| MDC ID | Metabolite Name                                      |
|--------|-----------------------------------------------------|
| 0125   | Ribulose 5-phosphate                                 |
| 0108   | ADP / 0273_3,5-ADP                                   |
| 0243   | IDP                                                 |
| 0132   | IMP                                                 |
| 0154   | O-Phosphoethanolamine                                |
| 0179   | Glucosamine 6-phosphate                              |
| 0147   | Gluconic acid                                       |
| 0246   | Nicotinamide hypoxanthine dinucleotide               |
| 0192   | Ciliatine                                           |
| 0159   | Tartaric acid                                       |
| 0367   | Sn-Glycero-3-phosphocholine                          |
| 0191   | Glucuronolactone                                     |
| 0200   | Galactitol                                          |
| 0020   | Citicoline                                           |
| 0312   | Glucosaminic acid                                   |
| 0341   | Methionine sulfoximine                               |
| 0048   | 4-Hydroxyproline                                     |
| 0149   | Dihydroorotic acid                                   |
| 0028   | Cystine                                             |
| 0013   | Aspartic acid                                       |
| 0223   | N-Methylaspartic acid                                |
| 0017   | 2,3-cyclic CMP                                       |
| 0168   | Thiourea                                            |
| 0092   | Orotic acid                                         |
| 0012   | Asparagine                                          |
| 0068   | Serine                                              |
| 0038   | Glutamine                                           |
| 0160   | Nicotinamide mononucleotide                          |
| 0234   | Nalpha-Acetylasparagine                              |
| 0026   | Cystathionine                                       |
| 0098   | Homoserine                                          |
| 0057   | Methionine Sulfoxide                                 |
| 0070   | Threonine / 0359_Alothreonine                       |
| 0322   | S-Carboxymethylcysteine                             |
| 0183   | Betaine                                             |
| 0226   | N-methylglutamic Acid                                |
| 0378   | N-Acetylserine                                       |
| 0039   | Glutamic acid                                       |
| 0073   | TMP                                                 |
| 0021   | Citrulline                                          |
| 0158   | dCMP                                                |
| 0064   | Proline                                             |
| 0336   | 3-Ureidopropionic acid                               |
| 0008   | Alanine                                             |
| Compound                                      |
|----------------------------------------------|
| 0146  Sarcosine                               |
| 0302  C6  sugar  amine                        |
| 0076  Uracil                                  |
| 0370  Trigonelline                            |
| 0242  N-Acetylaspartic acid                   |
| 0369  2,3-Diaminopropionic acid               |
| 0091  NAD                                     |
| 0358  5-Hydroxylysine                         |
| 0321  Orthanilic acid                         |
| 0143  Beta-Alanine                            |
| 0201  5-Oxoproline                            |
| 0164  dAMP                                    |
| 0023  Creatine                                |
| 0364  Citramalic acid                         |
| 0097  Xanthine                                |
| 0061  Ornithine                               |
| 0044  Histidine                               |
| 0371  3,4-Dihydroxyphenylglycol               |
| 0085  Fumaric acid                            |
| 0055  Lysine                                  |
| 0049  Hypoxanthine                            |
| 0325  N-Acetylglutamic acid                   |
| 0059  Nicotinic acid                          |
| 0077  Uridine                                 |
| 0373  2-Hydroxybutyric acid                   |
| 0036  Gamma-aminobutyric acid                 |
| 0140  Pipecolic acid                          |
| 0018  3,5-cyclic GMP                          |
| 0253  2,3-cyclic AMP                           |
