**Medium to use**

Two types of media were considered when performed the reconstructions, those based on cell culture media, and those based on the average concentration of the exchange metabolites from the HumanGEM model in normal human blood.

**Unconstrained elements**

This elements were considered to be freely accessible to the cells, **in all media**.

|  |  |  |
| --- | --- | --- |
| **Elements** | **Recon ID** | **ub** |
| **H2O** | h2o[e] | 1000 |
| **O2** | o2[e] | 1000 |
| **H** | h[e] | 1000 |

**Cell Cluture Media Used**

- Plasmax medium

- Article: Vande Voorde et al. *Improving the metabolic fidelity of cancer models with a physiological cell culture medium*. Science Advances. 2019;5: eaau7314 (10.1126/sciadv.aau7314)

- Detailed information gathered from supplementary table S1 (<https://advances.sciencemag.org/content/advances/suppl/2018/12/21/5.1.eaau7314.DC1/aau7314_SM.pdf>)

- Medium: [https://ximbio.com/reagent/156371/plasmaxsuptmsup-cell-culture-medium-coming-soon#datasheet](https://ximbio.com/reagent/156371/plasmaxsuptmsup-cell-culture-medium-coming-soon" \l "datasheet)

- HPLM

- Article: Cantor JR et al. *Physiologic Medium Rewires Cellular Metabolism and Reveals Uric Acid as an Endogenous Inhibitor of UMP Synthase*. Cell. 2017;169(2): 258-272.e17 ([doi.org/10.1016/j.cell.2017.03.023](https://doi.org/10.1016/j.cell.2017.03.023))

- Detailed information gathered from supplementary table S1 (<https://advances.sciencemag.org/content/advances/suppl/2018/12/21/5.1.eaau7314.DC1/aau7314_SM.pdf>)

- Medium:

- RPMI-1640:

- Article:

- Detailed information gathered from:[https://ss-usa.s3.amazonaws.com/c/308472537/media/187615dfb9b2320e9776486215674958/Plasmax%28TM%29%20formulation%20compared%20to%20historic%20media.pdf](https://ss-usa.s3.amazonaws.com/c/308472537/media/187615dfb9b2320e9776486215674958/Plasmax(TM) formulation compared to historic media.pdf)

- Medium:

**Note:** Several metabolites were added to these chemical defined media. The two essential fatty acids for human cells (Linoleate and Linolenate), fat-soluble vitamins (A, D, E and K), and lipoic acid. The vitamins are carried by binding proteins in serum, which is normally used with the chemically defined medium (fetal bovine serum – FBS, for example). The concentrations of these metabolites were set according to the *Serum Metabolome Database*, which is integrated in the *Human Metabolome Database* (<https://serummetabolome.ca/>). When more than one quantification is available, the average was calculated (database accessed on August 10th, 2020).

Tables summarising information on the media used. Some components will not be used in the models, either because they are not part of the metabolism (e.g. Phenol Red), or because they are not represented in HumanGEM, or even because they were excluded from HumanGEM\_consistent when removing blocked reactions (this last case will be highlighted in orange – malonate, calcium, magnesium, potassium, sodium, copper, zinc, phylloquinone (Vitamin K), D-serine, 1-Myristoylglycerophosphocholine, 1-Oleoylglycerophosphocholine (Delta 9), 1-Stearoylglycerophosphocholine, 1-Eicosatetraenoylglycerophosphocholine (Delta 8, 11, 14, 17), Sn1-Lpc (20:4), 1-Lignocericylglycerophosphocholine (24:0), Lysopc A C24, 1-Heptadecanoylglycerophosphocholine, (8Z,11Z,14Z)-Eicosatrienoic Acid, gluatarate, indoxyl sulfate, guanidine, 8-dehydrocholesterol, Oleoyl ethanolamine, Palmitoylethanolamide, Prostaglandin D3, Methanethiol, prostaglandin D1, beta-tocopherol, 1-Palmitoylglycerophosphocholine, 1-Palmitoleoylglycerophosphocholine (Delta 9), 1-Linoleoylglycerophosphocholine (Delta 9,12), 1-Octadeca-Trienoylglycerophosphocholine, Sn1-Lpc (18:3, Delta 6, 9, 12), 1-Octadeca-Trienoylglycerophosphocholine, Sn1-Lpc (18:3, Delta 9, 12, 15), 1-Eicosenoylglycerophosphocholine (Delta 11) ,Sn1-Lpc (20:1), 1-Eicosadienoylglycerophosphocholine (Delta 11,14), 1-Dihomo-Linolenoylglycerophosphocholine (20:3, Delta 8, 11, 14), Lysopc A C20:3, 1-Arachidonoyl-Glycero-3-Phosphocholine, 1-Eicosapentenoylglycerophosphocholine (Delta 5, 8, 11, 14, 17), Sn1-Lpc (20:5); 1-Docosatetraenoylglycerophosphocholine (Delta 7, 10, 13, 16), Sn1-Lpc (22:4); 1-Docosapentenoylglycerophosphocholine (Delta 4, 7, 10, 13, 16), Sn1-Lpc (22:5)-W6; 1-Docosapentenoylglycerophosphocholine (Delta 7, 10, 13, 16, 19), Sn1-Lpc (22:5)-W3; 1-Docosahexenoylglycerophosphocholine (Delta 4, 7, 10, 13, 16, 19), Sn1-Lpc (22:6); Lysopc A C28:0; Lysopc A C26:1 (Delta 5); Lysopc A C28:1 (Delta 5); Decenoyl carnitine; Octenoyl carnitine; Dodecenoyl carnitine; 3-Hydroxy-Octadecenoyl Carnitine; Cholesterol Ester; phosphatidate-LD-TAG pool; ). Concentrations for each medium are in M.

