

# Purine metabolites regulate leukemic cell sensitivity toward cytarabine

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Xiaowen Zhang,<sup>1\*</sup> Ang Jia,<sup>1\*</sup> Jianwei You,<sup>1\*</sup> Zixuan Zhuang,<sup>1</sup> Yinfei Wang,<sup>1</sup> Ting Liu,<sup>1</sup> Xingrong Du,<sup>1</sup> Linzhang Huang,<sup>1</sup> Peng Li,<sup>1,2</sup> Tong-Jin Zhao,<sup>1,2</sup> Craig T. Jordan,<sup>3</sup> Li Chen,<sup>1</sup> Ji-Hao Zhou<sup>4</sup> and Haobin Ye<sup>1</sup>

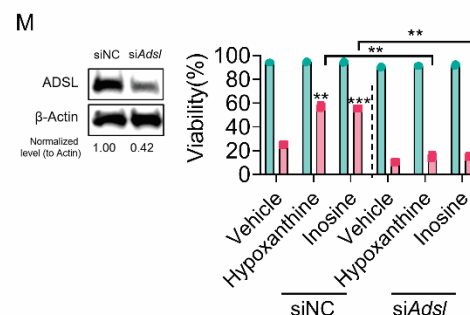
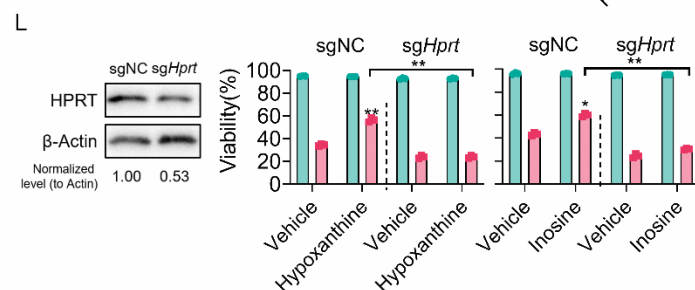
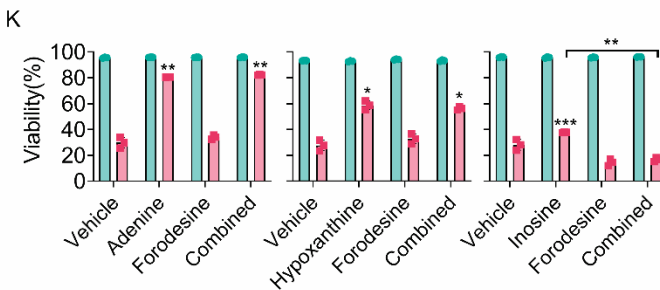
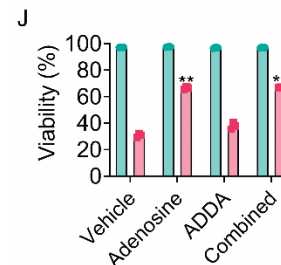
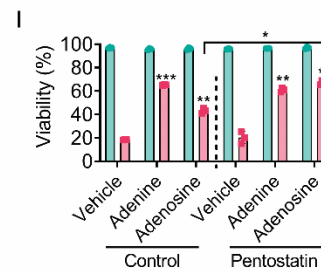
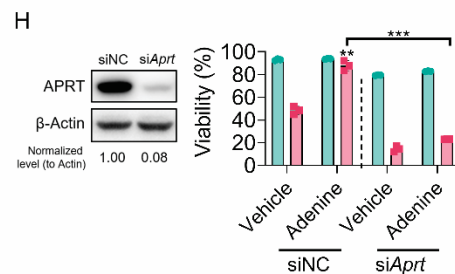
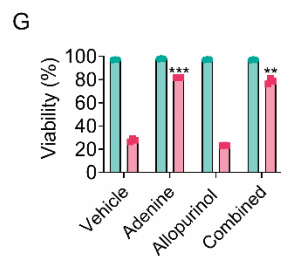
