Supplementary data 1

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Result**  |  **Metabolite** |  **Pr > F**  |  **p-value Pressure**  |  **Fold-Change Diver/Control**  |  **p-value****Diet**  |  **Fold-Change MAIZE/SOY**  |
|  D\*P\*I  |  4-QUINOLINECARBOXYLIC ACID  |  0.000  |  0.016915  | 0.84  |  0.00000  | 0.24 |
|  D\*P\*I  |  7-methylguanine  |  0.000  |  0.025681  | 0.79  |  0.00000  | 0.11 |
|  D\*P\*I  |  ARGININE  |  0.000  |  0.004173  | 0.54  |  0.00038  | 0.45 |
|  D\*P\*I  |  Gly-Gly  |  0.000  |  0.019005  | 0.59  |  0.00000  | 0.28 |
|  D\*P\*I  |  PYRROLE-2-CARBOXYLATE  |  0.000  |  0.021722  | 0.56  |  0.00000  | 32.77 |
|  D\*P\*I  |  THIOPURINE S-METHYLETHER  |  0.000  |  0.022229  | 4.83  |  0.00817  | 0.13 |
|  D\*P\*I  |  THYROTROPIN RELEASING HORMONE  |  0.000  |  0.033936  | 0.57  |  0.00000  | 0.02 |
|  P\*I  |  C18\_LysoPAF  |  0.000  |  0.000001  | 2.09  |  0.76634  | 0.96 |
|  P  |  ASPARTATE  |  0.006  |  0.002067  | 1.39  |  0.64983  | 0.95 |
|  P  |  CYTIDINE  |  0.022  |  0.009361  | 0.66  |  0.13505  | 0.79 |
|  P  |  glycocholic acid hydrate  |  0.003  |  0.000335  | 1.97  |  0.50852  | 0.89 |
|  P  |  L-Asparagine  |  0.017  |  0.005391  | 1.41  |  0.50206  | 0.92 |
|  P  |  RHAMNOSE  |  0.040  |  0.023204  | 1.54  |  0.10623  | 0.74 |
|  I  |  5b-cholanic acid-3-ONE  |  0.017  |  0.062888  | 0.84  |  0.47721  | 0.93 |
|  I  |  DEOXYGUANOSINE-MONOPHOSPHATE  |  0.019  |  0.919039  | 0.98  |  0.61697  | 1.10 |
|  I  |  GLUCOSE 6-PHOSPHATE  |  0.002  |  0.165031  | 0.73  |  0.11308  | 0.69 |
|  I  |  GLYCEROL 3-PHOSPHATE  |  0.005  |  0.261198  | 0.72  |  0.28514  | 0.73 |
|  D\*P  |  (\xB1)-a-Lipoic acid  |  0.001  |  0.034508  | 4.61  |  0.01076  | 0.12 |
|  D\*P  |  ADENOSINE-MONOPHOSPHATE  |  0.000  |  0.000776  | 1.90  |  0.00000  | 3.18 |
|  D\*P  |  CARNOSINE  |  0.000  |  0.001480  | 0.49  |  0.00012  | 0.41 |
|  D\*P  |  CHENODEOXYCHOLATE  |  0.000  |  0.037227  | 0.71  |  0.00016  | 1.97 |
|  D\*P  |  L-Glutamine  |  0.000  |  0.033810  | 0.59  |  0.00002  | 0.29 |
|  D\*P  |  L-Leucine  |  0.000  |  0.028156  | 0.74  |  0.00001  | 0.51 |
|  D\*P  |  METHYLTHIOADENOSINE  |  0.000  |  0.023341  | 0.74  |  0.00000  | 0.32 |
|  D\*P  |  N-ACETYLGALACTOSAMINE  |  0.000  |  0.001363  | 1.80  |  0.00069  | 1.87 |
|  D\*P  |  N-ACETYLNEURAMINATE  |  0.000  |  0.000597  | 2.05  |  0.00000  | 3.68 |
|  D\*P  |  N-Acetylneuraminic acid  |  0.000  |  0.047934  | 1.59  |  0.00016  | 2.70 |
|  D\*P  |  PROTOPORPHYRIN  |  0.000  |  0.015469  | 0.75  |  0.00000  | 1.93 |