Source table:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Elements** | **HumanGEM metabolite ID (extracelular)** | **Plasmax** | **HPLM** | **RPMI-1640** |
| **Proteinogenic Amino Acids** | L-Alanine | ala\_L[e] | 510 | 430 |  |
| L-Arginine | arg\_L[e] | 64 | 110 | 1149 |
| L-Asparagine | asn\_L[e] | 41 | 50 | 379 |
| L-Aspartic acid | asp\_L[e] | 6 | 20 | 150 |
| L-Cysteine | cys\_L[e] | 33 | 40 |  |
| L-Glutamate | glu\_L[e] | 98 | 80 | 136 |
| L-Glutamine | gln\_L[e] | 650 | 550 | 2055 |
| Glycine | gly[e] | 330 | 300 | 133 |
| L-Histidine | his\_L[e] | 120 | 110 | 97 |
| L-Isoleucine | ile\_L[e] | 140 | 70 | 382 |
| L-Leucine | leu\_L[e] | 170 | 160 | 382 |
| L-Lysine | lys\_L[e] | 220 | 200 | 219 |
| L-Methionine | met\_L[e] | 30 | 30 | 101 |
| L-Phenylalanine | phe\_L[e] | 68 | 80 | 91 |
| L-Proline | pro\_L[e] | 360 | 200 | 174 |
| L-Serine | ser\_L[e] | 140 | 150 | 286 |
| L-Threonine | thr\_L[e] | 240 | 140 | 168 |
| L-Tryptophan | trp\_L[e] | 78 | 60 | 25 |
| L-Tyrosine | tyr\_L[e] | 74 | 80 | 111 |
| L-Valine | val\_L[e] | 230 | 220 | 171 |
| **Non-proteinogenic Amino Acids** | -Aminobutyrate | C02356[e] | 41 | 20 |  |
| L-Citrulline | citr\_L[e] | 55 | 40 |  |
| L-Cystine | Lcystin[e] | 65 | 100 | 207.7 |
| L-Homocysteine | hcys\_L[e] | 9 |  |  |
| 4-Hydroxy-L-proline | 4hpro\_LT[e] | 13 | 20 | 152.7 |
| L-Ornithine | orn[e] | 80 | 10 |  |
| L-Pyroglutamate | 5oxpro[e] | 20 |  |  |
| **Amino Acids Derivatives** | L-Acetyl glycine | acgly[e] | 70 | 90 |  |
| L-Carnosine | carn[e] | 6 |  |  |
| Glutathione (reduced) | gthrd[e] | 37 | 25 | 3.3 |
| Taurine | taur[e] | 130 | 90 |  |
| N-Trimethylglycine (betaine) | glyb[e] | 72 | 70 |  |
| **Other Components** | Acetate | ac[e] | 42 | 40 |  |
| Acetone | acetone[e] | 55 | 60 |  |
| Acetyl carnitine | acrn[e] | 5 |  |  |
| Citrate | cit[e] | 114 | 130 |  |
| Carnitine | crn[e] | 46 | 40 |  |
| Creatine | creat[e] | 37 | 40 |  |
| Creatinine | crtn[e] | 74 | 75 |  |
| Formate | for[e] | 33 | 50 |  |
| Fructose | fru[e] |  | 40 |  |
| Galactose | gal[e] |  | 60 |  |
| D-Glucose | glc\_D[e] | 5560 | 5000 | 11111 |
| Glycerol | glyc[e] | 82 | 120 |  |
| 2-Hydroxybutyrate | 2hb[e] | 31 | 50 |  |
| 3-Hydroxybutyrate | bhb[e] | 77 | 50 |  |
| 3-Hydroxyisobutyrate | 3hmp[e] | 20 |  |  |
| Hypoxanthine | hxan[e] | 5 | 10 |  |
| Lactate | lac\_L[e]; lac\_D[e] | 500 | 1600 |  |
| Malonate | HC00319[e] |  | 10 |  |
| Methyl acetoacetate | acetoacetate + methyl group | 41 |  |  |
| Phenol Red | - | 25 | 14 | 13.3 |
| Pyruvate | pyr[e] | 100 | 50 |  |
| Succinate | succ[e] | 23 | 20 |  |
| Uracil | ura[e] | 2 |  |  |
| Urate | urate[e] | 270 | 350 |  |
| Urea | urea[e] | 3000 | 5000 |  |
| Uridine | uri[e] | 3 |  |  |
| **Inorganic Salts** | Ammonium Chloride | nh4[e] + cl[e] | 50 | 40 |  |
| Calcium Chloride | ca2[e] + 2 cl[e] | 1800 | 2350 |  |
| Calcium Nitrate | ca2[e] + 2 CE5643[e] |  | 40 | 424 |
| Magnesium Chloride | mg2[e] + 2 cl[e] |  | 480 |  |
| Magnesium Sulfate | mg2[e] + so4[e] | 813 | 350 | 407 |
| Potassium Chloride | k[e] + cl[e] | 5330 | 4100 | 5333 |
| Sodium Bicarbonate | na1[e] + hco3[e] | 26191 | 24000 | 23810 |
| Sodium Chloride | na1[e] + cl[e] | 118706 | 105000 | 103448 |
| Sodium Phosphate | 2 na1[e] + pi[e] | 1010 | 870 | 5634 |
| **Trace Elements** | Ammonium Metavanadate | nh4[e] + - | 0.0026 |  |  |
| Cupric Sulfate | cu2[e] + so4[e] | 0.0052 |  |  |
| Ferric NitrateZinc | fe3[e] + 3 CE5643[e] | 0.1238 |  |  |
| Ferric Sulfate | 2 fe3[e] + 3 so4[e] | 1.048 |  |  |
| Manganous Chloride | - + 2 cl[e] | 0.0002 |  |  |
| Sodium Selenite | 2 na1[e] + selni[e] | 0.0289 |  |  |
| Zinc Sulfate | zn2[e] + so4[e] | 1.5 |  |  |
| **Vitamins** | p-Aminobenzoate | m01342s |  | 7.3 | 7.3 |
| Ascorbate | ascb\_L[e] | 62 |  |  |
| D-Biotin | btn[e] | 4.1 | 0.8 | 0.820 |
| Choline | chol[e] | 7.1 | 21.5 | 21.4 |
| Folate | fol[e] | 2.3 | 2.3 | 2.27 |
| Myo-Inositol | inost[e] | 11.1 | 194.3 | 194.4 |
| Niacinamide | ncam[e] | 8.2 | 8.2 | 8.2 |
| D-Pantothenic acid hemicalcium | 2 pnto\_R[e] and ca2[e] | 4.2 | 1.05 | 0.52 |
| Pyridoxine | Pydxn[e] | 4.9 | 4.9 | 4.9 |
| Riboflavin | ribflv[e] | 0.3 | 0.5 | 0.53 |
| Thiamine | thm[e] | 3 | 3 | 3 |
| Vitamin B12 | **aquacob(III)alamin** | 0.005 | 0.0037 | 0.0037 |
| **Added Metabolites** | Lipoic acid | m02394s | 0.077 | 0.077 | 0.077 |
| Linoleate | m02387s | 343.1 | 343.1 | 343.1 |
| Linolenate | m02389s | 28.652 | 28.652 | 28.652 |
| Retinol (Vitamin A) | m02834s | 2.4 | 2.4 | 2.4 |
| -tocopherol (Vitamin E) | m01327s | 28.125 | 28.125 | 28.125 |
| γ-tocopherol (Vitamin E) | m01935s | 12.639 | 12.639 | 12.639 |
| Vitamin D2 | m03141s | 0.0028 | 0.0028 | 0.0028 |
| Vitamin D3 | m03142s | 0.0503 | 0.0503 | 0.0503 |
| Phylloquinone (Vitamin K) | m02744s | 0.00154 | 0.00154 | 0.00154 |

