 | 0.71 | 0.39 | 0.43 | 0.50 | 0.55 |
| 179 | 1.02 | 1.00 | 1.91 | 3.10 | 4.15 | 1.91 | 1.62 | 1.34 | 2.80 | 4.20 | 4.40 | 4.95 | 1.50 |
| 180 | 0.79 | 1.14 | 1.15 | 1.13 | 1.18 | 1.01 | 0.98 | 1.05 | 1.44 | 1.45 | 1.47 | 1.47 | 1.01 |
| 181 | 0.88 | 1.09 | 1.17 | 1.15 | 1.22 | 1.08 | 0.98 | 1.07 | 1.45 | 1.46 | 1.59 | 1.54 | 1.00 |
| 190 | 0.93 | 1.07 | 1.14 | 1.15 | 1.17 | 1.07 | 1.01 | 1.02 | 1.21 | 1.17 | 1.20 | 1.23 | 0.96 |
| 193 | 2.91 | 1.18 | 1.36 | 1.29 | 0.99 | 1.16 | 0.94 | 0.77 | 0.62 | 0.31 | 0.44 | 0.48 | 0.49 |
| 198 | 0.44 | 1.01 | 1.47 | 1.77 | 2.20 | 1.45 | 1.20 | 1.25 | 2.66 | 3.17 | 4.00 | 3.94 | 1.19 |
| 200 | 1.04 | 1.00 | 0.87 | 0.95 | 0.90 | 0.87 | 1.09 | 0.94 | 0.96 | 0.82 | 0.94 | 0.84 | 0.85 |
| 202 | 1.27 | 0.98 | 0.93 | 1.00 | 0.77 | 0.95 | 1.07 | 0.77 | 0.93 | 0.62 | 0.97 | 0.85 | 0.67 |
| 205 | 1.05 | 0.97 | 1.14 | 1.06 | 0.98 | 1.17 | 0.93 | 0.92 | 1.15 | 1.07 | 1.12 | 1.13 | 0.93 |
| 206 | 0.99 | 1.10 | 1.12 | 1.09 | 1.04 | 1.01 | 0.98 | 0.95 | 1.22 | 1.13 | 1.17 | 1.16 | 0.93 |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| 213 | 1.28 | 1.33 | 1.84 | 2.04 | 2.48 | **1.38** | 1.11 | 1.22 | 1.11 | 1.69 | 3.12 | 2.75 | 1.52 |
| 216 | 0.92 | 1.26 | **1.50** | 1.13 | 1.13 | 1.19 | **0.75** | 1.01 | 1.23 | 1.51 | **1.94** | 1.50 | 1.23 |
| 224 | 1.09 | 1.62 | 1.81 | 2.07 | 1.89 | 1.11 | 1.14 | 0.92 | 1.65 | 1.69 | 1.64 | 1.89 | 1.02 |
| 225 | 0.96 | 0.98 | 0.71 | 0.61 | 0.51 | 0.72 | 0.86 | 0.83 | 0.92 | 0.70 | 0.57 | 0.53 | 0.77 |
| 227 | 1.04 | 0.83 | 1.01 | 1.02 | 1.02 | 1.22 | 1.01 | 1.00 | 1.23 | 0.89 | 1.26 | 1.11 | 0.72 |
| 229 | 0.93 | 0.99 | 1.14 | 0.98 | 1.06 | 1.15 | 0.85 | 1.08 | 1.09 | 1.05 | 1.18 | 1.01 | 0.96 |
| 231 | 0.61 | 1.53 | 2.33 | 2.63 | 2.91 | 1.52 | 1.13 | 1.11 | **1.62** | 3.95 | 5.57 | 4.98 | 2.44 |
| 241 | 1.44 | 1.72 | **2.11** | 2.92 | 1.60 | 1.23 | 1.38 | **0.55** | 1.42 | 1.34 | 1.75 | 1.79 | 0.95 |
| 244 | 0.71 | 0.96 | 1.09 | 0.80 | 1.02 | 1.14 | 0.73 | **1.29** | 1.21 | 1.23 | 1.41 | **1.34** | 1.02 |
| 245 | 0.90 | 0.95 | 1.08 | 0.97 | 1.03 | 1.14 | 0.89 | 1.07 | 1.20 | 1.11 | **1.34** | **1.24** | 0.92 |
| 246 | 1.00 | 1.05 | 1.14 | **1.16** | 1.12 | 1.08 | 1.02 | 0.97 | **1.17** | 1.14 | 1.35 | 1.31 | 0.98 |
| 248 | 0.88 | 1.07 | **1.17** | 1.16 | **1.18** | 1.10 | 0.99 | 1.02 | 1.02 | 1.04 | 1.10 | 1.18 | 1.02 |
| 252 | 0.90 | 1.18 | 1.15 | 1.17 | 1.13 | 0.98 | 1.01 | 0.97 | 1.28 | 1.39 | 1.18 | 1.23 | 1.08 |
| 259 | 0.95 | 1.04 | 1.08 | 1.08 | 1.05 | 1.04 | 1.00 | 0.97 | 1.15 | 1.11 | 1.16 | **1.14** | 0.96 |
| 260 | **0.83** | 0.74 | 0.95 | 1.04 | 1.02 | 1.28 | 1.10 | 0.97 | 0.93 | 1.13 | 1.15 | **1.21** | **1.22** |
| 263 | 0.85 | 0.96 | 1.17 | 0.93 | 1.02 | 1.21 | **0.80** | 1.10 | **1.20** | **1.24** | 1.38 | 1.38 | 1.03 |
| 266 | 0.92 | 2.10 | 2.68 | 2.58 | 2.67 | 1.28 | 0.96 | 1.04 | 2.94 | 3.49 | 3.08 | 2.88 | 1.19 |
| 270 | 1.04 | 1.10 | **1.22** | 1.30 | 1.28 | 1.11 | 1.07 | 0.98 | 1.20 | 1.17 | 1.28 | **1.29** | 0.98 |
| 280 | 0.97 | 0.94 | 1.04 | 0.96 | 0.88 | 1.11 | 0.92 | 0.92 | 0.91 | 0.97 | 0.81 | 0.78 | 1.06 |
| 281 | 1.16 | 1.17 | 1.03 | 1.12 | 1.40 | 0.88 | 1.09 | 1.25 | 1.38 | 1.35 | 1.02 | 0.73 | 0.98 |
| 282 | 1.15 | 3.30 | 5.54 | 7.26 | 8.56 | 1.68 | 1.31 | 1.18 | 4.69 | 6.52 | 8.93 | 8.91 | 1.39 |
| 283 | 1.11 | 0.92 | 0.76 | 0.68 | 0.70 | 0.82 | 0.91 | 1.02 | 0.84 | 0.65 | 0.58 | 0.51 | **0.77** |
| 285 | 1.00 | 0.25 | 0.15 | 0.09 | 0.09 | **0.58** | 0.64 | 1.00 | 0.46 | 0.21 | 0.11 | 0.08 | 0.46 |
| 404 | 0.95 | 1.09 | 0.94 | 1.16 | 0.83 | 0.86 | 1.24 | **0.72** | 1.24 | 1.14 | 1.08 | 0.79 | 0.92 |
| 453 | 0.38 | 0.98 | 1.33 | 1.23 | 1.53 | 1.37 | 0.92 | **1.24** | 1.73 | 2.78 | 4.85 | 4.70 | 1.60 |
| 455 | 0.53 | **1.67** | 3.68 | 3.09 | 3.93 | 2.20 | 0.84 | 1.27 | 2.57 | 1.96 | 4.06 | 4.70 | 0.77 |
| 472 | 0.74 | 1.07 | 1.33 | 1.19 | 1.33 | **1.24** | 0.89 | 1.12 | 0.94 | 0.99 | 1.75 | 1.94 | 1.04 |
| 478 | 0.83 | 0.88 | 1.34 | 0.99 | 1.06 | 1.53 | 0.74 | 1.07 | 0.91 | 0.69 | 0.87 | 0.82 | 0.75 |
| 482 | 0.84 | **0.77** | 0.95 | 0.79 | 0.81 | 1.23 | 0.84 | 1.02 | 1.20 | 1.07 | **1.36** | 1.18 | 0.89 |
| 487 | 0.97 | 0.96 | 1.05 | 0.86 | 0.86 | 1.10 | 0.82 | 1.00 | 0.98 | 0.91 | 1.11 | 0.97 | 0.93 |
| 489 | 0.90 | 1.04 | 1.48 | 1.36 | 1.26 | 1.42 | 0.92 | 0.92 | 2.15 | 2.57 | 3.20 | 2.29 | 1.19 |
| 496 | 0.98 | 1.07 | 1.07 | 1.08 | 1.06 | 1.00 | 1.01 | 0.98 | 1.08 | 1.08 | 1.04 | 0.97 | 0.99 |
| 501 | 0.82 | 3.92 | 8.46 | 6.60 | 9.32 | 2.16 | 0.78 | 1.41 | 2.89 | 5.26 | 8.28 | 8.62 | 1.82 |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| ~~515~~ | 0.99 | 0.99 | 1.27 | 0.97 | 1.07 | 1.28 | 0.77 | 1.10 | 1.15 | 0.96 | 1.57 | 1.02 | 0.84 |
| 517 | 0.12 | 1.90 | 2.91 | 2.72 | 3.54 | 1.54 | 0.93 | 1.30 | 6.24 | 11.39 | 15.34 | 17.06 | 1.83 |