|  D\*P  |  PTERIN  |  0.000  |  0.029561  | 0.64  |  0.00010  | 0.42 |
|  D  |  (+)-Catechin hydrate  |  0.011  |  0.181077  | 1.28  |  0.02030  | 0.65 |
|  D  |  (2-AMINOETHYL)PHOSPHONATE  |  0.003  |  0.296803  | 0.77  |  0.00028  | 0.36 |
|  D  |  14-0\_LysoPE  |  0.000  |  0.732475  | 1.09  |  0.00000  | 0.23 |
|  D  |  16:0\_LysoPA  |  0.003  |  0.099656  | 0.62  |  0.00091  | 0.34 |
|  D  |  16-0\_LysoPE  |  0.000  |  0.993670  | 1.00  |  0.00000  | 0.26 |
|  D  |  16-0\_LysoPG  |  0.000  |  0.147703  | 0.76  |  0.00000  | 0.35 |
|  D  |  16-0\_LysoPI  |  0.006  |  0.427934  | 0.75  |  0.00062  | 0.21 |
|  D  |  17a-Ethynylestradiol  |  0.000  |  0.118138  | 0.87  |  0.00000  | 2.51 |
|  D  |  17a-Hydroxyprogesterone  |  0.005  |  0.184236  | 0.85  |  0.00079  | 0.64 |
|  D  |  18-1\_LysoPA  |  0.045  |  0.742986  | 0.90  |  0.00536  | 0.35 |
|  D  |  18-1\_LysoPE  |  0.000  |  0.455495  | 1.13  |  0.00003  | 0.45 |
|  D  |  1-METHYLADENOSINE  |  0.005  |  0.864207  | 1.03  |  0.00096  | 0.58 |
|  D  |  1-METHYL-L-HISTIDINE  |  0.025  |  0.051539  | 1.34  |  0.01878  | 1.43 |
|  D  |  1-Methyluric acid  |  0.009  |  0.971751  | 1.01  |  0.00081  | 0.23 |
|  D  |  2,6-quinolinediol  |  0.000  |  0.647492  | 0.85  |  0.00000  | 178.32 |
|  D  |  3-AMINO-4-HYDROXYBENZOATE  |  0.000  |  0.588934  | 0.90  |  0.00000  | 12.38 |
|  D  |  3-HYDROXYANTHRANILATE  |  0.000  |  0.506459  | 0.88  |  0.00000  | 12.84 |
|  D  |  4-IMIDAZOLEACETATE  |  0.007  |  0.088896  | 2.31  |  0.00802  | 4.39 |
|  D  |  5b-cholanic acid-3a-OL-12-ONE  |  0.000  |  0.487034  | 0.82  |  0.00007  | 3.89 |
|  D  |  5b-cholanic acid-3a-OL-7,12-DIONE  |  0.000  |  0.789038  | 0.98  |  0.00000  | 1.72 |
|  D  |  5'-DEOXYADENOSINE  |  0.000  |  0.890395  | 0.96  |  0.00002  | 0.13 |
|  D  |  5-hydroxyindole-3-acetic acid  |  0.000  |  0.503034  | 1.16  |  0.00000  | 6.64 |
|  D  |  ADENOSINE  |  0.000  |  0.230700  | 0.80  |  0.00002  | 0.40 |
|  D  |  BETA-ALANINE  |  0.001  |  0.078335  | 0.62  |  0.00030  | 0.33 |
|  D  |  BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE  |  0.009  |  0.824158  | 1.06  |  0.00309  | 0.42 |
|  D  |  CELLOBIOSE  |  0.018  |  0.106161  | 0.70  |  0.00594  | 0.53 |
|  D  |  CHOLATE  |  0.000  |  0.500183  | 0.93  |  0.00000  | 3.37 |
|  D  |  CORTEXOLONE  |  0.000  |  0.308736  | 1.43  |  0.00000  | 52.53 |
|  D  |  CYSTATHIONINE  |  0.030  |  0.227727  | 1.76  |  0.03581  | 0.35 |
|  D  |  CYSTEATE  |  0.000  |  0.117401  | 1.44  |  0.00000  | 0.25 |
|  D  |  CYSTEINE  |  0.019  |  0.051060  | 0.53  |  0.02349  | 2.14 |