Final media table used as base to calculate the respective exchange fluxes (µM). **Only Plasmax was used.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Elements** | **HumanGEM Exchange Reaction ID** | **Plasmax** | **HPLM** | **RPMI-1640** |
| L-Alanine | HMR\_9061 | 510 | 430 | 0 |
| L-Arginine | HMR\_9066 | 64 | 110 | 1149 |
| L-Asparagine | HMR\_9062 | 41 | 50 | 379 |
| L-Aspartic acid | HMR\_9070 | 6 | 20 | 150 |
| L-Cysteine | HMR\_9065 | 33 | 40 | 0 |
| L-Glutamate | HMR\_9071 | 98 | 80 | 136 |
| L-Glutamine | HMR\_9063 | 650 | 550 | 2055 |
| Glycine | HMR\_9067 | 330 | 300 | 133 |
| L-Histidine | HMR\_9038 | 120 | 110 | 97 |
| L-Isoleucine | HMR\_9039 | 140 | 70 | 382 |
| L-Leucine | HMR\_9040 | 170 | 160 | 382 |
| L-Lysine | HMR\_9041 | 220 | 200 | 219 |
| L-Methionine | HMR\_9042 | 30 | 30 | 101 |
| L-Phenylalanine | HMR\_9043 | 68 | 80 | 91 |
| L-Proline | HMR\_9068 | 360 | 200 | 174 |
| L-Serine | HMR\_9069 | 140 | 150 | 286 |
| L-Threonine | HMR\_9044 | 240 | 140 | 168 |
| L-Tryptophan | HMR\_9045 | 78 | 60 | 25 |
| L-Tyrosine | HMR\_9064 | 74 | 80 | 111 |
| L-Valine | HMR\_9046 | 230 | 220 | 171 |
| -Aminobutyrate | EX\_C02356[e] | 41 | 20 | 0 |
| L-Citrulline | HMR\_9201 | 55 | 40 | 0 |
| L-Cystine | HMR\_9363 | 65 | 100 | 207.7 |
| L-Homocysteine | EX\_hcys\_L[e] | 9 | 0 | 0 |
| 4-Hydroxy-L-proline | EX\_4hpro[e] | 13 | 20 | 152.7 |
| L-Ornithine | HMR\_9087 | 80 | 10 | 0 |
| L-Pyroglutamate | EX\_5oxpro[e] | 20 | 0 | 0 |
| L-Acetyl glycine | EX\_acgly[e] | 70 | 90 | 0 |
| L-Carnosine | EX\_carn[e] | 6 | 0 | 0 |
| Glutathione (reduced) | HMR\_9351 | 37 | 25 | 3.3 |
| TaurineCopper | HMR\_9418 | 130 | 90 | 0 |
| N-Trimethylglycine (betaine) | HMR\_9341 | 72 | 70 | 0 |
| Acetate | HMR\_9086 | 42 | 40 | 0 |
| Acetone | HMR\_9243 | 55 | 60 | 0 |
| Acetyl carnitine | EX\_acrn[e] | 5 | 0 | 0 |
| Citrate | HMR\_9286 | 114 | 130 | 0 |
| Carnitine | HMR\_9292 | 46 | 40 | 0 |
| Creatine | HMR\_9290 | 37 | 40 | 0 |
| Creatinine | HMR\_9460 | 74 | 75 | 0 |
| Formate | HMR\_9318 | 33 | 50 | 0 |
| Fructose | HMR\_9139 | 0 | 40 | 0 |
| Galactose | HMR\_9140 | 0 | 60 | 0 |
| D-Glucose | HMR\_9034 | 5560 | 5000 | 11111 |
| Glycerol | HMR\_9085 | 82 | 120 | 0 |
| 2-Hydroxybutyrate | HMR\_9216 | 31 | 50 | 0 |
| 3-Hydroxybutyrate | HMR\_9134 | 77 | 50 | 0 |
| 3-Hydroxyisobutyrate | EX\_3hmp[e] | 20 | 0 | 0 |
| Hypoxanthine | HMR\_9358 | 5 | 10 | 0 |
| Lactate | HMR\_9135 | 500 | 1600 | 0 |
| Lactate | HMR\_9136 | 500 | 1600 | 0 |
| Malonate | HC00319[e] | 0 | 10 | 0 |
| Acetoacetate | HMR\_9164 | 41 | 0 | 0 |
| Pyruvate | HMR\_9132 | 100 | 50 | 0 |
| Succinate | HMR\_9133 | 23 | 20 | 0 |
| Uracil | HMR\_9415 | 2 | 0 | 0 |
| Urate | HMR\_9437 | 270 | 350 | 0 |
| Urea | HMR\_9075 | 3000 | 5000 | 0 |
| Uridine | HMR\_9438 | 3 | 0 | 0 |
| Ammonia | HMR\_9439 | 50,0026 | 40 | 0 |
| Chloride ion | EX\_nh4[e] | 127686 | 114800 | 108781 |
| Calcium | HMR\_9082 | 1804.2 | 2391.05 | 424.52 |
| Nitrate | EX\_CE5643[e] | 0.3714 | 40 | 424 |
| Magnesium | EX\_mg2[e] | 813 | 830 | 407 |
| Sulfate | HMR\_9074 | 817.6492 | 350 | 407 |
| Potassium | HMR\_9081 | 5330 | 4100 | 5333 |
| Sodium | HMR\_9077 | 146917.058 | 130740 | 138526 |
| Hidrogen carbonate | HMR\_9078 | 26191 | 24000 | 23810 |
| Phosphate | HMR\_9072 | 1010 | 870 | 5634 |
| Copper | EX\_cu2[e] | 0.0052 | 0 | 0 |
| Iron3 | HMR\_9096 | 2.2198 | 0 | 0 |
| Zinc | HMR\_9080 | 1.5 | 0 | 0 |
| D-Pantothenic acid | HMR\_9145 | 8.4 | 2.1 | 1.04 |
| p-Aminobenzoate | EX\_anth[e] | 0 | 7.3 | 7.3 |
| Ascorbate | HMR\_9158 | 62 | 0 | 0 |
| D-Biotin | HMR\_9109 | 4.1 | 0.8 | 0.820 |
| Choline | HMR\_9083 | 7.1 | 21.5 | 21.4 |
| Folate | HMR\_9146 | 2.3 | 2.3 | 2.27 |
| Myo-Inositol | HMR\_9361 | 11.1 | 194.3 | 194.4 |
| Niacinamide | HMR\_9378 | 8.2 | 8.2 | 8.2 |
| Pyridoxine | HMR\_9144 | 4.9 | 4.9 | 4.9 |
| Riboflavin | HMR\_9143 | 0.3 | 0.5 | 0.53 |
| Thiamine | HMR\_9159 | 3 | 3 | 3 |
| Vitamin B12 | HMR\_9269 | 0.005 | 0.0037 | 0.0037 |
| Lipoic acid | HMR\_9167 | 0.077 | 0.077 | 0.077 |
| Linoleate | HMR\_9035 | 343.1 | 343.1 | 343.1 |
| Linolenate | HMR\_9036 | 28.652 | 28.652 | 28.652 |
| Retinol (Vitamin A) | HMR\_9147 | 2.4 | 2.4 | 2.4 |
| -tocopherol | HMR\_9151 | 28.125 | 28.125 | 28.125 |
| γ-tocopherol | HMR\_9153 | 12.639 | 12.639 | 12.639 |
| Vitamin D2 | HMR\_9441 | 0.0028 | 0.0028 | 0.0028 |
| Vitamin D3 | HMR\_9442 | 0.0503 | 0.0503 | 0.0503 |
| Phylloquinone (Vitamin K) | HMR\_9392 | 0.00154 | 0.00154 | 0.00154 |

**Blood medium**

The metabolite concentrations for this medium were based on the average concentration that the exchange metabolites from the HumanGEM model have in the human blood. This information was taken from the *Serum Metabolome Database*, which is integrated in the *Human Metabolome Database* (<https://serummetabolome.ca/>).

In total, 587 metabolites were considered for the medium.

More info on how data was filtered is elsewhere (serum\_concentration\_decisions.rtf and serum\_concentrations\_final.txt).

Final media table used as base to calculate the respective exchange fluxes (µM).