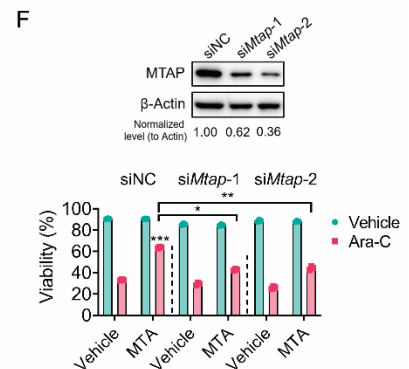
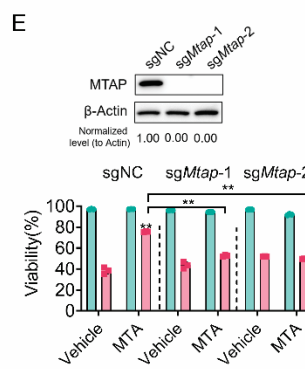
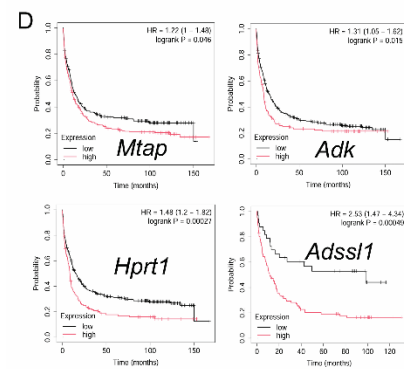
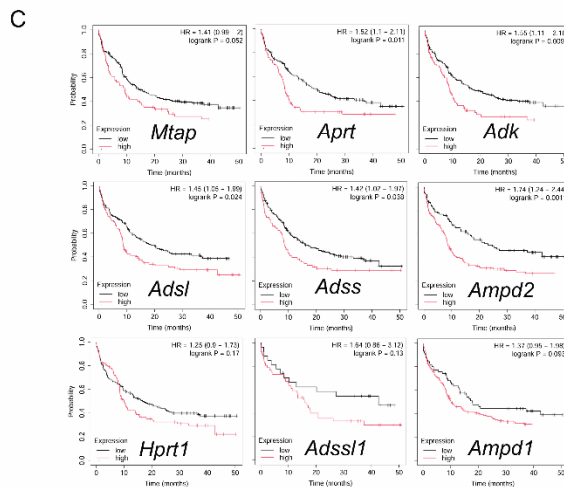
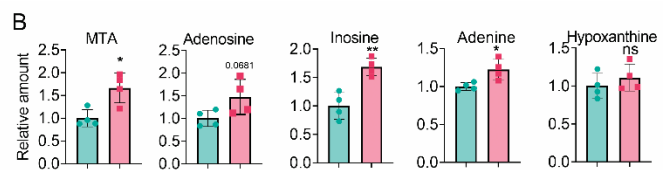
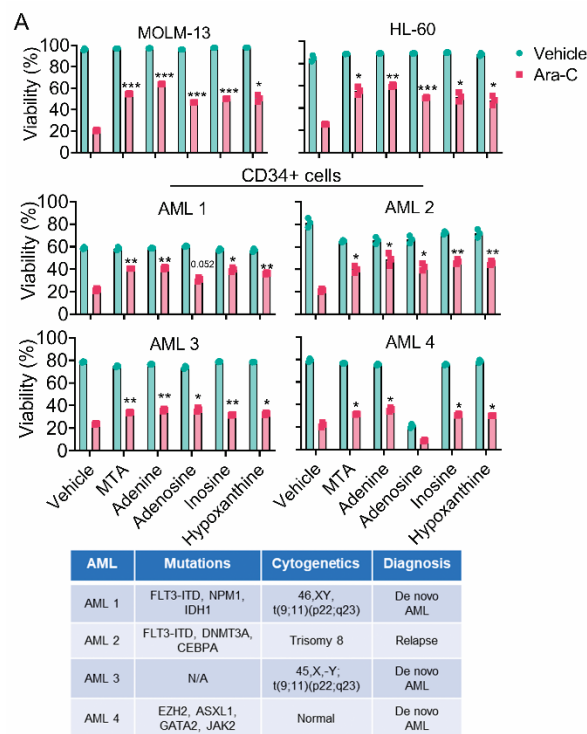
<sup>1</sup>State Key Laboratory of Genetic Engineering, Shanghai Key Laboratory of Metabolic Remodeling and Health, Institute of Metabolism and Integrative Biology, Shanghai Xuhui Central Hospital/Zhongshan-Xuhui Hospital, Fudan University, Shanghai, China; <sup>2</sup>Tianjian Laboratory of Advanced Biomedical Sciences, Zhengzhou University, Zhengzhou, Henan, China; <sup>3</sup>Division of Hematology, Department of Medicine, University of Colorado Anschutz Medical Campus, Aurora, CO, USA and <sup>4</sup>Department of