|  D  |  CYTIDINE MONOPHOSPHATE  |  0.030  |  0.813084  | 1.06  |  0.00362  | 0.46 |
|  D  |  DEOXYADENOSINE MONOPHOSPHATE  |  0.015  |  0.802912  | 0.93  |  0.00238  | 0.37 |
|  D  |  DEOXYGUANOSINE  |  0.001  |  0.608261  | 1.14  |  0.00012  | 3.21 |
|  D  |  DIPALMITOYLGLYCEROL  |  0.000  |  0.076276  | 0.71  |  0.00000  | 0.00 |
|  D  |  D-ORNITHINE  |  0.002  |  0.415139  | 1.17  |  0.00203  | 0.53 |
|  D  |  GALACTITOL  |  0.000  |  0.143402  | 0.86  |  0.00007  | 0.63 |
|  D  |  GALACTOSAMINE  |  0.000  |  0.305340  | 0.81  |  0.00001  | 0.34 |
|  D  |  GALACTOSE  |  0.002  |  0.687560  | 0.92  |  0.00018  | 0.41 |
|  D  |  GLYCINE  |  0.000  |  0.678738  | 0.95  |  0.00002  | 0.52 |
|  D  |  GUANINE  |  0.037  |  0.812269  | 1.05  |  0.00574  | 1.76 |
|  D  |  HIPPURATE  |  0.000  |  0.267146  | 0.69  |  0.00000  | 157.15 |
|  D  |  HISTIDINE  |  0.008  |  0.063139  | 0.82  |  0.00551  | 0.74 |
|  D  |  HYPOTAURINE  |  0.006  |  0.082473  | 2.30  |  0.00824  | 4.14 |
|  D  |  HYPOXANTHINE  |  0.004  |  0.102436  | 0.73  |  0.00093  | 0.50 |
|  D  |  INDOLE-3-ACETATE  |  0.000  |  0.531423  | 1.12  |  0.00000  | 32.36 |
|  D  |  INOSINE  |  0.000  |  0.394235  | 0.86  |  0.00000  | 0.30 |
|  D  |  LACTOSE  |  0.012  |  0.181366  | 0.54  |  0.00220  | 0.17 |
|  D  |  LITHOCHOLATE  |  0.000  |  0.859140  | 0.95  |  0.00007  | 3.62 |
|  D  |  L-Threo-3-Phenylserine (DL-3-Phenylserine)  |  0.000  |  0.949335  | 1.01  |  0.00000  | 4.12 |
|  D  |  L-tyrosine  |  0.002  |  0.337470  | 0.89  |  0.00063  | 0.64 |
|  D  |  MALTOSE  |  0.029  |  0.191824  | 0.69  |  0.00649  | 0.44 |
|  D  |  MANNITOL  |  0.000  |  0.072932  | 1.58  |  0.00004  | 0.29 |
|  D  |  N6-(DELTA2-ISOPENTENYL)-ADENINE  |  0.000  |  0.873562  | 0.99  |  0.00000  | 0.39 |
|  D  |  N-ACETYLASPARTATE  |  0.021  |  0.364345  | 0.85  |  0.00308  | 1.74 |
|  D  |  NERVONATE  |  0.000  |  0.538488  | 1.10  |  0.00000  | 0.26 |
|  D  |  PHENYLALANINE  |  0.000  |  0.295369  | 0.83  |  0.00004  | 0.43 |
|  D  |  PHOSPHORYLCHOLINE  |  0.017  |  0.858690  | 1.09  |  0.00245  | 0.12 |
|  D  |  Pro-Leu  |  0.006  |  0.198900  | 0.80  |  0.00085  | 0.54 |
|  D  |  RIBITOL  |  0.010  |  0.244591  | 1.64  |  0.00756  | 0.27 |
|  D  |  RIBOFLAVIN  |  0.019  |  0.132877  | 1.30  |  0.00616  | 0.60 |
|  D  |  RIBOSE  |  0.000  |  0.552413  | 0.93  |  0.00000  | 0.29 |
|  D  |  S-ADENOSYLMETHIONINE  |  0.000  |  0.086765  | 0.72  |  0.00000  | 0.20 |
|  D  |  S-HEXYL-GLUTATHIONE  |  0.000  |  0.978366  | 1.00  |  0.00000  | 0.21 |