| 0030  Cytosine                                |
| 0006  Adenylsuccinic acid                     |
| 0204  Methylguanidinhe                         |
| 0221  3-Hydroxymethylglutaric acid            |
| 0346  4-Imidazoleacetic acid                  |
| 0047  Homocystine                             |
| 0404  Maleic acid                             |
| 0438  2-Hydroxypyridine                       |
| 0305  Thiamine monophosphate                  |
| 0010  Arginine                                |
| 0170  3-Aminoisobutanoic acid                 |
| 0060  Ophthalmic acid                         |
| 0211  4-Acetamidobutanoic acid                |
| 0014  3,5-cyclic AMP                          |
| 0058  Nicotinamide                            |
| 0461  Pterin                                  |
| 0051  Inosine                                 |
| 0533  | Biotin                      |
| 0425  | Thiopurine S-methylether    |
| 0195  | Caffeine                    |
| 0421  | Caffeic acid                |
| 0537  | 5-Hydroxyindoleacetic acid  |
| 0050  | Isoleucine                  |
| 0459  | Hippuric acid               |
| 0489  | N-Acetylserotonin           |
| 0481  | Gentisic acid               |
| 0525  | 3-Hydroxyphenylacetic acid  |
| 0349  | 5-Hydroxytryptophan         |
| 0229  | Thyrotropin releasing hormone |
| 0163  | Pyridoxine                  |
| 0487  | Dethiobiotin                |
| 0007  | ADMA / SDMA Dimethylarginine |
| 0416  | Mandelic acid               |
| 0053  | Leucine                     |
| 0318  | 5-Deoxyadenosine            |
| 0295  | Normetanephrine             |
| 0503  | N-Acetylleucine             |
| 0338  | Norleucine                  |
| 0493  | Suberic acid                |
| 0430  | 2-Pyrocatechuic acid        |
| 0410  | Kynurenic acid              |
| 0033  | Dopamine                    |
| 0388  | Xanthurenic acid            |
| 0473  | 2-Aminophenol               |
| 0450  | 3-Indoleacetamide           |
| 0274  | 3-Nitrotyrosine             |
| 0506  | Salicylamide                |
| 0413  | N-Acetylserylalanine        |
| 0063  | Phenylalanine               |
| 0466  | Melilotic acid              |
| 0479  | Anthranilic acid            |
| 0433  | Ferulic acid                |
| 0422  | Lumichrome                  |
| 0505  | Salsolinol                  |
| 0173  | N-acetyltryptophan          |
| 0052  | Kynurenine                  |
| 0482  | Azelaic acid                |
| 0420  | Indoleacetic acid           |
| 0395  | Tyramine                    |
| 0403  | Melatonin                   |
| 0356  | Guanidinosuccinic acid      |
| 0432  | Indole-3-ethanol            |
| 0436  | 10-Hydroxydecanoic acid C10:0(OH) |
| Code  | Name                  |
|-------|-----------------------|
| 0396  | Cortisol              |
| 0467  | 3-Methoxytyramine     |
| 0069  | Serotonin             |
| 0454  | Lipoamide             |
| 0415  | 3,5-Diiodotyrosine    |
| 0074  | Tryptophan            |
| 0434  | Glycocholic acid      |
| 0423  | Tryptophanamide       |
| 0307  | S-Hexylglutathione    |
| 0449  | Hydrocortisone 21-acetate |
| 0463  | 3,5-Diiodothyronine   |

MDC = Molecular Determinants Core
| Compound name                                                                 |
|------------------------------------------------------------------------------|
| Ribulose 5-phosphate sodium salt                                              |
| Adenosine diphosphate                                                         |
| Inosine 5-diphosphate                                                         |
| 2-Inosine-5-monophosphate / Inosinic acid                                    |
| O-Phosphoethanolamine                                                         |
| D-GLUCOSAMINE 6-PHOSPHATE                                                    |
| GLUCONATE                                                                    |
| NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE                                        |
| (2-AMINOETHYL)PHOSPHONATE                                                    |
| Tartaric acid                                                                |
| SN-GLYCERO-3-PHOSPHOCHOLINE                                                   |
| D-GLUCURONOLACTONE                                                           |
| GALACTITOL                                                                   |
| Cytidine 5-Diphosphocholine / Citicoline / Choline 5-cytidine diphosphate    |