| 519 | 1.05 | 1.10 | 1.49 | 1.30 | 1.27 | 1.35 | 0.87 | 0.98 | 1.01 | 4.50 | 7.99 | 6.65 | 4.46 |
| 521 | 1.02 | 0.95 | 1.04 | 0.91 | 0.92 | 1.09 | 0.88 | 1.01 | 1.11 | 1.00 | 1.10 | 1.05 | 0.91 |
| 523 | 0.85 | 0.65 | 0.87 | 0.63 | 0.77 | 1.33 | 0.72 | 1.22 | 1.57 | 1.58 | 1.28 | 1.28 | 1.01 |
| 524 | 1.02 | 1.01 | 1.42 | 1.19 | 1.05 | 1.40 | 0.84 | 0.88 | 1.86 | 2.96 | 2.30 | 2.24 | **1.59** |
| 527 | 1.74 | 1.03 | 1.09 | 1.09 | 0.88 | 1.06 | 1.00 | **0.81** | 2.24 | 0.38 | 0.18 | 0.14 | 0.17 |
| 529 | 0.64 | 0.63 | 0.61 | 0.37 | 0.34 | 0.97 | 0.61 | 0.91 | 0.81 | 0.64 | 0.32 | 0.21 | 0.78 |
| 531 | 0.39 | 0.32 | 1.57 | **0.20** | **0.24** | 4.94 | **0.13** | 1.21 | 1.71 | 0.33 | 0.04 | 0.02 | 0.19 |
| 532 | 0.84 | 0.92 | 1.08 | 0.86 | 1.03 | 1.17 | 0.79 | 1.21 | 0.87 | 1.13 | 1.30 | 1.13 | 1.30 |
| 533 | 0.10 | 0.46 | 0.12 | 0.03 | 0.03 | 0.26 | 0.28 | 1.01 | 1.13 | 0.82 | 0.47 | 0.12 | 0.72 |
| 534 | 0.45 | 0.56 | 0.24 | 0.14 | 0.10 | 0.43 | 0.59 | 0.72 | 0.82 | **0.59** | 0.33 | 0.13 | 0.72 |
| 535 | 0.16 | 0.83 | 0.78 | 0.42 | 0.35 | 0.94 | 0.54 | 0.83 | 1.17 | **1.98** | 35.49 | 66.45 | 1.69 |
| 536 | 0.65 | 2.86 | 5.40 | 5.99 | 6.99 | 1.89 | 1.11 | 1.17 | 3.46 | 4.82 | 6.72 | 7.12 | 1.39 |
| 545 | 1.33 | 0.59 | 0.42 | 0.37 | 0.24 | 0.72 | 0.88 | 0.66 | 1.37 | 1.90 | 1.96 | 0.81 | 1.39 |
| 546 | 0.58 | 0.83 | 1.09 | 0.89 | 1.10 | **1.32** | 0.82 | 1.23 | 1.74 | 1.70 | 1.93 | 1.90 | 0.98 |
| 548 | 0.16 | 0.90 | 1.11 | 0.95 | 1.28 | 1.23 | 0.86 | 1.35 | 5.91 | 7.24 | 8.32 | 8.74 | 1.22 |
| 549 | 0.75 | 1.18 | 1.56 | 1.26 | 1.45 | **1.32** | 0.81 | 1.15 | 1.40 | 1.51 | 2.06 | 1.68 | 1.08 |
| 551 | 0.61 | 2.49 | 1.16 | 2.04 | 3.29 | 0.47 | 1.76 | 1.61 | 1.13 | 1.00 | 6.51 | 18.77 | 0.88 |
| 557 | 0.98 | 0.87 | 1.04 | 0.84 | 0.65 | 1.19 | 0.81 | 0.77 | 1.39 | 0.96 | 0.54 | 0.33 | 0.69 |
| 559 | **0.52** | 3.73 | 3.48 | 3.64 | 4.20 | 0.93 | 1.05 | 1.15 | 4.06 | **2.73** | 1.31 | 1.48 | 0.67 |
| 561 | 1.53 | 0.62 | 0.93 | 0.63 | 0.62 | 1.49 | 0.67 | 0.99 | 1.18 | 0.68 | 0.16 | 0.11 | 0.58 |
| 565 | 0.20 | 1.00 | 1.03 | 1.00 | 1.00 | 1.03 | 0.97 | 1.00 | 15.80 | 16.12 | 8.80 | 5.09 | 1.02 |
| 566 | 0.91 | 0.97 | 1.27 | 0.89 | 0.91 | 1.31 | **0.70** | 1.02 | **1.43** | 1.14 | **1.46** | 1.22 | 0.80 |
| 569 | 0.27 | 1.00 | 1.06 | 0.70 | 0.81 | 1.06 | 0.65 | 1.16 | 1.78 | 4.38 | 7.21 | 7.15 | **2.46** |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| 570 | 0.89 | 1.16 | 1.97 | 1.73 | 1.72 | 1.70 | 0.88 | 0.99 | 1.09 | 1.36 | 1.94 | 1.29 | 1.25 |
| 579 | 1.27 | 0.86 | 0.89 | 0.67 | 0.61 | 1.03 | **0.76** | 0.90 | 1.03 | 0.83 | **0.83** | 0.54 | 0.81 |
| 582 | 1.03 | 1.27 | 1.53 | 1.49 | 1.22 | 1.20 | 0.97 | 0.82 | 1.66 | 1.69 | 2.01 | 1.86 | 1.02 |
| 591 | 0.94 | 1.02 | **1.15** | 1.23 | 1.21 | 1.13 | 1.07 | 0.98 | 1.19 | **1.19** | 1.39 | 1.46 | 1.00 |
| 594 | 1.02 | 1.08 | **1.35** | **1.39** | 1.28 | 1.25 | 1.03 | 0.92 | 1.71 | 1.84 | 2.61 | 1.89 | 1.07 |
| 598 | 0.85 | **1.28** | 1.87 | 1.70 | 2.12 | 1.47 | 0.91 | 1.25 | 2.61 | 2.99 | 3.88 | 2.81 | 1.14 |
| 601 | 0.94 | 1.04 | 1.13 | 0.92 | 1.03 | 1.09 | 0.81 | 1.12 | **1.26** | 1.17 | 1.33 | 1.20 | 0.93 |
| 602 | 1.05 | 1.03 | 1.36 | 1.14 | 1.18 | 1.32 | 0.84 | 1.03 | 1.00 | 0.95 | 1.40 | 1.47 | 0.95 |
| 603 | 0.70 | 0.92 | 0.49 | 0.15 | 0.37 | **0.54** | 0.30 | 2.50 | 0.45 | 0.44 | 0.38 | 0.26 | 0.98 |
| 604 | 1.03 | 1.24 | **1.38** | 1.85 | 1.49 | 1.11 | 1.34 | 0.80 | 1.67 | 1.63 | 2.30 | 2.16 | 0.98 |
| 608 | 1.07 | 1.21 | 1.32 | 1.51 | 1.54 | 1.09 | 1.15 | 1.02 | 1.33 | 1.20 | **1.54** | **1.54** | 0.90 |
| 609 | 1.12 | 0.94 | 1.27 | 1.71 | 1.30 | 1.34 | 1.35 | 0.76 | 1.27 | 1.22 | 1.85 | 1.90 | 0.96 |
| 610 | 1.02 | 1.18 | 1.17 | 1.83 | 1.86 | 1.00 | 1.56 | 1.02 | 1.24 | 1.18 | 1.43 | 1.53 | 0.95 |
| 611 | 1.18 | 1.78 | 1.83 | 3.08 | 2.71 | 1.03 | 1.68 | 0.88 | 1.49 | 1.84 | 2.42 | 2.76 | 1.23 |
| 613 | 1.25 | **1.53** | 1.49 | 2.39 | 1.87 | 0.98 | **1.60** | 0.78 | 1.75 | **1.64** | 2.31 | 2.49 | 0.94 |
| 618 | 1.92 | 0.77 | 0.61 | **0.52** | **0.57** | 0.79 | 0.86 | 1.08 | 1.18 | 0.64 | 0.67 | 0.40 | 0.54 |
| 619 | 1.85 | 1.31 | 1.28 | 1.12 | 1.32 | 0.98 | 0.88 | 1.17 | 1.61 | 1.13 | 1.17 | 0.77 | 0.71 |
| 620 | 1.98 | 0.97 | 1.30 | 1.23 | 0.96 | 1.34 | 0.95 | 0.78 | 2.29 | 1.60 | **1.77** | 1.09 | 0.70 |
| 621 | **1.55** | 1.75 | 1.94 | 1.68 | **1.62** | 1.11 | 0.86 | 0.97 | 2.35 | 1.99 | 1.88 | **1.56** | 0.84 |
| 622 | 1.10 | 1.76 | 2.38 | 2.16 | 1.98 | 1.36 | 0.91 | 0.92 | 2.06 | 2.12 | 2.10 | 2.08 | 1.03 |
| 625 | 1.15 | 1.19 | 1.14 | 1.37 | 1.23 | 0.96 | 1.20 | 0.90 | **1.26** | **1.29** | 1.18 | 1.16 | 1.03 |
| 629 | 1.18 | 1.78 | 2.03 | 2.47 | 1.99 | 1.14 | 1.22 | 0.81 | 2.04 | 2.08 | 2.43 | 2.19 | 1.02 |