|  D  |  SHIKIMATE  |  0.000  |  0.360045  | 0.84  |  0.00001  | 0.37 |
|  D  |  STACHYOSE  |  0.026  |  0.519998  | 0.87  |  0.00382  | 1.95 |
|  D  |  THIAMINE MONOPHOSPHATE  |  0.012  |  0.441104  | 1.23  |  0.00188  | 0.39 |
|  D  |  THYMIDINE-MONOPHOSPHATE  |  0.003  |  0.189384  | 0.70  |  0.00096  | 0.37 |
|  D  |  trans-3-Hydroxycinnamic acid (m-Coumaric acid)  |  0.000  |  0.391325  | 0.87  |  0.00000  | 0.00 |
|  D  |  TRICOSANOATE  |  0.001  |  0.079588  | 1.44  |  0.00352  | 0.53 |
|  D  |  TRYPTOPHAN  |  0.000  |  0.514199  | 0.92  |  0.00000  | 0.46 |
|  D  |  URACIL 5-CARBOXYLATE  |  0.009  |  0.158574  | 0.72  |  0.00203  | 2.20 |
|  D  |  UREIDOPROPIONATE  |  0.002  |  0.579935  | 0.87  |  0.00021  | 0.33 |
|  D  |  URIDINE  |  0.000  |  0.413112  | 0.84  |  0.00001  | 0.31 |
|  D  |  URIDINE 5'-DIPHOSPHATE  |  0.039  |  0.300569  | 0.58  |  0.00825  | 5.59 |
|  D  |  URIDINE DIPHOSPHATE GLUCOSE  |  0.040  |  0.242693  | 0.54  |  0.01055  | 4.95 |
|  D  |  VITAMIN D2  |  0.000  |  0.801378  | 1.08  |  0.00000  | 0.15 |
|  D  |  XANTHOSINE  |  0.001  |  0.571578  | 1.20  |  0.00009  | 0.19 |
| D | XANTHURENATE |  0.000  |  0.264313  | 0.91  |  0.00000  | 0.12 |
|  D\*I  |  25-HYDROXYCHOLESTEROL  |  0.000  |  0.806121  | 0.97  |  0.00027  | 1.65 |
|  D\*I  |  4-GUANIDINOBUTANOATE  |  0.000  |  0.172833  | 0.74  |  0.00007  | 0.37 |
|  D\*I  |  D-RIBOSE 5-PHOSPHATE  |  0.000  |  0.161263  | 0.73  |  0.00544  | 0.52 |
|  D\*I  |  PYRIDOXAL  |  0.000  |  0.957266  | 1.01  |  0.00061  | 1.84 |
|  NS  |  14-0\_LysoPC  |  0.504  |  0.367100  | 0.72  |  0.25843  | 0.66 |
|  NS  |  16-0\_LysoPC  |  0.448  |  0.174065  | 0.76  |  0.50110  | 1.14 |
|  NS  |  16-0\_LysoPS  |  0.113  |  0.107407  | 3.60  |  0.29663  | 2.14 |
|  NS  |  18-0\_LysoPC  |  0.540  |  0.824382  | 0.95  |  0.16187  | 0.73 |
|  NS  |  18-0\_LysoPE  |  0.052  |  0.487502  | 1.21  |  0.01409  | 0.49 |
|  NS  |  18-1\_LysoPC  |  0.226  |  0.068226  | 0.69  |  0.29994  | 0.81 |
|  NS  |  18-1\_LysoPS  |  0.319  |  0.904019  | 1.06  |  0.17989  | 2.07 |
|  NS  |  2-DEOXY-D-GLUCOSE  |  0.204  |  0.256592  | 3.15  |  0.17421  | 0.23 |
|  NS  |  2-hydroxycaproic acid  |  0.157  |  0.029171  | 6.74  |  0.93859  | 1.05 |
|  NS  |  3-b-Hydroxyandrost-5-en-17-one (Dehydroepiandrosterone)  |  0.072  |  0.181534  | 0.90  |  0.03344  | 0.84 |
|  NS  |  4 carbamyl-1-methylpyridinium  |  0.297  |  0.882917  | 1.02  |  0.05988  | 0.73 |
|  NS  |  5b-cholanic acid-3a,12a-DIOL-7-ONE  |  0.215  |  0.874090  | 0.89  |  0.04022  | 7.51 |