|  |  |  |
| --- | --- | --- |
| **Elements** | **HumanGEM Exchange Reaction ID** | **Concentration** |
| (R)-3-hydroxybutanoate | HMR\_9134 | 702.5 |
| 12(S)-HPETE | EX\_12HPET[e] | 0.00145 |
| 13,16,19-docosatrienoic acid | EX\_M00341[e] | 0.004 |
| 13-cis-retinoyl-glucuronide | HMR\_9210 | 0.0066 |
| 1-methylnicotinamide | HMR\_9104 | 0.43 |
| 20alpha-hydroxy-4-pregnen-3-one | HMR\_9268 | 0.0291 |
| 25-Hydroxyvitamin D2 | HMR\_9214 | 9001.125 |
| 2-Hydroxybutyrate | HMR\_9216 | 42.225 |
| 2-Methylcitrate | HMR\_9217 | 0.0795 |
| 3,4-dihydroxyphenylethyleneglycol | HMR\_9218 | 0.00767 |
| 4-aminobutyrate | HMR\_9091 | 0.21 |
| 4-Hydroxy-debrisoquine | HMR\_9223 | 0.217 |
| 4-hydroxyphenylacetate | HMR\_9224 | 9.881 |
| 4-Pyridoxate | HMR\_9228 | 0.0210 |
| 5-alpha-dihydrotestosterone | HMR\_9229 | 0.00194 |
| 5-formyl-THF | HMR\_9100 | 0.0025 |
| 5-Hydroxy-L-tryptophan | HMR\_9094 | 0.018 |
| 5-methyl-THF | HMR\_9234 | 0.3 |
| Acetaldehyde | HMR\_9242 | 1 |
| Acetate | HMR\_9086 | 46.735 |
| Acetoacetate | HMR\_9132 | 152.0583 |
| Acetone | HMR\_9243 | 65.0333 |
| Adenine | HMR\_9253 | 0.47 |
| Adenosine | HMR\_9254 | 1.344 |
| ADP | HMR\_9255 | 160 |
| adrenaline | HMR\_9095 | 0.000738 |
| Adrenic acid | EX\_adrn[e] | 4.0728 |
| AKG | HMR\_9259 | 10.5 |
| Alanine | HMR\_9061 | 358.610 |
| Aldosterone | HMR\_9261 | 0.000678 |
| alpha-Tocopherol | HMR\_9151 | 32.430 |
| Alpha-Tocotrienol | HMR\_9152 | 4.23 |
| AMP | HMR\_9262 | 19.075 |
| Androsterone | HMR\_9263 | 0.0603 |
| Androsterone-glucuronide | HMR\_9264 | 0.437 |
| Arachidonate | EX\_arachd[e] | 171.0599 |
| Arginine | HMR\_9066 | 85.805 |
| Ascorbate | HMR\_9158 | 43.611 |
| Asparagine | HMR\_9062 | 53.135 |
| aspartate | HMR\_9070 | 21.723 |
| ATP | EX\_atp[e] | 1792.75 |
| Behenic acid | EX\_docosac[e] | 10.951 |
| beta-Alanine | HMR\_9260 | 2.635 |
| Betaine | HMR\_9341 | 72.545 |
| Bilirubin | HMR\_9273 | 44.813 |
| Biotin | HMR\_9109 | 0.0257 |
| Butyrate | HMR\_9809 | 1 |
| Ca2+ | HMR\_9082 | 2197.455 |
| Calcidiol | HMR\_9215 | 0.0684 |
| cAMP | HMR\_9275 | 0.0085 |
| cerotic acid | EX\_hexc[e] | 0.723 |
| cGMP | HMR\_9220 | 0.0055 |
| Chenodiol | HMR\_10026 | 1.0825 |
| Chloride | HMR\_9150 | 103044.444 |
| Cholate | HMR\_9280 | 0.84 |
| Cholesterol | HMR\_9285 | 3123.865 |
| Choline | HMR\_9083 | 13.275 |
| cis-cetoleic acid | EX\_M01582[e] | 0.0295 |
| cis-erucic acid | EX\_doco13ac[e] | 7.164 |
| cis-gondoic acid | EX\_CE2510[e] | 4.628 |
| cis-Vaccenic acid | EX\_vacc[e] | 98.6 |
| Citrate | HMR\_9286 | 125.713 |
| Citrulline | HMR\_9201 | 41.892 |
| CO2 | HMR\_9058 | 21328.571 |
| Coproporphyrin I | HMR\_9701 | 0.0081 |
| Coproporphyrin III | HMR\_9702 | 0.006 |
| Cortisol | HMR\_9293 | 0.346 |
| Creatine | HMR\_9290 | 50.453 |
| Creatinine | HMR\_9460 | 60.582 |
| cys-gly | HMR\_9279 | 51.878 |
| Cysteine | HMR\_9065 | 140.735 |
| Cystine | HMR\_9363 | 81.457 |
| Cytidine | HMR\_9295 | 0.175 |
| Cytosine | HMR\_9291 | 6.4 |
| D-Alanine | HMR\_9098 | 446.75 |
| debrisoquin | HMR\_9299 | 0.149 |
| decanoic acid | HMR\_9815 | 11 |
| Dehydroascorbic acid | HMR\_9301 | 5.772 |
| dehydroepiandrosterone sulfate | HMR\_9302 | 7.547 |
| Deoxycytidine | HMR\_9296 | 0.2 |
| Deoxyuridine | HMR\_9310 | 0.284 |
| D-glucitol | HMR\_9685 | 7.045 |
| DHA | EX\_crvnc[e] | 105.619 |
| dihomo-gamma-linolenate | EX\_dlnlcg[e] | 46.664 |
| Dopamine | HMR\_9092 | 0.000065 |
| D-Ornithine | HMR\_9454 | 89 |
| DPA | EX\_clpnd[e] | 30.728 |
| D-Serine | HMR\_9407 | 2.587 |
| eicosanoate | EX\_arach[e] | 7.278 |
| Elaidate | EX\_elaid[e] | 100 |
| EPA | EX\_tmndnc[e] | 143.446 |
| estradiol-17beta 3-glucuronide | HMR\_9129 | 0.0000387 |
| Estradiol-17beta | HMR\_9314 | 0.000272 |
| Estriol | HMR\_9452 | 0.00478 |
| Ethanol | HMR\_9099 | 23.833 |
| Ethanolamine | HMR\_9084 | 26.95 |
| Etiocholanolone | HMR\_9453 | 0.00125 |
| FAD | EX\_fad[e] | 0.07133 |
| Fe2+ | HMR\_9076 | 8922 |
| Folate | HMR\_9146 | 0.0237 |
| Formate | HMR\_9318 | 103.173 |
| Fructose | HMR\_9139 | 39.5 |
| Galactose | HMR\_9140 | 59.303 |
| Gamma-Linolenate | EX\_lnlncg[e] | 12.13 |
| GDP | HMR\_9340 | 16.5 |
| Glucosamine | HMR\_9168 | 0.29 |
| Glucose | HMR\_9034 | 4687.664 |
| glutamate | HMR\_9071 | 65.419 |
| Glutamine | HMR\_9063 | 587.715 |
| Glycerate | HMR\_9342 | 10 |
| Glycerol | HMR\_9085 | 140.733 |
| Glycine | HMR\_9067 | 456.676 |
| glycochenodeoxycholate | HMR\_9283 | 0.68 |
| Glycocholate | HMR\_9281 | 0.513 |
| Glycoursodeoxycholate | EX\_HC02196[e] | 0.145 |
| GSH | HMR\_9351 | 89.835 |
| GSSG | HMR\_9350 | 10.825 |
| GTP | HMR\_9352 | 56 |
| Guanosine | HMR\_9348 | 0.8 |
| H2O2 | HMR\_9354 | 10.5 |
| HCO3- | HMR\_9078 | 23027.679 |
| heptaglutamyl-folate(DHF) | HMR\_9239 | 0.0076 |
| hexanoic acid | HMR\_9811 | 17 |
| Histamine | EX\_hista[e] | 0.0753 |
| Histidine | HMR\_9038 | 120.661 |
| Homoserine | HMR\_9161 | 12 |
| Homovanillate | HMR\_9694 | 0.0596 |
| Hypoxanthine | HMR\_9358 | 6.322 |
| IMP | HMR\_9360 | 63 |
| Inosine | HMR\_9362 | 1.388 |
| Inositol | HMR\_9361 | 23.525 |
| Isoleucine | HMR\_9039 | 63.710 |
| K+ | HMR\_9081 | 4398.0952 |
| L-3-amino-isobutanoate | HMR\_9221 | 1.03 |