| 630 | **2.01** | 0.52 | 0.67 | 1.30 | 0.80 | 1.29 | 1.92 | 0.62 | 1.39 | 1.97 | 1.39 | 1.27 | 1.42 |
| 631 | 1.17 | 1.52 | 1.56 | 1.95 | 1.51 | 1.03 | **1.25** | 0.77 | 1.45 | 1.41 | 1.84 | 1.64 | 0.97 |
| 632 | 1.19 | **1.26** | 1.44 | 1.58 | 1.42 | 1.15 | 1.09 | 0.90 | 1.43 | 1.57 | 2.02 | 1.70 | 1.10 |
| 633 | 1.06 | 1.42 | 1.12 | **1.56** | 1.46 | 0.79 | 1.39 | 0.94 | 1.48 | **1.64** | 2.24 | **1.62** | 1.11 |
| 635 | 1.41 | 1.45 | 1.65 | 1.92 | 1.64 | 1.14 | 1.16 | 0.85 | 1.56 | 1.65 | 1.93 | 1.71 | 1.06 |
| 636 | 1.27 | 1.27 | **1.35** | 1.89 | 1.59 | 1.06 | **1.41** | 0.84 | **1.44** | **1.44** | 1.78 | 1.55 | 0.99 |
| 637 | **1.27** | 1.35 | 1.60 | 1.71 | 1.52 | 1.19 | 1.07 | 0.89 | 1.59 | 1.65 | 2.05 | 1.73 | 1.04 |
| 639 | 0.83 | 0.90 | 1.08 | 0.95 | 0.94 | 1.20 | 0.88 | 0.99 | 1.25 | **1.47** | **1.42** | 1.38 | 1.17 |
| 641 | 0.50 | 0.91 | 1.14 | 1.23 | 1.24 | 1.26 | 1.08 | 1.01 | 1.71 | 0.74 | 1.94 | **2.45** | 0.43 |
| 655 | 1.14 | **1.56** | **1.50** | 2.02 | 1.77 | 0.96 | 1.35 | 0.87 | 1.78 | 1.85 | 2.36 | 2.35 | 1.04 |
| 658 | 1.22 | **0.47** | 0.95 | 0.75 | 0.89 | **2.03** | 0.78 | 1.19 | 1.43 | 1.46 | 1.63 | 1.53 | 1.02 |
| 659 | 1.12 | 1.15 | 1.26 | 1.92 | **1.64** | 1.10 | 1.52 | 0.86 | 1.30 | 1.18 | 1.94 | 2.22 | 0.91 |
| 665 | 1.27 | 0.52 | 0.53 | 0.47 | 0.44 | 1.02 | 0.88 | 0.94 | 0.68 | 0.41 | 0.67 | 0.65 | 0.60 |
| 670.01 | 1.01 | 9.57 | 12.97 | 17.93 | 19.42 | 1.36 | 1.38 | 1.08 | 9.63 | 14.52 | 14.71 | 18.06 | 1.51 |
| 672 | 0.93 | 21.88 | 34.28 | 39.21 | 40.88 | 1.57 | 1.14 | 1.04 | 24.53 | 35.00 | 42.49 | 44.03 | 1.43 |
| 706 | 1.03 | 0.94 | 1.31 | 1.08 | 0.89 | 1.40 | 0.82 | 0.82 | 1.55 | **1.66** | 3.29 | 1.90 | 1.07 |
| 714 | 0.72 | 1.18 | 1.64 | 1.74 | 2.18 | 1.39 | 1.06 | 1.25 | 2.95 | 2.85 | 3.61 | 3.84 | 0.97 |
| 721 | 0.96 | 3.49 | 7.46 | 9.03 | 11.32 | 2.14 | 1.21 | 1.25 | 3.08 | 4.73 | 6.79 | 8.60 | 1.54 |
| 735 | 0.46 | 0.61 | 0.97 | 0.28 | 1.00 | 1.59 | 0.29 | 3.57 | 0.52 | 0.87 | 0.49 | 0.93 | 1.67 |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| 742 | 1.09 | 1.71 | 1.99 | 2.36 | 2.13 | 1.16 | 1.18 | 0.90 | 1.80 | 2.28 | 2.66 | 2.68 | 1.27 |
| 744 | 1.43 | 1.67 | 2.03 | 2.76 | 2.43 | 1.22 | **1.36** | 0.88 | 1.66 | 1.97 | 2.47 | 2.37 | 1.19 |
| 809 | 1.27 | 0.96 | 0.91 | 0.85 | **0.82** | 0.95 | 0.93 | 0.97 | 0.99 | 0.79 | **0.81** | 0.71 | 0.79 |
| 811 | 1.02 | 1.08 | **0.63** | 0.99 | 1.10 | **0.58** | **1.58** | 1.11 | 0.84 | 0.45 | 1.06 | 0.54 | 0.54 |
| 819 | 0.99 | 0.97 | 1.04 | 1.15 | 1.04 | 1.07 | 1.11 | 0.90 | 1.11 | 1.12 | 1.16 | 1.10 | 1.00 |
| 820 | 0.97 | 1.05 | 1.14 | 1.08 | 1.06 | 1.09 | 0.95 | 0.97 | 1.16 | 1.18 | 1.15 | 1.16 | 1.01 |
| 821 | 1.04 | 1.12 | **1.19** | **1.23** | **1.21** | 1.05 | 1.03 | 0.99 | 1.18 | 1.12 | **1.22** | 1.18 | 0.95 |
| 822 | 1.09 | 0.95 | 0.95 | 0.96 | 0.89 | 0.99 | 1.01 | 0.93 | **1.15** | 0.96 | 0.97 | **0.89** | 0.84 |
| 823 | 1.04 | 0.61 | 0.48 | 0.60 | **0.70** | 0.78 | 1.26 | 1.15 | 0.84 | 0.68 | 1.09 | 1.01 | 0.81 |
| 825 | 0.99 | 1.07 | 1.12 | 1.29 | 1.20 | 1.05 | 1.16 | 0.93 | 1.24 | 1.35 | 1.66 | 1.40 | 1.09 |
| 833 | 0.36 | 6.66 | 11.08 | 14.45 | 81.48 | 1.66 | 1.30 | 5.64 | **6.07** | 8.79 | 13.36 | 10.83 | 1.45 |
| 834 | 0.38 | 3.03 | 7.91 | 9.88 | 47.10 | 2.61 | 1.25 | 4.77 | 9.39 | 14.61 | 21.89 | 16.73 | 1.56 |
| 835 | 0.36 | **4.52** | 10.06 | 13.93 | 66.06 | 2.23 | 1.39 | 4.74 | 9.27 | 14.18 | 23.23 | 14.68 | 1.53 |
| 840 | 0.95 | 0.99 | 0.89 | 0.87 | 0.78 | 0.89 | 0.98 | 0.90 | 1.11 | 0.95 | 0.93 | 1.21 | 0.86 |
| 849 | 1.03 | 0.81 | 1.19 | 0.99 | 1.20 | 1.48 | 0.83 | 1.21 | 1.23 | 1.69 | 1.56 | 1.58 | **1.38** |
| 851 | 0.93 | 0.83 | 0.83 | 0.79 | 0.66 | 1.00 | 0.95 | 0.83 | 1.20 | 1.08 | 1.07 | 1.13 | 0.90 |
| 876 | 0.52 | 1.07 | 1.62 | 0.99 | **1.83** | 1.52 | 0.61 | **1.85** | **1.67** | **1.80** | 2.45 | 2.49 | 1.08 |
| 877 | 1.50 | 1.20 | 1.88 | 1.00 | 1.19 | 1.56 | 0.53 | 1.19 | 0.52 | 0.63 | 0.69 | 0.48 | 1.22 |
| 881 | 0.94 | 1.02 | 1.11 | 1.10 | 1.05 | 1.09 | 0.99 | 0.96 | **1.18** | 1.13 | 1.16 | 1.18 | 0.95 |
| 882 | 0.96 | 0.86 | 0.98 | 0.78 | **0.67** | 1.14 | 0.80 | 0.86 | 1.51 | 0.78 | 0.46 | 0.32 | 0.52 |
| 883 | 0.89 | 0.95 | 0.97 | 0.94 | 0.96 | 1.02 | 0.97 | 1.02 | 1.01 | 1.06 | 1.15 | **1.19** | 1.05 |
| 890 | 0.79 | 0.90 | 1.04 | 0.79 | 0.87 | 1.15 | **0.76** | 1.10 | 1.06 | 0.95 | 1.01 | 1.03 | 0.90 |
| 905 | 0.96 | 2.12 | 3.84 | 3.73 | 4.68 | 1.81 | 0.97 | 1.25 | 3.24 | 3.31 | 4.75 | 5.31 | 1.02 |
| 909 | **1.65** | 0.67 | 0.75 | 0.60 | **0.56** | 1.12 | 0.80 | 0.94 | 1.40 | 0.99 | 2.27 | 1.01 | 0.70 |
| 915 | 0.93 | 0.85 | 0.80 | 0.95 | 0.63 | 0.93 | 1.19 | 0.66 | 1.12 | 0.75 | 1.46 | 1.16 | 0.67 |
| 919 | 1.33 | 0.68 | 0.68 | **0.61** | 0.47 | 1.00 | 0.91 | 0.77 | 1.05 | 1.06 | 1.33 | 0.91 | 1.01 |