|  NS  |  5-HYDROXYMETHYLURACIL  |  0.078  |  0.528431  | 1.22  |  0.07187  | 0.56 |
|  NS  |  5-Hydroxynicotinic acid  |  0.067  |  0.493033  | 0.92  |  0.03805  | 0.77 |
|  NS  |  AGMATINE SULFATE  |  0.352  |  0.614662  | 0.87  |  0.47344  | 0.82 |
|  NS  |  ALLANTOIN  |  0.219  |  0.463348  | 1.19  |  0.17742  | 1.39 |
|  NS  |  ALPHA-D-GLUCOSE  |  0.193  |  0.684230  | 0.94  |  0.11210  | 0.77 |
|  NS  |  ANSERINE  |  0.071  |  0.012145  | 0.21  |  0.39680  | 0.65 |
|  NS  |  ARABINOSE  |  0.739  |  0.344180  | 1.22  |  0.83756  | 0.96 |
|  NS  |  ASPARAGINE  |  0.773  |  0.994029  | 1.00  |  0.30038  | 0.78 |
|  NS  |  BILIVERDIN  |  0.146  |  0.550638  | 1.20  |  0.02818  | 0.49 |
|  NS  |  BIOTIN  |  0.108  |  0.045432  | 1.44  |  0.16752  | 0.78 |
|  NS  |  C16  |  0.583  |  0.450731  | 0.70  |  0.56905  | 0.77 |
|  NS  |  C16\_PlasmLPC  |  0.567  |  0.393688  | 0.68  |  0.67347  | 0.83 |
|  NS  |  C18  |  0.193  |  0.293708  | 0.65  |  0.06398  | 0.46 |
|  NS  |  CADAVERINE  |  0.647  |  0.231606  | 1.30  |  0.67235  | 0.91 |
|  NS  |  CITRULLINE  |  0.121  |  0.162786  | 0.90  |  0.60369  | 1.04 |
|  NS  |  CORTISOL  |  0.042  |  0.060218  | 0.56  |  0.10431  | 1.65 |
|  NS  |  CORTISOL 21-ACETATE  |  0.324  |  0.095161  | 1.27  |  0.58488  | 0.93 |
|  NS  |  CREATINE  |  0.352  |  0.468751  | 0.69  |  0.73560  | 0.85 |
|  NS  |  DEOXYADENOSINE  |  0.261  |  0.926608  | 1.03  |  0.04892  | 1.96 |
|  NS  |  DEOXYCHOLATE  |  0.174  |  0.335756  | 0.86  |  0.05272  | 1.38 |
|  NS  |  DEOXYCYTIDINE  |  0.839  |  0.884440  | 0.98  |  0.65850  | 0.94 |
|  NS  |  DEOXYCYTIDINE MONOPHOSPHATE  |  0.310  |  0.918751  | 0.97  |  0.06111  | 0.58 |
|  NS  |  DPPC  |  0.192  |  0.065232  | 0.62  |  0.46067  | 1.21 |
|  NS  |  D-Raffinose (D-(+)-Raffinose pentahydrate )  |  0.142  |  0.030151  | 0.63  |  0.54995  | 0.88 |
|  NS  |  GLUCOSAMINE 6-SULFATE  |  0.102  |  0.027613  | 2.27  |  0.93946  | 1.03 |
|  NS  |  GLUCURONATE  |  0.183  |  0.037205  | 1.45  |  0.55331  | 0.90 |
|  NS  |  GLUTAMATE  |  0.440  |  0.723812  | 0.96  |  0.11302  | 1.20 |
|  NS  |  GLYCEROL-MYRISTATE  |  0.497  |  0.392090  | 0.79  |  0.56606  | 0.85 |
|  NS  |  Gly-Pro  |  0.272  |  0.078575  | 0.71  |  0.36087  | 0.84 |
|  NS  |  GUANOSINE  |  0.277  |  0.601062  | 0.93  |  0.06744  | 0.76 |
|  NS  |  HOMOSERINE  |  0.635  |  0.588505  | 1.15  |  0.24286  | 0.74 |
|  NS  |  KYNURENINE  |  0.059  |  0.021684  | 0.45  |  0.12797  | 0.60 |
|  NS  |  L-carnitine hydrochloride  |  0.188  |  0.078001  | 0.73  |  0.32135  | 0.84 |