| LacCer pool | HMR\_10027 | 10 |
| L-Arabinose | HMR\_9270 | 2.5 |
| L-Arabitol | HMR\_9241 | 2 |
| lauric acid | EX\_ddca[e] | 5.822 |
| L-Carnitine | HMR\_9292 | 40.938 |
| L-Dopa | HMR\_9219 | 0.00723 |
| Leucine | HMR\_9040 | 133.28 |
| Leukotriene B4 | HMR\_9365 | 0.00783 |
| Leukotriene C4 | HMR\_9366 | 0.00419 |
| Leukotriene E4 | HMR\_9368 | 0.00753 |
| lignocerate | EX\_lgnc[e] | 5.9583 |
| Limonene | HMR\_9369 | 0.19 |
| Linoleate | HMR\_9035 | 637.382 |
| Linolenate | HMR\_9036 | 28.652 |
| lipoic acid | HMR\_9167 | 0.077 |
| Lithocholate | EX\_HC02191[e] | 0.205 |
| L-Lactate | HMR\_9135 | 1612.554 |
| L-Metanephrine | HMR\_9373 | 0.0016 |
| Lysine | HMR\_9041 | 187.738 |
| Malonate | HMR\_9164 | 12.326 |
| Mannose | HMR\_9137 | 51.5 |
| margaric acid | EX\_hpdca[e] | 266.618 |
| mead acid | EX\_M02457[e] | 3.458 |
| Methanol | HMR\_9372 | 167.6 |
| Methionine | HMR\_9042 | 215.0466 |
| Methylimidazoleacetic acid | HMR\_9090 | 0.0846 |
| Myristic acid | EX\_ttdca[e] | 20.259 |
| Na+ | HMR\_9077 | 140381.818 |
| NAD+ | HMR\_9376 | 24.3 |
| NADH | EX\_nadh[e] | 22 |
| NADP+ | HMR\_9377 | 19.6 |
| Nervonic acid | EX\_nrvnc[e] | 26.0005 |
| NH3 | HMR\_9073 | 110.195 |
| Nicotinate | HMR\_9142 | 43.075 |
| Nitrite | HMR\_9149 | 19.736 |
| NO | HMR\_9381 | 0.000012 |
| noradrenaline | HMR\_9093 | 0.00281 |
| Norepinephrine sulfate | HMR\_9382 | 0.008 |
| octanoic acid | HMR\_9813 | 5.25 |
| Oleate | EX\_ocdcea[e] | 303.668 |
| omega-3-arachidonic acid | EX\_eicostet[e] | 0.007 |
| Omeprazole | HMR\_9387 | 0.34 |
| Ornithine | HMR\_9087 | 78.271 |
| Orotate | HMR\_9690 | 2.945 |
| Palmitate | EX\_hdca[e] | 487.0738 |
| Palmitolate | EX\_hdcea[e] | 50.341 |
| Pantothenate | HMR\_9145 | 2.744 |
| pentadecylic acid | EX\_ptdca[e] | 100.781 |
| Phenylacetylglutamine | HMR\_9391 | 3.34 |
| Phenylalanine | HMR\_9043 | 69.45 |
| phylloquinone (Vitamin K) | HMR\_9392 | 0.00145 |
| physeteric acid | EX\_M02745[e] | 1.5 |
| Phytanic acid | HMR\_9037 | 4.697 |
| PPi | EX\_ppi[e] | 1.8 |
| Progesterone | HMR\_9393 | 2.368 |
| Proline | HMR\_9068 | 198.863 |
| Propanoate | HMR\_9808 | 1.25 |
| Prostaglandin A1 | EX\_HC02202[e] | 0.000074 |
| Prostaglandin A2 | EX\_HC02203[e] | 0.000955 |
| Prostaglandin B2 | EX\_HC02205[e] | 0.000446 |
| Prostaglandin D2 | HMR\_9395 | 0.000193 |
| Prostaglandin E1 | HMR\_9396 | 0.0000037 |
| Prostaglandin E2 | HMR\_9397 | 0.000731 |
| Prostaglandin F2alpha | HMR\_9398 | 0.000251 |
| Putrescine | EX\_ptrc[e] | 0.156 |
| Pyridoxal-phosphate | HMR\_9691 | 0.0344 |
| Pyridoxine | HMR\_9144 | 0.025 |
| Pyruvate | HMR\_9133 | 72.693 |
| retinoate | HMR\_9404 | 0.107 |
| retinol | HMR\_9147 | 84.879 |
| Retinoyl-glucuronide | HMR\_9405 | 0.0066 |
| Ribitol | HMR\_9401 | 1.167 |
| Riboflavin | HMR\_9143 | 0.350 |
| Ribose | HMR\_9406 | 2.3 |
| Sarcosine | HMR\_9131 | 0.7 |
| Serine | HMR\_9069 | 139.7 |
| Serotonin | HMR\_9412 | 0.754 |
| Spermidine | EX\_spmd[e] | 4.776 |
| Spermine | HMR\_9715 | 2.604 |
| Sphingosine | EX\_sphings[e] | 0.05 |
| Stearate | EX\_ocdca[e] | 286.289 |
| Stearidonic acid | EX\_strdnc[e] | 0.212 |
| Succinate | HMR\_9415 | 14.275 |
| Sucrose | HMR\_9416 | 1.8 |
| Sulfate | HMR\_9074 | 352.75 |
| Taurine | HMR\_9418 | 103.561 |
| Taurochenodesoxycholate | HMR\_9284 | 0.3 |
| taurocholate | HMR\_9282 | 0.24 |
| taurolithocholate | EX\_HC02192[e] | 1.212 |
| Testosterone | HMR\_9429 | 0.00593 |
| THF | HMR\_9421 | 0.0025 |
| Thiamin | HMR\_9159 | 0.160 |
| Thiocyanate | HMR\_9420 | 31.83 |
| Thiosulfate | HMR\_9432 | 51.15 |
| Threonine | HMR\_9044 | 147.783 |
| Thromboxane A2 | HMR\_9433 | 0.00024 |
| Thymidine | HMR\_9423 | 0.205 |
| Thyroxine | HMR\_9424 | 6.518 |
| Tricosanoic acid | EX\_M03045[e] | 0.033 |
| triiodothyronine | HMR\_9427 | 0.000986 |
| tryptophan | HMR\_9045 | 61.0829 |
| Tyrosine | HMR\_9064 | 77.788 |
| UDP | HMR\_9435 | 41 |
| Uracil | HMR\_9437 | 1.135 |
| urate | HMR\_9075 | 283.0244 |
| Urea | HMR\_9438 | 3749.0856 |
| Uridine | HMR\_9439 | 9.107 |
| Valeric acid | HMR\_9810 | 0.6 |
| Valine | HMR\_9046 | 216.567 |
| Vitamin D2 | HMR\_9441 | 0.00275 |
| Vitamin D3 | HMR\_9442 | 0.0459 |
| Xanthurenate | HMR\_9693 | 0.011 |
| xylitol | HMR\_9138 | 1.589 |
| Phytanate | EX\_phyt[e] | 4.697 |
| Formaldehyde | EX\_fald[e] | 16.3 |
| Coproporphyrinogen I | EX\_HC01610[e] | 0.015 |
| Chenodeoxycholate | EX\_C02528[e] | 1.0825 |
| Glucuronate | EX\_glcur[e] | 165 |
| Decanoyl carnitine | EX\_c10crn[e] | 0.237 |
| O-Butyrylcarnitine | EX\_c4crn[e] | 0.238 |
| L-Octanoylcarnitine | EX\_c8crn[e] | 0.210 |
| trans-4-hydroxy-L-proline | EX\_4hpro[e] | 21.565 |
| Taurodeoxycholate | EX\_tdechola[e] | 0.062 |
| Carnosine | EX\_carn[e] | 3.23 |
| 3alpha,12alpha-dihydroxy-5beta-cholanate | EX\_dchac[e] | 0.45 |
| FMN | EX\_fmn[e] | 0.0106 |
| 4-Hydroxyphenylpyruvate | EX\_34hpp[e] | 0.37 |
| 3-methyl-2-oxobutyrate | EX\_3mob[e] | 12.5 |
| 2-oxo-3-methylvalerate | EX\_3mop[e] | 20.35 |
| 4-methyl-2-oxopentanoate | EX\_4mop[e] | 26.5 |
| 5-oxoproline | EX\_5oxpro[e] | 19.5 |
| SAH | EX\_ahcys[e] | 0.244 |
| anthranilate | EX\_anth[e] | 0.0155 |
| malate | EX\_mal\_L[e] | 7.6 |