| 920 | 0.49 | 5.76 | 9.20 | 13.64 | 35.01 | 1.60 | 1.48 | 2.57 | 8.54 | 13.05 | 14.00 | 11.73 | 1.53 |
| 922 | 0.56 | **2.84** | 7.25 | 9.12 | 24.26 | 2.55 | 1.26 | **2.66** | 7.30 | 10.02 | 11.26 | 7.91 | 1.37 |
| 923 | 0.39 | **3.40** | 6.52 | 7.20 | 21.36 | 1.92 | 1.10 | 2.97 | 6.91 | 10.88 | 12.35 | 10.37 | 1.58 |
| 926 | 0.29 | 1.28 | 2.06 | 2.02 | 5.76 | 1.60 | 0.98 | **2.86** | 2.06 | 5.22 | 6.62 | 7.59 | **2.54** |
| 929 | 0.68 | 4.44 | 13.73 | 20.75 | 43.62 | **3.09** | 1.51 | 2.10 | 10.27 | 11.68 | 21.94 | 13.82 | 1.14 |
| 930 | 0.43 | 3.32 | 6.52 | 8.98 | 27.45 | 1.96 | 1.38 | 3.06 | 12.38 | 22.87 | 27.13 | 25.19 | 1.85 |
| 934 | 0.45 | 4.27 | 11.26 | 16.01 | 49.02 | 2.64 | 1.42 | 3.06 | 10.28 | 17.49 | 24.04 | 19.45 | 1.70 |
| 935 | 0.55 | 1.55 | **4.31** | 5.40 | 16.42 | 2.78 | 1.25 | 3.04 | 6.94 | 11.86 | 15.48 | 13.89 | 1.71 |
| 936 | 0.55 | **3.66** | 11.74 | 17.24 | 51.40 | 3.21 | 1.47 | 2.98 | 13.39 | 15.11 | 31.18 | 17.59 | 1.13 |
| 937 | 0.47 | 1.62 | **3.26** | 3.99 | 11.41 | 2.01 | 1.22 | 2.86 | **4.23** | 4.98 | 8.32 | 5.76 | 1.18 |
| 938 | 1.33 | 0.88 | 0.94 | 0.95 | 0.71 | 1.07 | 1.00 | 0.75 | 1.07 | 1.08 | 1.75 | 1.04 | 1.00 |
| 939 | 0.41 | 1.65 | 2.01 | 3.80 | 9.61 | 1.22 | 1.89 | 2.53 | **4.19** | 7.98 | 8.53 | 7.94 | **1.90** |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| 945 | **0.26** | 1.78 | 2.71 | **3.81** | 13.65 | 1.52 | 1.41 | 3.58 | 4.42 | 7.52 | 8.41 | 8.59 | 1.70 |
| 970 | 1.35 | 1.69 | 1.24 | 1.21 | 1.26 | 0.73 | 0.98 | 1.04 | 1.58 | 1.82 | 1.57 | 1.47 | 1.15 |
| 1004 | 0.92 | 0.92 | 1.17 | 0.87 | 0.96 | 1.26 | **0.74** | 1.11 | 1.26 | 1.18 | **1.36** | 1.25 | 0.94 |
| 1005 | 0.95 | 0.93 | 1.09 | 1.02 | 0.97 | 1.18 | 0.93 | 0.95 | 1.27 | 1.17 | 1.32 | 1.17 | 0.92 |
| 1018 | 0.73 | 0.83 | 0.99 | 0.76 | 0.81 | 1.19 | 0.77 | 1.07 | 1.39 | 1.30 | **1.31** | **1.53** | 0.94 |
| 1020 | 0.88 | 0.96 | 1.19 | 0.91 | 0.97 | **1.23** | 0.76 | 1.07 | 1.11 | 1.09 | **1.24** | 1.21 | 0.98 |
| 1024 | 0.85 | 0.97 | 1.71 | 0.97 | 0.72 | 1.75 | 0.57 | 0.74 | 1.09 | 1.13 | 1.59 | 1.51 | 1.04 |
| 1034 | 0.96 | 1.23 | 1.23 | 1.03 | **1.33** | 1.00 | 0.84 | **1.29** | 1.11 | 0.72 | 1.01 | 1.15 | 0.65 |
| 1057 | 0.80 | **1.75** | 2.37 | 1.56 | 1.05 | 1.36 | 0.66 | 0.68 | 0.94 | **1.62** | 1.48 | 1.17 | 1.71 |
| 1059 | 0.40 | 0.97 | 1.28 | 1.22 | 1.52 | 1.33 | 0.95 | 1.24 | 0.91 | 0.96 | 1.76 | 1.49 | 1.06 |
| 1098 | 0.33 | 1.10 | 3.84 | 9.09 | 19.10 | 3.49 | 2.36 | 2.10 | 72.66 | 70.11 | 86.08 | 75.62 | 0.96 |
| 1101 | 0.63 | 2.13 | 3.73 | 2.11 | 2.17 | 1.75 | 0.56 | 1.03 | 1.58 | 2.67 | 4.07 | 4.19 | 1.69 |
| 1105 | 0.70 | 0.85 | 0.73 | 0.68 | 0.63 | 0.85 | 0.94 | 0.92 | 1.11 | 0.89 | **0.80** | 0.52 | 0.80 |
| 1106 | 0.79 | 0.55 | 1.08 | 1.06 | 0.73 | 1.96 | 0.99 | 0.69 | 1.94 | 2.23 | 2.28 | 2.08 | 1.15 |
| 1114 | 1.46 | 1.05 | 1.68 | 1.96 | 1.87 | 1.60 | 1.17 | 0.96 | 1.00 | 0.64 | 1.33 | 1.31 | **0.64** |
| 1116 | 1.84 | 0.97 | 1.06 | 0.94 | 0.74 | 1.10 | 0.88 | 0.79 | 0.79 | 0.58 | **0.68** | 0.51 | 0.74 |
| 1128 | 1.27 | 1.08 | 1.19 | 1.15 | 1.15 | 1.10 | 0.96 | 1.01 | 1.28 | 1.06 | 1.24 | **0.75** | 0.82 |
| 1149 | 1.23 | 0.91 | 0.97 | 0.92 | 0.77 | 1.07 | 0.94 | **0.84** | 1.08 | 0.80 | 0.97 | 0.81 | 0.73 |
| 1150 | 1.49 | 0.74 | 0.39 | 1.22 | 1.03 | 0.53 | **3.09** | 0.84 | 1.06 | 0.71 | 1.75 | 1.15 | 0.67 |
| 1180 | 0.97 | **1.23** | 1.32 | 1.55 | 1.43 | 1.07 | 1.18 | 0.92 | 1.65 | 1.56 | 1.52 | 1.76 | 0.94 |
| 1181 | 1.02 | 0.80 | 0.88 | 1.23 | 1.06 | 1.09 | 1.40 | 0.86 | 1.32 | 1.71 | 1.84 | 1.60 | 1.30 |
| 1199 | 0.83 | 0.85 | 1.04 | 0.92 | 0.88 | 1.22 | 0.89 | 0.95 | 1.26 | **1.28** | 1.64 | 1.53 | 1.01 |
| 1202 | 1.25 | 1.19 | 1.41 | 1.06 | 1.32 | 1.18 | 0.75 | 1.25 | 1.20 | 0.99 | 1.40 | 0.90 | 0.83 |
| 1212 | 0.33 | 3.22 | **4.05** | **4.83** | 15.46 | 1.26 | 1.19 | 3.20 | 4.28 | 6.33 | **5.14** | 4.00 | 1.48 |
| 1216 | 0.68 | 1.29 | 0.96 | 1.50 | 1.89 | 0.75 | 1.57 | 1.26 | 3.22 | 4.16 | 4.31 | 2.88 | 1.29 |
| 1221 | 0.93 | 0.96 | 1.15 | **1.34** | 1.05 | 1.20 | 1.16 | 0.79 | 1.48 | 1.17 | **1.35** | 1.40 | 0.79 |
| 1224 | 1.30 | 1.20 | 1.10 | 1.15 | 1.50 | 0.92 | 1.05 | 1.30 | 1.25 | 0.51 | 0.47 | 0.44 | 0.41 |
| 1232 | 1.00 | 1.11 | 1.08 | 1.08 | 0.95 | 0.98 | 0.99 | 0.88 | 1.29 | 1.14 | 1.07 | 0.87 | 0.88 |
| 1242 | 0.95 | 0.93 | 0.98 | 1.03 | 0.97 | 1.06 | 1.05 | 0.94 | 1.12 | 1.06 | **1.14** | 1.06 | 0.94 |

| | | ANVOA Contrasts | | | | | | | ANVOA Contrasts | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T2-28 T1-28 | C-7 C-0 | C-14 C-0 | C-21 C-0 | C-28 C-0 | C-14 C-7 | C-21 C-14 | C-28 C-21 | T1-7 T1-0 | T1-14 T1-0 | T1-21 T1-0 | T1-28 T1-0 | T1-14 T1-7 |
| ~~1242.1~~ | 0.92 | 1.21 | 0.97 | 0.89 | 0.97 | 0.80 | 0.92 | 1.10 | 0.91 | 1.05 | 0.85 | 0.91 | 1.17 |