| GLUCOSAMINATE                                                                |
| METHIONINE SULFOXIMINE                                                        |
| 4-Hydroxy-L-Proline                                                           |
| Dihydroorotic acid                                                           |
| Cystine                                                                      |
| Aspartic acid                                                                |
| N-METHYL-D-ASPARTIC ACID                                                      |
| Cytidine 2,3-Cyclic Monophosphate / 2,3-Cyclic CMP                            |
| Thiourea                                                                     |
| Orotic acid                                                                  |
| L-Asparagine                                                                 |
| Serine                                                                       |
| Glutamine                                                                    |
| Nicotinamide mononucleotide                                                   |
| N-ALPHA-ACETYL-L-ASPARAGINE                                                   |
| Cystathionine                                                                |
| Homoserine                                                                   |
| Methionine sulfoxide                                                          |
| Threonine/Allothreonine                                                       |
| S-CARBOXYMETHYL-L-CYSTEINE                                                    |
| BETAINE                                                                      |
| N-METHYL-L-GLUTAMATE                                                          |
| N-ACETYL-DL-SERINE                                                            |
| Glutamic acid                                                                |
| Thymidine 5’-monophosphate / 5-Thymidyllic acid                              |
| Citrulline                                                                   |
| 2-Deoxyctydine 5-monophosphate                                                |
| Proline                                                                      |
| 3-UREIDOPROPIONATE                                                           |
| Alanine                                                                      |
| Compound                              |
|---------------------------------------|
| Sarcosine                            |
| C6 sugar amine                        |
| Uracil                                |
| TRIGONELLINE                          |
| N-AMIDINO-L-ASPARTATE                 |
| DL-2,3-Diaminopropionic acid monohydrochloride |
| Nicotinamide adenine dinucleotide     |
| DL-5-HYDROXYLYSINE                    |
| ANILINE-2-SULFONIC ACID               |
| Beta-Alanine                          |
| 5-OXO-D-PROLINE                       |
| Deoxyadenosine monophosphate          |
| Creatine                              |
| CITRAMALATE                           |
| Xanthine                              |
| Ornithine                             |
| Histidine                             |
| 3,4-DIHYDROXYPHENYL GLYCOL           |
| Fumaric acid                          |
| Lysine                                |
| Hypoxanthine / 6-Hydroxypurine        |
| N-ACETYL-DL-GLUTAMIC ACID             |
| Nicotinic acid                        |
| Uridine                               |
| 2-HYDROXYBUTYRIC ACID                 |
| Gamma-aminobutyric acid / 4-aminobutanoic acid |
| Pipecolic acid                        |
| Guanosine 3,5-Cyclic Monophosphate / 3,5-Cyclic GMP |
| ADENOSINE 2,3-CYCLIC MONOPHOSPHATE    |
| Cytosine                              |
| Adenylosuccinic acid / Adenylsuccinic acid |
| METHYLGUANIDINE                       |
| 3-HYDROXY-3-METHYLGLUTARATE           |
| 4-IMIDAZOLEACETIC ACID                |
| Homocystine                           |
| MALEIC ACID                           |
| 2-HYDROXYPYRIDINE                     |
| THIAMINE MONOPHOSPHATE                |
| Arginine                              |
| 3-Aminoisobutanoic acid               |
| Ophthalmic acid                       |
| 4-ACETAMIDOButanoate                  |
| Adenosine 3,5-Cyclic Monophosphate / 3,5-Cyclic AMP |
| Nicotinamide                          |
| PTERIN                                |
| Inosine                               |
| PTERIN                                |