Hematology, Shenzhen People’s Hospital, The Second Clinical Medical College of Jinan University, The First Affiliated Hospital of Southern University of Science and Technology, Shenzhen, Guangdong, China

*\*XZ, AJ and JY contributed equally as first authors.*

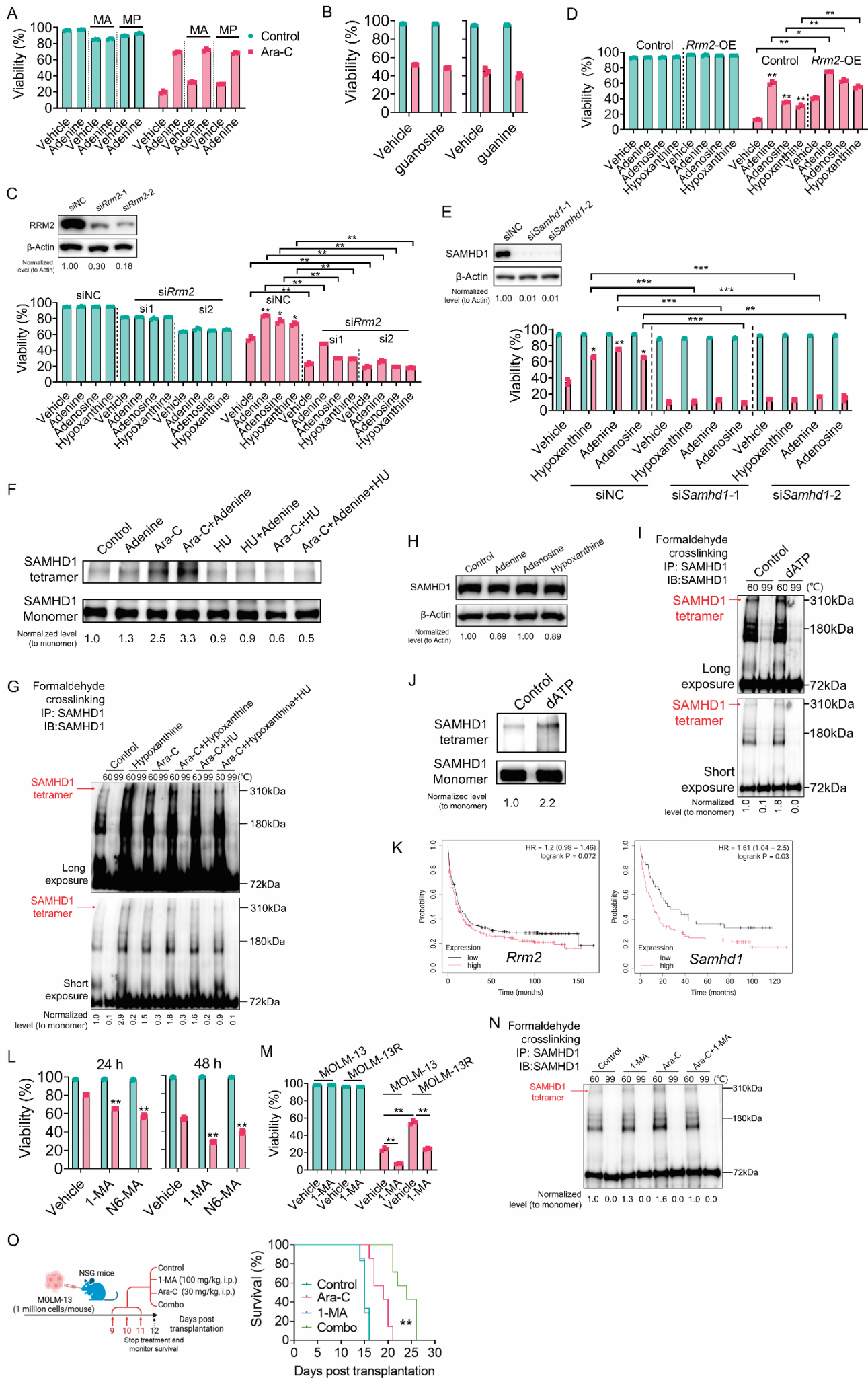
Correspondence:  
H. YE - haobin\_ye@fudan.edu.cn  
J. ZHOU - zhoujihao@aliyun.com  
L. CHEN - chenli\_imib@fudan.edu.cn