| 1243 | 0.84 | 0.92 | 1.12 | 1.33 | 1.09 | 1.22 | 1.19 | 0.82 | 1.14 | 1.12 | 1.19 | 1.25 | 0.99 |
| 1266 | 0.84 | 0.84 | 1.03 | **0.68** | 0.72 | 1.22 | **0.67** | 1.06 | 0.97 | 1.19 | 1.55 | 1.25 | 1.23 |
| 1288 | 0.96 | 1.23 | 1.12 | **1.19** | 1.05 | 0.91 | 1.06 | 0.88 | 1.23 | **1.17** | 1.30 | **1.17** | 0.95 |
| 1300 | 0.93 | 1.04 | 1.08 | 1.09 | 1.01 | 1.03 | 1.01 | 0.92 | 1.12 | 1.05 | 1.13 | 1.11 | 0.93 |
| 1318 | 0.82 | 1.05 | 1.23 | 0.98 | 1.02 | 1.17 | 0.80 | 1.04 | 1.23 | 1.08 | **1.40** | **1.29** | 0.88 |
| 1360 | 1.20 | 0.94 | 0.86 | 0.86 | 0.62 | 0.92 | 1.00 | 0.73 | 1.24 | 0.82 | 0.82 | **0.51** | 0.66 |
| 1469 | 1.07 | 0.93 | 1.12 | 1.10 | 1.06 | **1.20** | 0.98 | 0.97 | 1.09 | 1.07 | 1.26 | 1.02 | 0.99 |
| 1531 | 0.90 | 0.86 | 0.93 | **0.66** | **0.70** | 1.08 | 0.71 | 1.06 | 1.39 | 1.03 | 1.36 | 0.92 | 0.74 |
| 1565 | 1.08 | 0.91 | 0.98 | 1.00 | 0.91 | 1.08 | 1.01 | 0.91 | 1.15 | 1.04 | **1.18** | 1.15 | 0.90 |
| 1584 | 0.99 | 0.97 | 0.95 | 0.94 | 0.93 | 0.98 | 1.00 | 0.99 | 1.17 | 1.09 | 1.14 | 1.22 | 0.94 |
| 1585 | 0.71 | 0.82 | 0.95 | 0.81 | 0.89 | 1.16 | 0.86 | 1.10 | 0.74 | 1.02 | 0.96 | 1.06 | 1.39 |
| 1612 | 0.91 | 0.98 | 1.01 | 1.02 | 0.92 | 1.03 | 1.01 | 0.91 | 1.13 | 1.08 | 1.22 | 1.13 | 0.95 |
| 1613 | 0.87 | 1.17 | 1.14 | 1.09 | 1.08 | 0.97 | 0.96 | 0.99 | 1.21 | **1.29** | 1.15 | 1.24 | 1.07 |
| 1614 | 1.05 | 0.98 | 1.08 | 1.16 | 1.13 | 1.10 | 1.07 | 0.97 | 1.00 | 0.90 | 1.16 | 1.11 | 0.90 |
| 1615 | 1.02 | 1.12 | 1.28 | 1.41 | 0.94 | 1.15 | 1.10 | 0.67 | 1.13 | 1.69 | 0.83 | 1.20 | 1.49 |
| 1632 | 0.44 | 1.19 | 1.72 | 1.79 | 2.21 | 1.45 | 1.04 | 1.24 | 1.68 | 2.49 | 4.21 | 4.84 | 1.48 |
| 1662 | 1.13 | 0.92 | 0.82 | 0.86 | 0.84 | 0.90 | 1.04 | 0.99 | 1.21 | 1.07 | **1.23** | 1.00 | 0.89 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| 1 | 1.38 | 1.11 | 1.24 | 1.63 | 1.78 | 2.38 | **1.31** | 1.10 | **1.33** |
| 3 | 0.75 | 1.25 | 1.16 | 1.11 | 1.81 | 1.39 | 0.96 | 1.63 | 0.76 |
| 4 | 1.24 | 0.91 | 0.97 | 1.39 | 0.87 | 0.90 | 1.43 | 0.62 | 1.03 |
| 7 | 0.97 | 0.99 | 1.11 | 1.20 | 0.82 | 1.18 | 1.08 | 0.68 | 1.45 |
| 8 | 1.18 | 0.99 | 1.13 | 1.16 | 1.07 | 1.14 | 1.03 | 0.93 | 1.06 |
| 17 | 0.94 | 1.08 | 1.14 | 1.19 | 1.02 | 1.16 | 1.05 | 0.86 | 1.14 |
| 22 | 1.03 | 1.03 | 1.00 | 1.07 | 0.97 | 1.02 | 1.07 | 0.90 | 1.05 |
| 24 | 1.18 | 0.79 | 0.95 | 1.14 | 1.24 | 1.13 | 1.21 | 1.08 | 0.91 |
| 25 | 1.09 | 0.97 | 0.93 | 0.91 | **0.78** | 0.64 | 0.97 | 0.86 | 0.82 |
| 26 | 1.07 | 1.18 | 0.99 | 1.13 | 0.84 | 0.46 | 1.15 | 0.74 | **0.55** |
| 27 | 1.23 | 0.97 | 1.12 | **1.26** | 1.17 | 1.25 | 1.13 | 0.92 | 1.07 |
| 39 | 1.02 | 0.98 | 0.90 | 1.01 | 0.85 | 1.04 | 1.12 | 0.85 | 1.22 |
| 44 | 0.83 | 0.96 | **0.88** | 0.78 | 0.68 | 0.60 | **0.88** | 0.87 | **0.88** |
| 45 | 1.02 | 1.05 | 1.02 | 0.87 | 0.80 | 1.01 | 0.85 | 0.92 | 1.26 |
| 50 | 1.46 | 0.84 | 1.01 | 0.92 | 1.03 | 0.99 | 0.91 | 1.12 | 0.96 |
| 69 | 1.06 | 1.07 | 1.11 | 1.13 | 1.29 | 0.86 | 1.02 | 1.14 | 0.67 |
| 74 | 0.96 | 1.00 | 1.05 | 0.89 | 0.99 | 1.07 | 0.84 | 1.12 | 1.08 |
| 75 | 1.03 | 1.09 | 0.98 | 0.92 | 0.92 | 0.87 | 0.93 | 1.00 | 0.95 |
| 80 | 0.97 | 0.68 | 0.97 | 0.72 | 0.75 | 0.75 | 0.75 | 1.03 | 1.00 |
| 83 | 0.99 | 1.07 | 1.09 | 1.24 | 1.16 | **1.19** | 1.14 | 0.93 | 1.03 |
| 88 | 1.18 | 0.86 | 0.93 | 0.95 | 0.87 | 0.93 | 1.02 | 0.92 | 1.07 |
| 99 | 0.97 | 1.09 | 1.04 | **1.18** | 1.08 | 1.18 | 1.14 | 0.91 | 1.09 |
| 128 | 1.11 | **0.81** | 0.91 | 0.97 | 0.94 | 0.99 | 1.07 | 0.97 | 1.06 |
| 135 | 1.00 | 1.01 | 0.96 | 0.92 | **0.82** | 0.89 | 0.96 | 0.90 | 1.09 |
| 144 | 0.81 | 0.99 | 1.18 | 1.10 | 1.14 | 0.97 | 0.94 | 1.04 | 0.85 |
| 145 | 1.00 | 1.04 | 1.02 | 1.13 | 1.05 | 1.05 | 1.11 | 0.93 | 1.00 |
| 151 | 1.09 | 1.05 | 1.00 | 0.95 | **0.84** | 0.99 | 0.95 | 0.89 | 1.17 |
| 164 | 1.04 | 1.03 | 0.92 | 1.21 | 1.00 | 0.94 | **1.31** | 0.82 | 0.95 |
| 170 | 1.14 | 0.79 | 0.88 | 0.87 | 0.92 | 0.98 | 0.99 | 1.06 | 1.06 |
| 172 | 1.44 | 1.06 | 1.16 | 1.14 | 0.82 | 0.76 | 0.98 | 0.72 | 0.92 |
| 173 | 1.10 | 1.17 | 1.11 | 1.22 | 1.17 | 1.14 | 1.10 | 0.96 | 0.98 |
| 179 | 1.05 | 1.13 | 1.00 | 1.91 | 2.97 | 5.07 | 1.91 | 1.55 | 1.71 |
| 180 | 1.01 | 1.00 | 1.00 | 1.08 | 1.01 | 1.11 | 1.08 | 0.94 | 1.10 |
| 181 | 1.08 | 0.97 | 1.05 | 1.12 | 1.08 | **1.23** | 1.06 | 0.96 | 1.14 |
| 190 | 1.02 | 1.03 | 1.04 | **1.15** | 1.01 | 1.09 | 1.10 | 0.88 | 1.09 |
| 193 | **1.41** | 1.10 | 1.15 | 1.26 | 0.95 | 0.92 | 1.09 | 0.75 | 0.98 |
| 198 | 1.26 | 0.98 | 0.87 | 1.10 | **1.40** | 2.16 | 1.26 | 1.27 | 1.55 |
| 200 | 1.15 | 0.89 | 0.92 | **0.84** | 0.74 | 0.79 | 0.91 | 0.88 | 1.06 |
| 202 | 1.57 | 0.87 | 0.88 | 0.86 | 0.73 | 0.98 | 0.97 | 0.85 | 1.35 |
| 205 | 1.05 | 1.01 | 0.94 | 0.93 | 0.89 | 1.12 | 0.99 | 0.95 | **1.26** |