| Chemical Name                          |
|---------------------------------------|
| Purine                                |
| Methionine                            |
| N-ALLYL-ACETYL-L-LYSINE               |
| Creatinine                            |
| Carnitine                             |
| O-SUCCINYL-L-HOMOSERINE               |
| 6-HYDROXYNICOTINATE                   |
| ITACONATE                             |
| Glutathione oxidized / Glutathione disulfide |
| 3-METHOXY-4-HYDROXYMANDELATE          |
| Guanosine                             |
| 5-METHYLCYTOSINE HYDROCLORIDE         |
| 2-DEOXYGUANOSINE                      |
| Cytidine                              |
| Thymidine                             |
| N-ACETYLPUTRESCINE                    |
| 5-AMINOPENTANOATE                     |
| 4-QUINOLINECARBOXYLIC ACID            |
| Pantothentic acid                     |
| 4-PYRIDOXATE                         |
| INDOXYL SULFATE                       |
| ETHYLMALONIC ACID                     |
| SELENOMETHIONINE                      |
| PYRIDOXAMINE                          |
| THEOBROMINE                           |
| 2-HYDROXY-4-(METHYLTHIO)BUTYRIC ACID  |
| DEOXYCYTIDINE                         |
| OCTOPAMINE                            |
| Adenine                               |
| Adenosine                             |
| 1-METHYLADENOSINE                     |
| 3,4-DIHYDROXYBENZOATE                 |
| PARAXANTHINE                          |
| 3-(4-HYDROXYPHENYL)LACTATE            |
| Tyrosine                              |
| UROCANATE                             |
| 3-HYDROXYKYNURENINE                   |
| N-ACETYL-DL-METHIONINE                |
| 4-AMINOBENZOATE                       |
| 3-METHYLADENINE                       |
| PYRIDOXAL                             |
| Epinephrine / Adrenaline              |
| PYRROLE-2-CARBOXYLATE                 |
| 2-QUINOLINECARBOXYLIC ACID            |
| 3-METHOXY-L-TYROSINE                  |
| 6-CARBOXYHEXANOATE                    |
| BIOTIN                                  |
|-----------------------------------------|
| THIOPURINE S-METHYLEETHER               |
| CAFFEINE                                |
| CAFFEATE                                |
| 5-HYDROXYINDOLEACETATE                 |
| Isoleucine                              |
| HIPPURATE                               |
| N-ACETYLSEROTONIN                       |
| 2,5-DIHYDROXYBENZOATE                  |
| 3-HYDROXYYPHENYLACETATE                |
| 5-HYDROXY-L-TRYPTOPHAN                  |
| THYROTROPIN RELEASING HORMONE           |
| Pyridoxine                              |
| DETHIOBIOTIN                            |
| Dimethylarginine                        |
| MANDELIC ACID                           |
| Leucine                                 |
| 5-DEOXYADENOSINE                        |
| DL-NORMETANEPHRINE                      |
| N-ACETYL-L-LEUCINE                      |
| NORLEUCINE                              |
| SUBERIC ACID                            |
| 2,3-DIHYDROXYBENZOATE                  |
| 4-HYDROXY-2-QUINOLINECARBOXYLIC ACID    |
| Hydroxytyramine / Dopamine              |
| XANTHURENIC ACID                        |
| 2-AMINOPHENOL                           |
| INDOLE-3-ACETAMIDE                      |
| 3-NITRO-L-TYROSINE                      |
| SALICYLMAMIDE                           |
| N-ACETYL-L-PHENYLALANINE                |
| Phenylalanine                           |
| 3-(2-HYDROXYPHENYL)PROPAENOATE          |
| ANTHRANILATE                            |
| FERULATE                                |
| LUMICHEMOME                             |
| 1-METHYL-6,7-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINE |
| N-acetyl-D-tryptophan                   |
| Kynurenine                              |
| AZELAIC ACID                            |
| N-ACETYLYL-ASPARTIC ACID                |
| TYRAMINE                                |
| MELATONIN                               |
| INDOLE-3-ACETATE                        |
| INDOLE-3-ETHANOL                        |
| 10-HYDROXYDECANOATE                     |
| CORTISOL       |
|----------------|
| 3-METHOXYTYRAMINE |
| Serotonin       |
| LIPOAMIDE      |
| 3,5-DIIODO-L-TYROSINE |
| Tryptophan     |
| GLYCOCHOLATE   |
| L-TRYPTOPHANAMIDE |
| S-HEXYL-GLUTATHIONE |
| CORTISOL 21-ACETATE |
| 3,5-DIIODO-L-THYRONINE |
| Metabolite                        | ratio | TH   |
|----------------------------------|-------|------|
| Carnitine                        | 0.77  | 7040 |