|  NS  |  L-Methionine  |  0.315  |  0.941626  | 0.99  |  0.06708  | 1.21 |
|  NS  |  L-Serine  |  0.195  |  0.566287  | 1.07  |  0.04209  | 0.78 |
|  NS  |  LYSINE  |  0.788  |  0.909300  | 1.02  |  0.54274  | 0.92 |
|  NS  |  LYXOSE  |  0.500  |  0.387658  | 1.20  |  0.42496  | 1.19 |
|  NS  |  MELATONIN  |  0.158  |  0.849605  | 1.05  |  0.11153  | 0.68 |
|  NS  |  MYOINOSITOL  |  0.895  |  0.832251  | 1.03  |  0.64255  | 1.08 |
|  NS  |  N-ACETYLASPARAGINE  |  0.405  |  0.577437  | 1.21  |  0.64242  | 0.85 |
|  NS  |  N-Acetyl-D-sphingosine  |  0.704  |  0.617723  | 0.88  |  0.32592  | 0.77 |
|  NS  |  N-ACETYLGLUCOSAMINE  |  0.064  |  0.378799  | 1.11  |  0.02928  | 1.29 |
|  NS  |  N-ALPHA-ACETYLLYSINE  |  0.337  |  0.414849  | 1.16  |  0.10020  | 1.36 |
|  NS  |  OXOGLUTARATE  |  0.579  |  0.284922  | 1.35  |  0.50056  | 1.21 |
|  NS  |  PANTOTHENATE  |  0.797  |  0.435127  | 1.20  |  0.54011  | 0.87 |
|  NS  |  PHOSPHOENOLPYRUVATE  |  0.108  |  0.393366  | 1.79  |  0.25467  | 0.45 |
|  NS  |  PIPECOLATE  |  0.503  |  0.799048  | 0.94  |  0.27797  | 0.78 |
|  NS  |  pregnenolone sulfate  |  0.374  |  0.330324  | 1.44  |  0.21441  | 1.61 |
|  NS  |  PUTRESCINE  |  0.085  |  0.827288  | 1.04  |  0.05212  | 0.67 |
|  NS  |  PYROGLUTAMATE  |  0.662  |  0.233418  | 0.81  |  0.76704  | 1.05 |
|  NS  |  QUINATE  |  0.132  |  0.874850  | 1.03  |  0.02098  | 0.61 |
|  NS  |  SACCHARATE  |  0.067  |  0.271705  | 1.29  |  0.01971  | 0.57 |
|  NS  |  SORBOSE  |  0.074  |  0.890665  | 1.02  |  0.01010  | 0.63 |
|  NS  |  SPHINGANINE  |  0.127  |  0.754922  | 0.96  |  0.02898  | 1.38 |
|  NS  |  taurocholic acid (iso1)  |  0.151  |  0.039165  | 4.43  |  0.67149  | 1.29 |
|  NS  |  THYMIDINE  |  0.107  |  0.832415  | 0.97  |  0.01472  | 0.66 |
|  NS  |  THYMINE  |  0.066  |  0.162483  | 1.47  |  0.09259  | 1.59 |
|  NS  |  TRYPTAMINE  |  0.268  |  0.618877  | 1.18  |  0.07621  | 0.54 |
|  NS  |  URIDINE DIPHOSPHATE-N-ACETYLGLUCOSAMINE  |  0.248  |  0.512963  | 0.81  |  0.64655  | 1.16 |
|  NS  |  URIDINE MONOPHOSPHATE  |  0.645  |  0.498612  | 0.81  |  0.79667  | 0.92 |
|  NS  |  XANTHINE  |  0.373  |  0.247487  | 0.81  |  0.21873  | 0.80 |

Supplementary data 2

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| **Comparison of metabolite lists** |
|  **Venn diagram of the present study**  | **Venn diagram of the previous study (deMaistre et al, 2020)** |
|   |   |
| n=112 | n=127 |
|  (\xB1)-a-Lipoic acid | (\xB1)-a-Lipoic acid |
|  (+)-Catechin hydrate  | (+)-Catechin hydrate |
|  (2-AMINOETHYL)PHOSPHONATE  | (2-AMINOETHYL)PHOSPHONATE |