| 206 | 1.04 | 0.99 | 0.89 | 0.91 | 0.85 | 0.91 | 1.02 | 0.93 | 1.07 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| 213 | 1.84 | 0.88 | 1.21 | 1.73 | 2.69 | 2.84 | **1.43** | 1.56 | 1.05 |
| 216 | 1.28 | 0.77 | 1.01 | 0.97 | 1.25 | 1.08 | 0.96 | **1.29** | 0.87 |
| 224 | 0.97 | 1.16 | 1.51 | 1.49 | 1.29 | 1.79 | 0.98 | 0.87 | 1.39 |
| 225 | **0.81** | 0.92 | 0.85 | 0.70 | 0.51 | 0.49 | 0.82 | 0.72 | 0.97 |
| 227 | **1.41** | 0.89 | 0.78 | **0.67** | 0.91 | 0.88 | 0.86 | 1.34 | 0.97 |
| 229 | 1.13 | 0.85 | 1.02 | 1.08 | 1.03 | 0.96 | 1.07 | 0.95 | 0.93 |
| 231 | 1.41 | 0.89 | 1.56 | 3.20 | 4.19 | 3.86 | 2.05 | 1.31 | 0.92 |
| 241 | 1.30 | 1.03 | 0.97 | 1.08 | 0.97 | 2.44 | 1.11 | 0.90 | 2.51 |
| 244 | 1.14 | 0.96 | 1.07 | 1.14 | 1.01 | 0.83 | 1.07 | 0.88 | 0.82 |
| 245 | 1.21 | 0.92 | 0.99 | 1.10 | 0.98 | 1.01 | 1.11 | 0.89 | 1.03 |
| 246 | **1.18** | 0.97 | 1.08 | 1.00 | 0.95 | 1.13 | 0.93 | 0.95 | 1.20 |
| 248 | 1.06 | 1.07 | 1.06 | 1.03 | 1.01 | 1.09 | 0.98 | 0.98 | 1.08 |
| 252 | **0.85** | 1.04 | 0.90 | 0.93 | 1.03 | 0.92 | 1.03 | 1.11 | 0.90 |
| 259 | 1.05 | 0.98 | 1.00 | 0.98 | **0.88** | 0.97 | 0.99 | 0.90 | 1.09 |
| 260 | 1.02 | 1.05 | 1.06 | 1.01 | 1.04 | 0.98 | 0.96 | 1.02 | 0.94 |
| 263 | 1.11 | 1.00 | 1.19 | 1.23 | 1.14 | 1.12 | 1.03 | 0.93 | 0.98 |
| 266 | 0.88 | 0.94 | 2.13 | 2.91 | 2.82 | 2.47 | **1.36** | 0.97 | 0.88 |
| 270 | 1.10 | 1.01 | 1.07 | 1.15 | 1.03 | 1.16 | 1.07 | 0.89 | 1.13 |
| 280 | 0.84 | 0.96 | **0.76** | 1.00 | 0.83 | 0.71 | **1.32** | 0.83 | 0.86 |
| 281 | 0.75 | 0.72 | 1.15 | 0.91 | 1.05 | 0.83 | 0.79 | 1.16 | 0.79 |
| 282 | 1.37 | 1.00 | 3.45 | 5.56 | 6.89 | 10.26 | 1.61 | **1.24** | 1.49 |
| 283 | 0.89 | 0.89 | **0.80** | 0.72 | 0.62 | 0.58 | 0.90 | 0.87 | 0.92 |
| 285 | **0.52** | 0.70 | 0.28 | 0.12 | 0.10 | 0.09 | 0.41 | 0.82 | 0.89 |
| 404 | 0.95 | **0.73** | 0.71 | 0.77 | 0.83 | 0.67 | 1.08 | 1.08 | 0.81 |
| 453 | 1.74 | 0.97 | 1.19 | 1.50 | 1.42 | 1.65 | **1.26** | 0.95 | 1.16 |
| 455 | 2.07 | 1.16 | 1.87 | 2.34 | 2.63 | 2.39 | 1.25 | 1.12 | 0.91 |
| 472 | 1.78 | 1.11 | 1.08 | 1.23 | 1.21 | 1.19 | 1.14 | 0.98 | 0.98 |
| 478 | 1.26 | 0.94 | 1.13 | 1.15 | 0.95 | 0.90 | 1.02 | 0.82 | 0.94 |
| 482 | 1.26 | 0.87 | 1.00 | 1.10 | 0.96 | 0.96 | 1.10 | 0.88 | 0.99 |
| 487 | 1.22 | 0.87 | 0.94 | 0.97 | 0.88 | 0.88 | 1.03 | 0.90 | 1.00 |
| 489 | 1.25 | 0.72 | 1.16 | 1.13 | 0.86 | 1.03 | 0.98 | 0.76 | 1.20 |
| 496 | 0.96 | 0.94 | 0.96 | 1.02 | 0.96 | 0.96 | 1.07 | 0.94 | 1.00 |
| 501 | **1.58** | 1.04 | 4.73 | 7.83 | 9.08 | 7.87 | **1.66** | 1.16 | 0.87 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| ~~515~~ | 1.63 | 0.65 | 1.08 | 1.06 | 0.91 | 0.90 | 0.98 | 0.86 | 0.99 |
| 517 | 1.35 | 1.11 | **1.60** | 1.97 | 2.39 | 2.61 | 1.24 | 1.21 | 1.09 |
| 519 | **1.78** | 0.83 | 1.13 | 1.07 | 0.66 | 1.10 | 0.95 | 0.62 | **1.66** |
| 521 | 1.09 | 0.95 | 0.96 | 1.00 | 0.89 | 0.98 | 1.04 | 0.89 | 1.11 |
| 523 | 0.81 | 1.00 | 0.81 | 0.76 | 0.87 | 0.88 | 0.94 | 1.14 | 1.02 |
| 524 | 0.78 | 0.97 | 1.08 | 1.06 | 0.74 | 1.06 | 0.98 | 0.70 | 1.44 |
| 527 | 0.47 | 0.81 | 1.02 | 0.92 | 0.73 | 0.85 | 0.89 | **0.79** | 1.17 |
| 529 | 0.50 | **0.64** | 0.64 | 0.38 | 0.21 | 0.25 | 0.59 | 0.55 | 1.20 |
| 531 | 0.13 | 0.41 | 2.65 | 0.90 | 1.78 | 0.77 | 0.34 | 1.98 | 0.43 |
| 532 | 1.15 | 0.87 | 1.21 | **1.46** | 0.95 | 1.04 | 1.20 | 0.65 | 1.10 |
| 533 | **0.58** | 0.25 | 0.35 | 0.07 | 0.01 | 0.01 | 0.19 | 0.22 | 0.95 |
| 534 | 0.56 | 0.40 | 0.38 | 0.12 | 0.06 | 0.08 | 0.32 | 0.50 | 1.25 |
| 535 | 17.89 | 1.87 | 1.32 | 0.95 | 0.41 | 0.38 | 0.72 | **0.44** | 0.93 |
| 536 | 1.39 | 1.06 | 3.01 | 4.71 | 5.21 | 6.14 | 1.56 | 1.11 | 1.18 |
| 545 | 1.03 | 0.41 | 0.73 | 0.47 | 0.43 | 0.47 | 0.65 | 0.91 | 1.09 |
| 546 | 1.13 | 0.99 | 0.88 | 0.96 | 0.98 | 0.92 | 1.09 | 1.03 | 0.93 |
| 548 | 1.15 | 1.05 | 1.23 | 1.08 | 1.00 | 1.35 | 0.88 | 0.92 | 1.36 |
| 549 | 1.36 | 0.82 | 1.13 | 1.36 | **1.31** | **1.31** | 1.20 | 0.96 | 1.00 |
| 551 | 6.51 | **2.88** | 1.10 | **2.71** | 1.58 | 1.11 | 2.46 | 0.58 | 0.71 |
| 557 | 0.56 | 0.61 | 0.93 | 0.78 | 0.73 | 0.62 | 0.84 | 0.94 | 0.85 |
| 559 | 0.48 | 1.13 | **0.49** | 0.81 | 0.93 | 0.89 | 1.64 | 1.16 | 0.95 |
| 561 | 0.23 | 0.68 | 1.24 | 0.81 | 0.85 | 0.82 | 0.65 | 1.05 | 0.97 |
| 565 | 0.55 | 0.58 | 1.00 | 1.00 | 1.19 | 1.00 | 1.00 | 1.19 | 0.84 |
| 566 | 1.28 | 0.84 | 0.89 | 1.14 | 0.85 | 1.01 | 1.29 | **0.74** | 1.20 |
| 569 | 1.64 | 0.99 | 1.13 | 0.95 | 0.77 | 1.61 | 0.84 | 0.81 | 2.08 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| 570 | 1.43 | 0.66 | 0.87 | 1.32 | 1.15 | 1.35 | **1.52** | 0.87 | 1.17 |
| 579 | 1.00 | 0.65 | 0.85 | 0.80 | 0.68 | 0.63 | 0.94 | 0.85 | 0.93 |
| 582 | **1.19** | 0.93 | 1.47 | 1.51 | 1.43 | 1.73 | 1.03 | 0.95 | 1.21 |