| 5-Hydroxyindoleacetate | EX\_5hoxindoa[e] | 0.0516 |
| Glyceraldehyde | EX\_glyald[e] | 1476 |
| PEP | EX\_pep[e] | 12.5 |
| guanidinoacetate | EX\_gudac[e] | 4.890 |
| Kynurenine | EX\_Lkynr[e] | 2.681 |
| 4-hydroxy-2-quinolinecarboxylic acid | EX\_kynate[e] | 0.0265 |
| Quinolinate | EX\_quln[e] | 0.47 |
| phosphocholine | EX\_cholp[e] | 2.2 |
| L-Cystathionine | EX\_cyst\_L[e] | 0.364 |
| Dimethylglycine | EX\_dmgly[e] | 2.5 |
| ethanolamine-phosphate | EX\_ethamp[e] | 11.5 |
| Fumarate | EX\_fum[e] | 1.223 |
| sn-glycerol-3-PC | EX\_g3pc[e] | 34 |
| Isocitrate | EX\_icit[e] | 6 |
| L-2-aminoadipate | EX\_L2aadp[e] | 1.368 |
| Xanthine | EX\_xan[e] | 19.731 |
| Xanthosine | EX\_xtsn[e] | 5.08 |
| Homocysteine | EX\_hcys\_L[e] | 8.808 |
| Retinal | EX\_retinal[e] | 0.155 |
| Argininosuccinate | EX\_argsuc[e] | 2.1 |
| O-Acetylcarnitine | EX\_acrn[e] | 6.473 |
| O-propanoylcarnitine | EX\_pcrn[e] | 0.414 |
| octadecenoylcarnitine(5) | EX\_odecrn[e] | 0.295 |
| L-Palmitoylcarnitine | EX\_pmtcrn[e] | 0.117 |
| Azelaic acid | EX\_C08261[e] | 27 |
| Hippurate | EX\_bgly[e] | 11.413 |
| 1-Myristoylglycerophosphocholine | EX\_pcholmyr\_hs[e] | 16.659 |
| 1-Oleoylglycerophosphocholine (Delta 9) | EX\_pcholole\_hs[e] | 24.124 |
| 1-Stearoylglycerophosphocholine | EX\_pcholste\_hs[e] | 32.756 |
| 1-Eicosatetraenoylglycerophosphocholine (Delta 8, 11, 14, 17), Sn1-Lpc (20:4) | EX\_pcholn204\_hs[e] | 5.373 |
| 1-Lignocericylglycerophosphocholine (24:0), Lysopc A C24 | EX\_pcholn24\_hs[e] | 0.291 |
| 1-Heptadecanoylglycerophosphocholine | EX\_pcholhep\_hs[e] | 1.558 |
| 15(S)-HPETE | EX\_15HPET[e] | 0.00106 |
| 4-hydroxyphenyllactate | EX\_34hpl[e] | 0.64 |
| 3-Hydroxyisobutyrate | EX\_3hmp[e] | 20.5 |
| hydracrylate | EX\_3hpp[e] | 4.1 |
| 3-Methoxytyramine | EX\_3moxtyr[e] | 0.0025 |
| 4-Acetamidobutanoate | EX\_4aabutn[e] | 0.5 |
| 5,6-dihydrouracil | EX\_56dura[e] | 0.313 |
| 5-Aminolevulinate | EX\_5aop[e] | 0.35 |
| provitamin D3 | EX\_7dhchsterol[e] | 5 |
| N-Acetylornithine | EX\_acorn[e] | 1.0933 |
| Adipic acid | EX\_adpac[e] | 0.09 |
| Allantoin | EX\_alltn[e] | 2.1 |
| SAM | EX\_amet[e] | 0.0855 |
| (S)-2-aminobutanoate | EX\_C02356[e] | 22.8 |
| 13(S)-HPODE | EX\_C04717[e] | 0.00601 |
| 5(S)-HETE | EX\_C04805[e] | 0.501 |
| Prostaglandin J2 | EX\_C05957[e] | 0.0000495 |
| Lipoxin A4 | EX\_C06314[e] | 0.0000785 |
| Anandamide | EX\_C11695[e] | 2.0393 |
| 5,6-EET | EX\_C14768[e] | 0.00356 |
| 8,9-EET | EX\_C14769[e] | 0.000627 |
| 14,15-EET | EX\_C14771[e] | 0.000942 |
| 9(10)-EpOME | EX\_C14825[e] | 0.00305 |
| 12(13)-EpOME | EX\_C14826[e] | 0.00645 |
| 6-oxo-prostaglandin F1alpha | EX\_CE0955[e] | 0.000269 |
| beta-hydroxy-beta-methylbutyrate | EX\_CE2028[e] | 4 |
| 3-O-methyldopa | EX\_CE2176[e] | 0.089 |
| 6-trans-LTB4 | EX\_CE2445[e] | 0.000185 |
| (8Z,11Z,14Z)-Eicosatrienoic Acid | EX\_CE2516[e] | 46.664 |
| Cis,Cis-11,14-Eicosadienoic Acid | EX\_CE4843[e] | 9.0358 |
| methylmalonate | EX\_HC00900[e] | 0.174 |
| Homogentisate | EX\_hgentis[e] | 0.043 |
| L-Pipecolate | EX\_Lpipecol[e] | 6.23 |
| Lathosterol | EX\_lthstrl[e] | 5.903 |
| (R)-mevalonate | EX\_mev\_R[e] | 0.0323 |
| L-hydroxylysine | EX\_pcollg5hlys[e] | 1.5 |
| Sebacicacid | EX\_sebacid[e] | 0.091 |
| Suberic acid | EX\_subeac[e] | 1.87 |
| Urocanate | EX\_urcan[e] | 0.43 |
| Galactitol | EX\_galt[e] | 0.59 |
| Glycolate | EX\_glyclt[e] | 34.05 |
| Indoleacetate | EX\_ind3ac[e] | 0.983 |
| Phenylacetate | EX\_pac[e] | 54.997 |
| 3-phosphoserine | EX\_pser\_L[e] | 17 |
| Normetanephrine | EX\_normete\_L[e] | 0.00034 |
| 16alpha-hydroxyestrone | EX\_C05300[e] | 0.00078 |
| N-acetylneuraminate | EX\_acnam[e] | 1.285 |
| 2-oxobutyrate | EX\_2obut[e] | 7.11 |
| D-gluconic acid | EX\_glcn[e] | 3.295 |
| 4-Hydroxybenzoate | EX\_4hbz[e] | 4.809 |
| 3,4-dihydroxyphenylacetate | EX\_34dhpha[e] | 0.0101 |
| Phenylpyruvate | EX\_phpyr[e] | 2.75 |
| Tyramine | EX\_tym[e] | 0.00500 |
| 2-hydroxyphenylacetate | EX\_2hyoxplac[e] | 0.503 |
| Lanosterol | EX\_lanost[e] | 0.48 |
| Vanillylmandelate | EX\_3mox4hoxm[e] | 0.035 |
| Glyoxalate | EX\_glx[e] | 3.05 |
| Isovalerylglycine | EX\_CE4968[e] | 0.17 |
| 4-androstene-3,17-dione | EX\_andrstndn[e] | 0.00369 |
| 5alpha-androstane-3,17-dione | EX\_andrstandn[e] | 0.00036 |
| 5alpha-androstane-3alpha,17beta-diol | EX\_CE2209[e] | 0.000475 |
| 2-methoxyestradiol-17beta | EX\_C05302[e] | 0.01 |
| 21-hydroxyallopregnanolone | EX\_CE5072[e] | 0.0052 |
| 11-deoxycortisol | EX\_11docrtsl[e] | 0.0039 |
| Pregnenolone | EX\_prgnlone[e] | 0.0143 |
| Allopregnanolone | EX\_CE2211[e] | 0.00373 |
| 17alpha-hydroxyprogesterone | EX\_17ahprgstrn[e] | 0.00507 |
| 17alpha-hydroxypregnenolone | EX\_17ahprgnlone[e] | 0.00682 |
| 5alpha-pregnane-3,20-dione | EX\_C03681[e] | 0.03605 |
| Pregnenolone sulfate | EX\_prgnlones[e] | 0.13 |
| Methylamine | EX\_mma[e] | 1 |
| N-methylhistamine | EX\_mhista[e] | 0.00034 |
| 4-hydroxy-2-nonenal | EX\_CE2006[e] | 0.11 |
| Salsolinol | EX\_C09642[e] | 0.00131 |
| Selenomethionine | EX\_selmeth[e] | 0.69 |
| quinonoid dihydrobiopterin | EX\_CE2705[e] | 0.006 |
| 1,3-Diaminopropane | EX\_13dampp[e] | 0.04 |
| N1-Acetylspermidine | EX\_N1aspmd[e] | 0.007 |