|   | 14-0\_LysoPC  |
|  14-0\_LysoPE  | 14-0\_LysoPE |
|  16:0\_LysoPA  |   |
|   | 16-0\_LysoPC  |
|  16-0\_LysoPE  | 16-0\_LysoPE |
|  16-0\_LysoPG  | 16-0\_LysoPG |
|  16-0\_LysoPI  | 16-0\_LysoPI |
|  17a-Ethynylestradiol  | 17a-Ethynylestradiol |
|  17a-Hydroxyprogesterone  | 17a-Hydroxyprogesterone |
|   | 18-0\_LysoPC  |
|   | 18-0\_LysoPE  |
|  18-1\_LysoPA  | 18-1\_LysoPA |
|   | 18-1\_LysoPC  |
|  18-1\_LysoPE  | 18-1\_LysoPE  |
|  1-METHYLADENOSINE  | 1-METHYLADENOSINE |
|  1-METHYL-L-HISTIDINE  | 1-METHYL-L-HISTIDINE |
|  1-Methyluric acid  | 1-Methyluric acid |
|  2,6-quinolinediol  | 2,6-quinolinediol |
|  25-HYDROXYCHOLESTEROL  | 25-HYDROXYCHOLESTEROL |
|   | 2-hydroxycaproic acid |
|  3-AMINO-4-HYDROXYBENZOATE  | 3-AMINO-4-HYDROXYBENZOATE |
|  3-HYDROXYANTHRANILATE  | 3-HYDROXYANTHRANILATE |
|  4-GUANIDINOBUTANOATE  | 4-GUANIDINOBUTANOATE |
|  4-IMIDAZOLEACETATE  | 4-IMIDAZOLEACETATE |
|  4-QUINOLINECARBOXYLIC ACID  | 4-QUINOLINECARBOXYLIC ACID |
|   | 5b-cholanic acid-3a,12a-DIOL-7-ONE |
|  5b-cholanic acid-3a-OL-12-ONE  | 5b-cholanic acid-3a-OL-12-ONE |
|  5b-cholanic acid-3a-OL-7,12-DIONE  | 5b-cholanic acid-3a-OL-7,12-DIONE |
|  5b-cholanic acid-3-ONE  |   |
|  5'-DEOXYADENOSINE  | 5'-DEOXYADENOSINE |
|   | 5-hydroxyindole-3-acetic acid |
|   | 5-HYDROXYMETHYLURACIL |
|  5-hydroxyindole-3-acetic acid  | 5-Hydroxynicotinic acid |
|  7-methylguanine  | 7-methylguanine |
|  ADENOSINE  | ADENOSINE |
|  ADENOSINE-MONOPHOSPHATE  | ADENOSINE-MONOPHOSPHATE |
|   | ANSERINE |
|  ARGININE  |   |
|  ASPARTATE |   |
|  BETA-ALANINE  | BETA-ALANINE |
|  BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE  | BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE |
|   | C16  |
|   | C16\_PlasmLPC  |
|   | C18  |
|  C18\_LysoPAF  | C18\_LysoPAF |
|  CARNOSINE  | CARNOSINE |
|  CELLOBIOSE  |   |
|  CHENODEOXYCHOLATE  |   |
|  CHOLATE  | CHOLATE |
|   | CITRULLINE |
|  CORTEXOLONE  | CORTEXOLONE |
|   | CREATINE  |
|  CYSTATHIONINE  | CYSTATHIONINE |
|  CYSTEATE  | CYSTEATE |
|  CYSTEINE  | CYSTEINE |
|  CYTIDINE  |   |
|  CYTIDINE MONOPHOSPHATE  | CYTIDINE MONOPHOSPHATE |
|  DEOXYADENOSINE MONOPHOSPHATE  | DEOXYADENOSINE MONOPHOSPHATE |
|   | DEOXYCYTIDINE MONOPHOSPHATE |
|  DEOXYGUANOSINE  | DEOXYGUANOSINE |
|  DEOXYGUANOSINE-MONOPHOSPHATE  |   |
|  DIPALMITOYLGLYCEROL  | Dipalmitoylglycerol |
|  D-ORNITHINE  | D-ORNITHINE |
|   | DPPC  |
|  D-RIBOSE 5-PHOSPHATE  | D-RIBOSE 5-PHOSPHATE |
|  GALACTITOL  | GALACTITOL |
|  GALACTOSAMINE  | GALACTOSAMINE |
|  GALACTOSE  |   |
|  GLUCOSE 6-PHOSPHATE  | GLUCOSE 6-PHOSPHATE |