| 591 | 1.17 | 1.05 | 1.06 | 1.08 | 0.96 | **1.19** | 1.02 | 0.89 | 1.24 |
| 594 | 1.42 | **0.72** | 1.12 | 1.12 | 1.13 | 1.83 | 1.00 | 1.01 | 1.62 |
| 598 | **1.30** | 0.72 | 1.40 | 1.38 | 1.40 | 1.91 | 0.98 | 1.02 | **1.36** |
| 601 | 1.14 | 0.90 | 1.08 | 1.12 | 1.00 | 0.93 | 1.03 | 0.89 | 0.93 |
| 602 | 1.47 | 1.05 | 1.13 | **1.25** | 1.16 | 1.19 | 1.11 | 0.92 | 1.03 |
| 603 | 0.86 | 0.69 | 0.90 | 0.63 | 0.49 | 0.23 | 0.69 | 0.78 | 0.46 |
| 604 | **1.41** | 0.94 | 1.38 | 1.25 | 1.31 | 2.00 | 0.90 | 1.06 | 1.52 |
| 608 | 1.28 | 1.00 | 1.60 | 1.44 | 1.34 | 2.03 | 0.90 | 0.93 | **1.52** |
| 609 | **1.52** | 1.02 | 1.19 | 0.94 | 1.13 | 1.84 | 0.79 | 1.20 | **1.63** |
| 610 | 1.21 | 1.07 | 1.58 | 1.18 | 1.55 | 2.09 | 0.75 | 1.31 | 1.35 |
| 611 | 1.31 | 1.14 | **1.52** | 1.84 | 1.87 | 3.19 | 1.21 | 1.01 | 1.71 |
| 613 | 1.41 | 1.08 | **1.57** | **1.62** | 1.83 | 2.94 | 1.03 | 1.13 | **1.61** |
| 618 | 1.05 | 0.60 | 0.88 | 0.68 | **0.53** | 0.62 | 0.77 | 0.79 | 1.17 |
| 619 | 1.04 | 0.65 | 1.57 | 1.61 | 1.08 | 1.39 | 1.02 | 0.67 | 1.29 |
| 620 | 1.11 | 0.62 | 1.99 | 2.85 | 2.60 | 2.87 | 1.44 | 0.91 | 1.10 |
| 621 | 0.94 | 0.83 | 1.95 | 2.44 | 1.89 | 2.26 | 1.25 | 0.77 | 1.20 |
| 622 | 0.99 | 0.99 | 1.77 | 2.27 | 1.78 | 1.98 | 1.28 | 0.79 | 1.11 |
| 625 | 0.91 | 0.98 | 1.15 | 1.23 | 1.20 | 1.40 | 1.07 | 0.98 | 1.16 |
| 629 | 1.17 | 0.90 | 1.69 | 1.84 | 1.69 | 2.12 | 1.09 | 0.92 | 1.25 |
| 630 | 0.71 | 0.91 | 0.84 | 1.13 | 1.17 | **2.11** | 1.35 | 1.03 | 1.80 |
| 631 | 1.31 | 0.89 | 1.38 | 1.37 | 1.27 | 1.80 | 0.99 | 0.93 | 1.42 |
| 632 | **1.29** | 0.84 | **1.26** | 1.18 | 1.08 | 1.63 | 0.94 | 0.91 | 1.52 |
| 633 | 1.37 | 0.72 | 1.51 | 1.28 | 1.51 | 1.90 | 0.85 | 1.18 | 1.26 |
| 635 | 1.17 | 0.88 | **1.40** | 1.47 | 1.25 | 2.11 | 1.05 | 0.86 | 1.68 |
| 636 | 1.24 | 0.87 | 1.45 | 1.25 | 1.31 | 1.99 | 0.86 | 1.05 | 1.52 |
| 637 | 1.24 | 0.84 | 1.40 | 1.34 | 1.19 | 1.78 | 0.95 | 0.89 | 1.50 |
| 639 | 0.97 | 0.97 | 1.16 | 1.16 | 1.25 | 1.23 | 1.01 | 1.07 | 0.99 |
| 641 | 2.62 | 1.26 | 1.00 | 0.47 | 0.76 | 0.79 | 0.47 | 1.60 | 1.05 |
| 655 | 1.27 | 1.00 | 1.35 | 1.25 | 1.25 | 2.20 | 0.92 | 1.00 | 1.75 |
| 658 | 1.11 | 0.94 | 1.03 | 0.51 | 0.94 | 1.31 | 0.50 | 1.85 | 1.39 |
| 659 | **1.65** | 1.14 | 1.34 | 1.06 | 1.26 | 2.22 | 0.79 | 1.20 | **1.75** |
| 665 | 1.64 | 0.98 | 1.93 | 0.91 | 1.62 | 1.69 | 0.47 | 1.79 | 1.04 |
| 670.01 | 1.01 | 1.23 | 8.66 | 12.28 | 13.05 | 17.23 | 1.42 | 1.06 | 1.32 |
| 672 | 1.21 | 1.04 | 20.38 | 25.50 | 25.76 | 35.35 | 1.25 | 1.01 | 1.37 |
| 706 | 1.98 | **0.58** | 0.81 | 0.78 | 0.62 | 0.95 | 0.96 | 0.79 | 1.55 |
| 714 | 1.27 | 1.06 | 1.07 | 1.70 | **1.44** | 2.31 | 1.59 | 0.85 | 1.61 |
| 721 | **1.44** | 1.27 | 2.76 | 4.39 | 5.74 | 7.70 | 1.59 | 1.31 | 1.34 |
| 735 | 0.56 | 1.92 | 0.27 | 0.43 | 0.68 | 0.36 | 1.59 | 1.57 | 0.54 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| 742 | 1.17 | 1.01 | 1.79 | 2.05 | 1.84 | 3.00 | 1.14 | 0.90 | 1.63 |
| 744 | 1.25 | 0.96 | 1.95 | 2.06 | 1.83 | 3.14 | 1.06 | 0.89 | 1.72 |
| 809 | 1.03 | **0.87** | 0.87 | 0.80 | 0.66 | 0.74 | 0.91 | **0.83** | 1.12 |
| 811 | 2.34 | 0.51 | 1.09 | 1.97 | 0.95 | 0.90 | 1.81 | 0.48 | 0.94 |
| 819 | 1.03 | 0.95 | 0.93 | 1.06 | **0.82** | 0.96 | 1.14 | 0.77 | 1.17 |
| 820 | 0.97 | 1.02 | 1.02 | 1.07 | 0.95 | 1.07 | 1.05 | 0.88 | 1.13 |
| 821 | 1.09 | 0.97 | 0.96 | 0.98 | 0.92 | 1.06 | 1.01 | 0.94 | 1.16 |
| 822 | 1.01 | 0.92 | **0.88** | 0.85 | 0.73 | 0.82 | 0.96 | 0.85 | 1.13 |
| 823 | **1.61** | 0.92 | 0.55 | 0.62 | 0.48 | 0.82 | 1.12 | 0.77 | 1.72 |
| 825 | 1.23 | 0.84 | 1.01 | 1.05 | 1.01 | 1.00 | 1.03 | 0.97 | 0.99 |
| 833 | 1.52 | 0.81 | 2.03 | 3.45 | 4.07 | **3.72** | 1.70 | 1.18 | 0.91 |
| 834 | 1.50 | 0.76 | 2.58 | **4.84** | 5.74 | 5.02 | 1.88 | 1.19 | 0.88 |
| 835 | 1.64 | 0.63 | 2.72 | 4.32 | 5.10 | **4.49** | 1.59 | 1.18 | 0.88 |
| 840 | 0.98 | 1.30 | 0.88 | 0.93 | 0.89 | 1.03 | 1.06 | 0.95 | 1.16 |
| 849 | 0.92 | 1.02 | 0.98 | 0.90 | 1.02 | 1.11 | 0.91 | 1.14 | 1.08 |
| 851 | 0.98 | 1.06 | 0.73 | 0.63 | 0.62 | **0.68** | 0.87 | 0.98 | 1.09 |
| 876 | 1.36 | 1.02 | 1.45 | 1.88 | 1.52 | 1.09 | 1.29 | 0.81 | 0.72 |
| 877 | 1.08 | 0.70 | 0.98 | 1.32 | 0.80 | 0.98 | 1.35 | **0.61** | 1.23 |
| 881 | 1.03 | 1.01 | 1.11 | 1.00 | 0.96 | 1.12 | 0.90 | 0.97 | 1.16 |
| 882 | 0.59 | 0.70 | 0.83 | 0.83 | 0.69 | 0.80 | 0.99 | 0.84 | 1.16 |
| 883 | 1.08 | 1.04 | 0.91 | 0.87 | 0.82 | 0.91 | 0.95 | 0.94 | 1.12 |
| 890 | 1.06 | 1.02 | 1.04 | 1.17 | 1.01 | 0.90 | 1.12 | 0.86 | 0.89 |
| 905 | 1.44 | 1.12 | **2.37** | 3.43 | 3.36 | 4.88 | 1.45 | 0.98 | 1.45 |
| 909 | 2.30 | 0.45 | 0.69 | **0.53** | 0.59 | 0.75 | 0.77 | 1.11 | 1.27 |
| 915 | 1.95 | 0.79 | 0.85 | 0.34 | **0.41** | 0.48 | **0.40** | 1.20 | 1.17 |