| 5-Hydroxytryptophol | EX\_CE1918[e] | 0,0009 |
| 5-Methoxytryptophol | EX\_CE6205[e] | 0.00012475 |
| Calcitriol | EX\_1a25dhvitd3[e] | 0.00008 |
| 12-hydroxy-arachidonate | EX\_12harachd[e] | 0.0834 |
| 18-hydroxy-arachidonate | EX\_18harachd[e] | 0.000273 |
| 5-guanidino-2-oxopentanoate | EX\_5g2oxpt[e] | 0.123 |
| dehydroepiandrosterone | EX\_dhea[e] | 0.0133 |
| Estrone | EX\_estrone[e] | 0.000163 |
| 2-Hydroxyestrone | EX\_C05298[e] | 0.00017 |
| 24-Hydroxycholesterol | EX\_xol24oh[e] | 0.0620 |
| 26-Hydroxycholesterol | EX\_xol27oh[e] | 0.284 |
| Desmosterol | EX\_dsmsterol[e] | 1.834 |
| Cholesterol-sulfate | EX\_chsterols[e] | 5.4 |
| 13-cis-Retinoate | EX\_13\_cis\_retn[e] | 0.003 |
| 2,5-dihydroxybenzoate | EX\_HC00460[e] | 0.825 |
| formyl-N-acetyl-5-methoxykynurenamine | EX\_fna5moxam[e] | 0.000065 |
| peroxynitrite | EX\_CE5643[e] | 38.683 |
| gamma-Glutamyl-cysteine | EX\_glucys[e] | 9.983 |
| Melatonin | EX\_melatn[e] | 0.000587 |
| 6-Hydroxymelatonin | EX\_6hoxmelatn[e] | 0.00024 |
| Picolinic acid | EX\_C10164[e] | 0.299 |
| Uroporphyrin I | EX\_C05767[e] | 0.0063 |
| Porphobilinogen | EX\_ppbng[e] | 0.06 |
| propane-1,2-diol | EX\_12ppd\_R[e] | 8.933 |
| L-xylulose | EX\_xylu\_L[e] | 9 |
| D-Xylulose | EX\_xylu\_D[e] | 2.5 |
| malonic-dialdehyde | EX\_CE0737[e] | 2.335 |
| imidazole-4-acetate | EX\_im4ac[e] | 0.1 |
| Sphinganine | EX\_sphgn[e] | 0.011 |
| 2-arachidonoylglycerol | EX\_C13856[e] | 7.8 |
| Pristanic acid | EX\_prist[e] | 1.675 |
| 12,13-hydroxyoctadec-9(z)-enoate | EX\_CE2049[e] | 0.00878 |
| 9,10-hydroxyoctadec-12(Z)-enoate | EX\_CE2047[e] | 0.0502 |
| 11-deoxycorticosterone | EX\_11docrtstrn[e] | 0.0368 |
| 3-iodo-L-tyrosine | EX\_3ityr\_L[e] | 0.00069 |
| Tetrahydrobiopterin | EX\_thbpt[e] | 0.0093 |
| D-Xylose | HMR\_9203 | 2443.1 |
| sn-glycerol-3-phosphate | EX\_glyc3p[e] | 30 |
| Sulfite | HMR\_9088 | 1.23 |
| protoporphyrin | EX\_ppp9[e] | 0.76 |
| Squalene | EX\_sql[e] | 1.9 |
| Sphingosine-1-phosphate | HMR\_9411 | 0.278 |
| PRPP | EX\_prpp[e] | 5.31 |
| UDP-glucose | EX\_udpg[e] | 155 |
| UMP | HMR\_9436 | 184 |
| 2-phospho-D-glycerate | EX\_2pg[e] | 1.6 |
| 3-(3-Hydroxy-Phenyl)Propionate | EX\_3hpppn[e] | 0.144 |
| 2-Hydroxy-Isovalerate | EX\_2hiv[e] | 8.633 |
| 17alpha-hydroxypregnenolone sulfate | EX\_CE1352[e] | 2 |
| 3-Hydroxy-glutarate | EX\_3ohglutac[e] | 0.15 |
| 3-Methylhistidine | EX\_3mhis[e] | 2.85 |
| Acetyl-glycine | EX\_acgly[e] | 89.57 |
| Mg2+ | EX\_mg2[e] | 865.610 |
| beta-Carotene | HMR\_9276 | 35.258 |
| D-Arabitol | EX\_abt\_D[e] | 1.5 |
| Dodecanedioic acid | EX\_dodecanac[e] | 109.91 |
| Succinylacetone | EX\_sucaceto[e] | 0.0815 |
| Cu2+ | EX\_cu2[e] | 16.221 |
| Glutarate | EX\_glutar[e] | 0.567 |
| Hexadecanedioic acid | EX\_hexdiac[e] | 0.11 |
| L-Homocystine | EX\_Lhcystin[e] | 8.52 |
| Homocitrulline | EX\_hmcr[e] | 5 |
| Indoxyl sulfate | EX\_inds[e] | 8.245 |
| Isovaleryl carnitine | EX\_ivcrn[e] | 0.216 |
| glycolithocholate | EX\_HC02193[e] | 0.009 |
| Hexanoy lcarnitine | EX\_c6crn[e] | 0.0603 |
| 4-Hydroxy-butyrate | EX\_4ohbut[e] | 24.6 |
| 3-hydroxy-L-kynurenine | EX\_hLkynr[e] | 0.05 |
| Glycogen | HMR\_9729 | 41.2 |
| Oxypurinol | EX\_oxyp[e] | 50 |
| tetrahydrobiopterin | EX\_thbpt[e] | 0.011 |
| 3-Phospho-D-glycerate | EX\_3pg[e] | 52.7 |
| Stearoylcarnitine | EX\_stcrn[e] | 0.05 |
| Tauroursodeoxycholate | EX\_HC02195[e] | 2 |
| Ursodeoxycholate | EX\_HC02194[e] | 0.16 |
| Dihydrofolate | HMR\_9303 | 0.005 |
| Fructose-1,6-bisphosphate | EX\_fdp[e] | 2.5 |
| Ubiquinol | EX\_q10h2[e] | 0.4 |
| ubiquinone | EX\_q10[e] | 1.179 |
| gamma-butyrobetaine | EX\_4tmeabutn[e] | 10 |
| Keratan sulfate I | HMR\_9113 | 0.14 |
| methylglyoxal | HMR\_9375 | 55.295 |
| D-Lactate | HMR\_9136 | 9.13 |
| CO | HMR\_9288 | 72 |
| Sphinganine-1-phosphate | HMR\_9410 | 0.055 |
| GMP | HMR\_9343 | 0.0097 |
| nicotinamide | HMR\_9378 | 0.235 |
| Estrone 3-sulfate | HMR\_9317 | 0.00233 |
| Pi | HMR\_9072 | 902.816 |
| Pyridoxamine | HMR\_9399 | 0.164 |
| DHAP | EX\_dhap[e] | 13.85 |
| 3-Hydroxyanthranilate | EX\_3hanthrn[e] | 0.079 |
| Gamma-Tocopherol | HMR\_9153 | 11.564 |
| 5,10-Methylene-THF | EX\_mlthf[e] | 0.01 |
| Pyridoxal | HMR\_9400 | 0.251 |
| CDP | EX\_cdp[e] | 36 |
| Corticosterone | HMR\_9294 | 0.027 |
| Guanidine | EX\_M02035[e] | 0.29 |
| 3,4-Dihydroxymandelate | EX\_34dhoxmand[e] | 0.011 |
| Benzoate | EX\_bz[e] | 20.785 |
| N-acetyl-L-cysteine | EX\_CE1310[e] | 4 |
| gamma-carboxyethyl-hydroxychroman | EX\_CE1926[e] | 0.16 |
| tetradecenoylcarnitine(5) | EX\_ttdcrn[e] | 0.077 |
| 8-Dehydrocholesterol | EX\_CE1297[e] | 0.65 |
| 4-coumarate | EX\_T4hcinnm[e] | 0.201 |
| Hyaluronate | HMR\_9122 | 0.053 |
| Cyanate | EX\_cynt[e] | 0.045 |
| hydrogen-cyanide | HMR\_9160 | 4.85 |
| Oleoyl ethanolamine | EX\_oleth[e] | 23.402 |
| Palmitoylethanolamide | EX\_pmeth[e] | 12.557 |
| Aminoacetone | EX\_aact[e] | 60 |
| N8-Acetylspermidine | EX\_n8aspmd[e] | 0.05 |
| dihydrobiopterin | EX\_dhbpt[e] | 4.18 |
| Homocysteine-thiolactone | EX\_CE1401[e] | 0.00282 |
| Oxalate | HMR\_9165 | 10.29 |
| Tiglyl carnitine | EX\_c51crn[e] | 0.0508 |