| Kynurenine                       | 0.72  | 2787 |
| Betaine                          | 0.75  | 34139|
| 5-Oxoproline                     | 0.57  | 4523 |
| Kynurenic acid                   | 0.58  | 688  |
| Cystathionine                    | 0.66  | 832  |
| Lysine                           | 0.73  | 75089|
| Pipecolic acid                   | 0.75  | 6030 |
| Orotic acid                      | 0.66  | 141  |
| Tyrosine                         | 0.84  | 27027|
| Aspartic acid                    | 1.55  | 1946 |
| Threonine Allothreonine          | 0.84  | 6984 |
| Dihydrooortic acid               | 0.76  | 86   |
| Hydroxyphenyllactic acid         | 0.8   | 161  |
| Serine                           | 1.26  | 15572|
| N-methylglutamic acid            | 0.76  | 293  |
| Creatinine                       | 0.9   | 13184|
| Urocanic acid                    | 2.9   | 281  |
| Hippuric acid                    | 0.68  | 464  |
| Leucine                          | 0.8   | 10132|
| N-alpha-acetyllysine             | 0.84  | 2360 |
| Histidine                        | 0.86  | 39296|
| Indole-3-ethanol                 | 1.42  | 53   |
| N-Acetylleucine                  | 0.78  | 185  |
| Glycocholic acid                 | 0.56  | 760  |
| Arginine                         | 0.82  | 11144|
| Theobromine                      | 0.76  | 270  |
| Citrulline                       | 0.81  | 3452 |
| Ciliatine                        | 0.81  | 100  |
| Alanine                          | 0.85  | 3227 |
| Proline                          | 0.91  | 82020|
| Guanidinosuccinic acid           | 1.14  | 517  |
| Asparagine                       | 1.09  | 4141 |
| Paraxanthine                     | 0.85  | 823  |
| Cystine                          | 1.21  | 2005 |
| Cortisol                         | 1.31  | 110  |
| 4-Hydroxyproline                 | 0.94  | 5341 |
| Isoleucine                       | 0.9   | 7903 |
| Sn-Glycero-3-phosphocholine      | 0.8   | 3030 |
| Galactitol                       | 0.8   | 63   |
| Creatine                         | 0.91  | 11716|
| Uracil                           | 1.24  | 69   |
| Glutamine                        | 0.95  | 82328|
| Caffeine                         | 0.91  | 5719 |
| Compound                               | Value | Significance |
|----------------------------------------|-------|--------------|
| Tryptophan                             | 0.96  | 17154        |
| Nicotinamide                           | 1.13  | 260          |
| 2,3-Diaminopropionic acid              | 0.99  | 164974       |
| Glutamic acid                          | 1.04  | 50288        |
| Melilotic acid                         | 0.97  | 10526        |
| Methionine                             | 1.03  | 3515         |
| 1-Methyladenosine                      | 0.98  | 1800         |
| Phenylalanine                          | 0.98  | 130908       |
| 5-Hydroxylysine                        | 0.97  | 126          |
| Methionine Sulfoxide                   | 1.03  | 334          |
| Asymmetric and Symmetric Dimethylarginine | 1.02 | 1737        |
| C6 sugar amine                         | 0.97  | 524          |
| Ornithine                              | 1     | 28414        |

TH=therapeutic hypothermia
| No TH | p-value |
|-------|---------|
| 5430  | 0.01    |
| 1996  | 0.01    |
| 25725 | 0.02    |
| 2594  | 0.02    |
| 402   | 0.03    |
| 553   | 0.05    |
| 55047 | 0.05    |
| 4503  | 0.07    |
| 93    | 0.07    |
| 22613 | 0.08    |
| 3012  | 0.1     |
| 5834  | 0.13    |
| 65    | 0.13    |
| 128   | 0.14    |
| 19564 | 0.15    |
| 222   | 0.15    |
| 11852 | 0.16    |
| 816   | 0.17    |
| 314   | 0.19    |
| 8088  | 0.2     |
| 1992  | 0.2     |
| 33803 | 0.23    |
| 75    | 0.23    |
| 145   | 0.24    |
| 425   | 0.26    |
| 9130  | 0.29    |
| 206   | 0.3     |
| 2788  | 0.33    |
| 81    | 0.36    |
| 2757  | 0.37    |
| 74299 | 0.4     |
| 588   | 0.42    |
| 4528  | 0.45    |
| 695   | 0.5     |
| 2419  | 0.5     |
| 145   | 0.51    |
| 5010  | 0.52    |
| 7147  | 0.54    |
| 2438  | 0.57    |
| 50    | 0.59    |
| 10714 | 0.62    |
| 86    | 0.65    |
| 78433 | 0.67    |
| 5207  | 0.71    |
| Value  | Probability |
|--------|-------------|
| 16553  | 0.75        |
| 294    | 0.77        |
| 163098 | 0.79        |
| 52497  | 0.81        |
| 10222  | 0.82        |
| 3611   | 0.83        |
| 1770   | 0.85        |
| 127924 | 0.86        |
| 122    | 0.9         |
| 344    | 0.9         |
| 1778   | 0.92        |
| 509    | 0.95        |
| 28516  | 0.98        |