| 919 | 1.26 | 0.68 | 0.69 | 0.51 | 0.52 | 0.56 | 0.74 | 1.02 | 1.07 |
| 920 | 1.07 | 0.84 | 4.08 | **5.20** | 8.12 | 6.42 | 1.27 | 1.56 | 0.79 |
| 922 | 1.12 | 0.70 | **3.34** | 4.26 | 6.59 | 6.56 | 1.28 | 1.55 | 1.00 |
| 923 | 1.14 | 0.84 | 1.93 | 3.11 | 4.03 | 3.60 | 1.61 | 1.30 | 0.89 |
| 926 | 1.27 | 1.15 | 1.69 | 1.78 | **3.46** | 2.22 | 1.05 | 1.94 | 0.64 |
| 929 | 1.88 | 0.63 | 2.49 | 2.26 | 5.93 | 6.83 | 0.90 | 2.63 | 1.15 |
| 930 | 1.19 | 0.93 | 2.56 | 3.00 | 7.07 | 5.34 | 1.17 | 2.36 | 0.75 |
| 934 | 1.37 | 0.81 | 2.27 | 2.54 | 5.85 | 5.47 | 1.12 | 2.31 | 0.93 |
| 935 | 1.31 | 0.90 | 1.61 | 1.28 | 4.11 | **3.04** | 0.79 | **3.22** | 0.74 |
| 936 | 2.06 | 0.56 | 2.35 | 2.09 | 5.40 | 5.77 | 0.89 | 2.59 | 1.07 |
| 937 | 1.67 | 0.69 | 1.90 | 1.70 | 2.69 | 2.46 | 0.89 | 1.59 | 0.92 |
| 938 | **1.63** | **0.60** | 0.80 | **0.60** | **0.61** | 0.86 | 0.76 | 1.02 | 1.40 |
| 939 | 1.07 | 0.93 | 2.66 | 2.31 | 4.75 | **3.27** | 0.87 | 2.06 | 0.69 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| 945 | 1.12 | 1.02 | 3.16 | 3.53 | 6.63 | 3.77 | 1.12 | 1.88 | 0.57 |
| 970 | 0.86 | 0.94 | 1.08 | 1.33 | 1.44 | 1.83 | 1.23 | 1.08 | 1.28 |
| 1004 | 1.15 | 0.92 | 1.00 | 1.10 | 0.98 | 0.99 | 1.10 | 0.89 | 1.01 |
| 1005 | 1.13 | 0.89 | 0.85 | 0.96 | 0.86 | 0.93 | 1.13 | 0.90 | 1.08 |
| 1018 | 1.01 | 1.17 | 1.11 | 1.43 | 1.05 | 0.96 | 1.29 | 0.73 | 0.92 |
| 1020 | 1.14 | 0.97 | 1.02 | 1.11 | 1.00 | 1.02 | 1.09 | 0.90 | 1.02 |
| 1024 | 1.40 | 0.95 | 0.54 | 0.73 | 0.65 | 0.74 | 1.36 | 0.88 | 1.14 |
| 1034 | 1.41 | 1.13 | **0.78** | 0.89 | 0.80 | 0.92 | 1.14 | 0.90 | 1.14 |
| 1057 | 0.92 | 0.79 | 0.36 | 0.36 | 0.90 | 0.73 | 1.00 | 2.52 | 0.81 |
| 1059 | 1.82 | 0.85 | 0.75 | 1.13 | 0.79 | **0.45** | 1.51 | 0.70 | 0.57 |
| 1098 | 1.23 | 0.88 | 1.13 | 4.90 | 15.19 | 30.64 | 4.33 | 3.10 | 2.02 |
| 1101 | 1.53 | 1.03 | 2.01 | 2.94 | 2.01 | 2.62 | **1.46** | 0.69 | 1.30 |
| 1105 | 0.90 | 0.66 | **0.75** | 0.52 | 0.38 | 0.32 | 0.69 | 0.73 | 0.84 |
| 1106 | 1.02 | 0.92 | 1.17 | 1.13 | 1.60 | 2.27 | 0.97 | 1.42 | 1.42 |
| 1114 | 2.07 | 0.98 | 1.15 | 1.15 | 1.13 | 1.90 | 1.00 | 0.98 | **1.68** |
| 1116 | 1.18 | 0.74 | 0.90 | 0.71 | **0.67** | 0.81 | 0.79 | 0.94 | 1.22 |
| 1128 | 1.18 | 0.61 | 0.89 | 0.89 | 0.62 | 0.81 | 1.01 | 0.69 | 1.31 |
| 1149 | **1.22** | **0.83** | 0.92 | **0.83** | 0.73 | 0.88 | 0.90 | 0.88 | **1.21** |
| 1150 | **2.45** | 0.66 | 0.46 | 0.49 | 0.50 | 0.71 | 1.08 | 1.01 | 1.42 |
| 1180 | 0.97 | 1.16 | 1.29 | 1.42 | 1.43 | 1.98 | 1.10 | 1.01 | 1.39 |
| 1181 | 1.07 | 0.87 | 0.96 | 0.79 | 0.69 | 0.87 | 0.83 | 0.87 | 1.27 |
| 1199 | 1.28 | 0.93 | 0.99 | 1.05 | 0.95 | 1.06 | 1.06 | 0.90 | 1.12 |
| 1202 | 1.41 | 0.65 | 1.09 | 0.94 | 0.98 | 1.17 | 0.86 | 1.04 | 1.20 |
| 1212 | 0.81 | 0.78 | 1.29 | 1.63 | 2.59 | 1.14 | 1.26 | 1.59 | 0.44 |
| 1216 | 1.04 | 0.67 | 1.06 | 1.75 | **2.04** | 1.60 | 1.65 | 1.16 | 0.78 |
| 1221 | 1.15 | 1.04 | 1.13 | 1.13 | 1.18 | 1.22 | 1.00 | 1.04 | 1.03 |
| 1224 | 0.92 | 0.93 | 1.04 | 1.66 | 1.98 | 1.03 | 1.59 | 1.19 | 0.52 |
| 1232 | 0.94 | **0.81** | 0.98 | 0.95 | **0.81** | **0.80** | 0.97 | 0.85 | 0.99 |
| 1242 | 1.08 | 0.93 | 1.01 | 0.98 | 0.90 | 0.95 | 0.97 | 0.93 | 1.05 |

| | | | ANVOA Contrasts | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PATHWAY SORT | T1-21 T1-14 | T1-28 T1-21 | T2-7 T2-0 | T2-14 T2-0 | T2-21 T2-0 | T2-28 T2-0 | T2-14 T2-7 | T2-21 T2-14 | T2-28 T2-21 |
| ~~1242.1~~ | 0.81 | 1.07 | 0.92 | 0.98 | 0.90 | 0.82 | 1.07 | 0.91 | 0.91 |
| 1243 | 1.06 | 1.05 | 1.01 | 1.01 | 0.95 | 1.00 | 1.00 | 0.94 | 1.05 |
| 1266 | 1.30 | 0.81 | 0.93 | 0.97 | 0.97 | 0.83 | 1.05 | 0.99 | 0.86 |
| 1288 | 1.11 | 0.90 | 0.90 | 0.91 | 0.84 | 0.93 | 1.01 | 0.92 | 1.12 |
| 1300 | 1.08 | 0.98 | 0.95 | 0.97 | **0.86** | 0.93 | 1.01 | 0.89 | 1.08 |
| 1318 | 1.30 | 0.93 | 1.11 | 1.19 | 1.04 | 0.97 | 1.08 | 0.87 | 0.94 |
| 1360 | 1.00 | 0.62 | 1.01 | 0.90 | **0.54** | **0.58** | 0.89 | 0.60 | 1.07 |
| 1469 | 1.17 | **0.81** | 0.95 | 0.95 | 0.91 | 1.00 | 1.00 | 0.95 | 1.10 |
| 1531 | 1.33 | **0.68** | 1.01 | 0.59 | **0.65** | 0.57 | 0.59 | 1.10 | 0.87 |
| 1565 | 1.14 | 0.97 | 0.93 | 0.88 | 0.76 | 0.97 | 0.95 | 0.87 | 1.27 |
| 1584 | 1.04 | 1.07 | 1.09 | 1.01 | 0.89 | 1.11 | 0.93 | 0.88 | 1.25 |
| 1585 | 0.94 | 1.10 | 0.89 | 0.94 | 0.88 | 0.74 | 1.06 | 0.93 | **0.84** |
| 1612 | 1.14 | 0.93 | 0.90 | 0.91 | **0.84** | 0.84 | 1.01 | 0.93 | 1.00 |
| 1613 | 0.89 | 1.08 | 1.07 | 1.18 | 1.11 | 1.05 | 1.10 | 0.94 | 0.94 |
| 1614 | 1.29 | 0.96 | 0.84 | **1.40** | 0.86 | 1.06 | 1.66 | 0.61 | 1.23 |
| 1615 | **0.49** | 1.45 | 1.23 | 0.95 | 0.82 | 1.02 | 0.77 | 0.86 | 1.24 |
| 1632 | 1.69 | 1.15 | **1.29** | 1.69 | 1.87 | 2.15 | **1.31** | 1.11 | 1.15 |
| 1662 | 1.15 | **0.81** | **0.82** | 0.94 | 0.87 | 0.95 | 1.15 | 0.93 | 1.09 |