| 9-cis-Retinoate | EX\_CE1617[e] | 0.0049 |
| sulfochenodeoxycholate | EX\_HC02220[e] | 0.1 |
| sulfoglycolithocholate | EX\_HC02197[e] | 0.06 |
| Ursodeoxycholic acid 3-sulfate | EX\_udca3s[e] | 19.095 |
| Prostaglandin F1alpha | EX\_HC02214[e] | 0.000376 |
| Androsterone sulfate | EX\_CE6031[e] | 11.1 |
| Cortisone | EX\_cortsn[e] | 0.0472 |
| Prostaglandin D3 | EX\_HC02210[e] | 0.000123 |
| LTD4 | HMR\_9367 | 0.0129 |
| Methanethiol | EX\_ch4s[e] | 5.7 |
| Thromboxane B2 | EX\_HC02180[e] | 0.147 |
| H2S | HMR\_9103 | 51.65 |
| aquacob(III)alamin | HMR\_9269 | 0.000272 |
| 3,5-Diiodo-L-tyrosine | EX\_35diotyr[e] | 0.0036 |
| Alpha-D-Glucose 1,6-bisphosphate | HMR\_9461 | 98 |
| Retinyl-ester | EX\_retfa[e] | 0.103 |
| Retinyl palmitate | EX\_M02837[e] | 0.0561 |
| D-3-amino-isobutanoate | HMR\_9222 | 1.643 |
| L-3-amino-isobutanoate | HMR\_9221 | 1.643 |
| Dopamine 4-O-sulfate | EX\_dopa4sf[e] | 0.0027 |
| 15-Keto-prostaglandin F2a | EX\_15kprostgf2[e] | 0.000199 |
| 11-Dehydro-thromboxane B2 | EX\_CE1447[e] | 0.00275 |
| Hepoxilin A3 | EX\_C04849[e] | 0.000114 |
| globoside | HMR\_9336 | 2.15 |
| 15(S)-HETrE | EX\_CE2537[e] | 0.000461 |
| Leukotriene B5 | EX\_CE7083[e] | 0.000079 |
| 5(S)-HEPE | EX\_CE7085[e] | 0.000728 |
| Prostaglandin D1 | EX\_HC02208[e] | 0.00001 |
| 3,4-Dihydroxyphenylethanol | EX\_34dhpe[c] | 0.16 |
| 25-Hydroxycholesterol | EX\_xol25oh[e] | 0.0105 |
| Dopamine 3-O-sulfate | HMR\_9308 | 0.0265 |
| Beta-tocopherol | EX\_bvite[e] | 0.2 |
| (S)-Glycerate | EX\_glyc\_S[e] | 2 |
| Ecgonine-methyl ester | EX\_egme[e] | 0.237 |
| Leukotriene F4 | HMR\_9163 | 0.000305 |
| D-Aspartate | HMR\_9097 | 11.786 |
| 14,15-DiHETE | EX\_CE7172[e] | 0.00113 |
| 15(R)-HEPE | EX\_CE7081[e] | 0.000599 |
| 15(S)-HEPE | EX\_CE7082[e] | 0.000599 |
| 5,15-DiHETE | EX\_CE7096[e] | 0.000340 |
| 1-Palmitoylglycerophosphocholine | EX\_pcholpalm\_hs[e] | 92.985 |
| 1-Palmitoleoylglycerophosphocholine (Delta 9) | EX\_pcholpalme\_hs[e] | 2.694 |
| 1-Linoleoylglycerophosphocholine (Delta 9,12) | EX\_pchollinl\_hs[e] | 33.683 |
| 1-Octadeca-Trienoylglycerophosphocholine, Sn1-Lpc (18:3, Delta 6, 9, 12) | EX\_pcholn1836\_hs[e] | 0.234 |
| 1-Octadeca-Trienoylglycerophosphocholine, Sn1-Lpc (18:3, Delta 9, 12, 15) | EX\_pcholn183\_hs[e] | 1.239 |
| 1-Eicosenoylglycerophosphocholine (Delta 11) ,Sn1-Lpc (20:1) | EX\_pcholn201\_hs[e] | 0.526 |
| 1-Eicosadienoylglycerophosphocholine (Delta 11,14) | EX\_pcholeic\_hs[e] | 0.712 |
| 1-Dihomo-Linolenoylglycerophosphocholine (20:3, Delta 8, 11, 14), Lysopc A C20:3 | EX\_pcholn203\_hs[e] | 2.496 |
| 1-Arachidonoyl-Glycero-3-Phosphocholine | EX\_pcholar\_hs[e] | 7.317 |
| 1-Eicosapentenoylglycerophosphocholine (Delta 5, 8, 11, 14, 17), Sn1-Lpc (20:5) | EX\_pcholn205\_hs[e] | 1.608 |
| 1-Docosatetraenoylglycerophosphocholine (Delta 7, 10, 13, 16), Sn1-Lpc (22:4) | EX\_pcholn224\_hs[e] | 0.064 |
| 1-Docosapentenoylglycerophosphocholine (Delta 4, 7, 10, 13, 16), Sn1-Lpc (22:5)-W6 | EX\_pcholn2254\_hs[e] | 0.107 |
| 1-Docosapentenoylglycerophosphocholine (Delta 7, 10, 13, 16, 19), Sn1-Lpc (22:5)-W3 | EX\_pcholn225\_hs[e] | 0.743 |
| 1-Docosahexenoylglycerophosphocholine (Delta 4, 7, 10, 13, 16, 19), Sn1-Lpc (22:6) | EX\_pcholn226\_hs[e] | 2.78 |
| Lysopc A C28:0 | EX\_pcholn28\_hs[e] | 0.465 |
| Lysopc A C26:1 (Delta 5) | EX\_pcholn261\_hs[e] | 1.01 |
| Lysopc A C28:1 (Delta 5) | EX\_pcholn281\_hs[e] | 0.62 |
| 11,12-EET | EX\_C14770[e] | 0.000542 |
| 12(S)-HHT | EX\_CE1243[e] | 0.00203 |
| (18R)-HEPE | EX\_CE7090[e] | 0.000138 |
| 3-Hydroxy butyryl carnitine | EX\_3bcrn[e] | 0.082 |
| Glutaryl carnitine | EX\_c5dc[e] | 0.0275 |
| Decenoyl carnitine | EX\_c101crn[e] | 0.217 |
| Hexadecenoylcarnitine(9) | EX\_hdd2crn[e] | 0.0317 |
| Octenoyl carnitine | EX\_c81crn[e] | 0.2 |
| Dodecenoyl carnitine | EX\_ddece1crn[e] | 0.193 |
| Dodecanedioyl carnitine | EX\_c12dc[e] | 0.227 |
| 3-Hydroxyhexadecenoylcarnitine | EX\_3hdececrn[e] | 0.01 |
| 3-Hydroxy Trans7,10-Hexadecadienoyl Carnitine | EX\_3thexddcoacrn[e] | 0.015 |
| 3-Hydroxyhexadecanoylcarnitine | EX\_3hexdcrn[e] | 0.0125 |
| 3-Hydroxy-Octadecenoyl Carnitine | EX\_3octdece1crn[e] | 0.0115 |
| Fe3+ | HMR\_9096 | 17.778 |
| Zinc | HMR\_9080 | 11.716 |
| (13Z)-eicosenoic acid | EX\_M00017[e] | 11.722 |
| NH4+ | EX\_nh4[e] | 38.5 |
| 3-Hydroxy-3-Methyl-Glutarate | EX\_3h3mglt[e] | 46 |
| 10Z-Heptadecenoic acid | EX\_M00003[e] | 1.03 |
| (11Z,14Z,17Z)-eicosatrienoic acid | EX\_M00010[e] | 0.341 |
| 15-deoxy-PGD2 | EX\_CE5304[e] | 0.00194 |
| 3-Hydroxy-isovaleryl carnitine | EX\_3ivcrn[e] | 0.266 |
| 9-Eicosenoic acid | EX\_M01235[e] | 11.722 |
| GM3 | EX\_gm3\_hs[e] | 5.067 |
| Ceramide pool | EX\_crm\_hs[e] | 8.880 |
| Glucosylceramide pool | EX\_gluside\_hs[e] | 9.6 |
| Cholesterol Ester | EX\_xolest\_hs[e] | 3927.455 |
| 1,2-diacylglycerol-LD-TAG pool | EX\_dag\_hs[e] | 556.701 |
| phosphatidate-LD-TAG pool | EX\_pa\_hs[e] | 1.739 |
| PC-LD pool | EX\_pchol\_hs[e] | 37110.332 |
| PI pool | EX\_pail\_hs[e] | 352.362 |
| PS-LD pool | EX\_ps\_hs[e] | 17.481 |
| SM pool | EX\_sphmyln\_hs[e] | 1084.343 |
| TAG-extraction | HMR\_9023 | 7136.410 |
| PG-CL pool | EX\_pglyc\_hs[e] | 35.772 |