|  GLYCEROL 3-PHOSPHATE  |   |
|   | GLYCEROL-MYRISTATE |
|  GLYCINE  | GLYCINE |
|  glycocholic acid hydrate  |   |
|  Gly-Gly  | Gly-Gly  |
|   | Gly-Pro  |
|  GUANINE  | GUANINE |
|   | GUANOSINE |
|  HIPPURATE  | Hippurate |
|  HISTIDINE  | HISTIDINE |
|  HYPOTAURINE  | HYPOTAURINE |
|  HYPOXANTHINE  | HYPOXANTHINE |
|  INDOLE-3-ACETATE  | INDOLE-3-ACETATE |
|  INOSINE  | INOSINE |
|   | KYNURENINE |
|  LACTOSE  |   |
|  L-Asparagine  |   |
|   | L-carnitine hydrochloride |
|  L-Glutamine  | L-Glutamine |
|  LITHOCHOLATE  | LITHOCHOLATE |
|  L-Leucine  | L-Leucine |
|   | L-Methionine |
|   | L-Serine |
|  L-Threo-3-Phenylserine (DL-3-Phenylserine)  | L-Threo-3-Phenylserine (DL-3-Phenylserine) |
|  L-tyrosine  | L-tyrosine |
|  MALTOSE  |   |
|  MANNITOL  | MANNITOL |
|  METHYLTHIOADENOSINE  | METHYLTHIOADENOSINE |
|   | MYOINOSITOL  |
|  N6-(DELTA2-ISOPENTENYL)-ADENINE  | N6-(DELTA2-ISOPENTENYL)-ADENINE |
|   | N-ACETYLASPARAGINE |
|  N-ACETYLASPARTATE  | N-ACETYLASPARTATE |
|  N-ACETYLGALACTOSAMINE  | N-ACETYLGALACTOSAMINE |
|   | N-ACETYLGLUCOSAMINE |
|  N-ACETYLNEURAMINATE  | N-ACETYLNEURAMINATE |
|  N-Acetylneuraminic acid  | N-Acetylneuraminic acid |
|  NERVONATE  | NERVONATE |
|  PHENYLALANINE  | PHENYLALANINE |
|   | PHOSPHOENOLPYRUVATE |
|  PHOSPHORYLCHOLINE  | PHOSPHORYLCHOLINE |
|   | PIPECOLATE  |
|  Pro-Leu  |   |
|  PROTOPORPHYRIN  | PROTOPORPHYRIN |
|  PTERIN  | PTERIN |
|   | PUTRESCINE |
|  PYRIDOXAL  | PYRIDOXAL |
|   | PYROGLUTAMATE |
|  PYRROLE-2-CARBOXYLATE  | PYRROLE-2-CARBOXYLATE |
|  RHAMNOSE  |   |
|  RIBITOL  | RIBITOL |
|  RIBOFLAVIN  | RIBOFLAVIN |
|  RIBOSE  | RIBOSE |
|  S-ADENOSYLMETHIONINE  | S-ADENOSYLMETHIONINE |
|  S-HEXYL-GLUTATHIONE  | S-HEXYL-GLUTATHIONE |
|  SHIKIMATE  | SHIKIMATE |
|  STACHYOSE  |   |
|  THIAMINE MONOPHOSPHATE  | THIAMINE MONOPHOSPHATE |
|  THIOPURINE S-METHYLETHER  | THIOPURINE S-METHYLETHER |
|   | THYMIDINE |
|  THYMIDINE-MONOPHOSPHATE  | THYMIDINE-MONOPHOSPHATE |
|  THYROTROPIN RELEASING HORMONE  | THYROTROPIN RELEASING HORMONE |
|  trans-3-Hydroxycinnamic acid (m-Coumaric acid)  | trans-3-Hydroxycinnamic acid (m-Coumaric acid) |
|  TRICOSANOATE  | TRICOSANOATE |
|  TRYPTOPHAN  | TRYPTOPHAN |
|  URACIL 5-CARBOXYLATE  | URACIL 5-CARBOXYLATE |
|  UREIDOPROPIONATE  | UREIDOPROPIONATE |
|  URIDINE  |   |
|  URIDINE 5'-DIPHOSPHATE  | URIDINE 5'-DIPHOSPHATE |
|  URIDINE DIPHOSPHATE GLUCOSE  | URIDINE DIPHOSPHATE GLUCOSE |
|  VITAMIN D2  | VITAMIN D2 |
|   | XANTHINE |
|  XANTHOSINE  | XANTHOSINE |
| XANTHURENATE | XANTHURENATE |