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### **Figure S1. Purine metabolites induce chemoresistance**

**(A)** Different leukemic cell lines and CD34+ AML patient cells were treated with Ara-C (0.2  $\mu$ M) combined with the indicated purine metabolites (10  $\mu$ M). Viability was accessed 48 h post-treatment (n=3). Information on the AML samples is provided. **(B)** BM serum was isolated from control and chemotherapy-treated mice. The levels of BM serum metabolites were examined (n=4). **(C-D)** Survival analysis was conducted on two AML patient cohorts, GSE12417 (C) and GSE37642 (D), based on the expression levels of enzymes involved in purine metabolism. **(E-F)** Methylthioadenosine phosphorylase (MTAP) was knocked out (KO) by sgRNAs (E) and knocked down (KD) by siRNAs (F) in leukemic cells. The protective effect of MTA against Ara-C was determined (n=3). **(G)** Leukemic cells were treated with Ara-C combined with adenine or the xanthine dehydrogenase (XDH) inhibitor Allopurinol (10  $\mu$ M). Viability was accessed 48 h post-treatment (n=3). **(H)** Adenine phosphoribosyltransferase (APRT) was KD by siRNAs in leukemic cells. The protective effect of adenine was determined (n=3). **(I-J)** MOLM-13 leukemic cells were treated with Ara-C combined with adenine, adenosine, the adenosine deaminase (ADA) inhibitor Pentostatin (10 nM) (I), or the Adenosyl homocysteinase (AHCY) inhibitor ADDA (100 nM) (J). Viability was accessed 48 h post-treatment (n=3). **(L)** Control and hypoxanthine guanine phosphoribosyltransferase (HPRT) KD leukemic cells were treated with Ara-C combined with hypoxanthine (10  $\mu$ M) or inosine (10  $\mu$ M). Viability was accessed 48 h post treatment (n=3). **(M)** Adenylosuccinate lyase (ADSL) was KD in leukemic cells, followed by Ara-C treatment combined with inosine or hypoxanthine. Viability was accessed 48 h post treatment (n=3). All data are represented as mean  $\pm$  SD. Quantification is provided for each gel image. \*,  $p \leq 0.05$ ; \*\*,  $p \leq 0.01$ ; \*\*\*,  $p \leq 0.001$ ; \*\*\*\*,  $p \leq 0.0001$ .



**Figure S2. Purine metabolites-mediated Ara-C resistance is via RRM2-induced tetramerization of SAMHD1**

**(A)** MOLM-13 leukemic cells were treated with Ara-C and adenine, with or without inosine-5'-monophosphate dehydrogenase (IMPDH) inhibitors mycophenolic acid (MA) (10  $\mu$ M) or Merimepodib (MP) (10  $\mu$ M). Viability was accessed 48 h post treatment (n=3). **(B)** MOLM-13 cells were treated with Ara-C combined with guanosine (10  $\mu$ M) or guanine (10  $\mu$ M). Viability was accessed 48 h post treatment (n=3). **(C-D)** The protective effect of purine metabolites against Ara-C was examined in RRM2 KD (C) and RRM2 overexpression (OE) (D) leukemic cells (n=3). **(E)** *Samhd1* was KD by siRNAs in leukemic cells. The protective effect of purine metabolites was determined (n=3). **(F)** SAMHD1 tetramerization was examined in leukemic cells under the indicated conditions by Native PAGE. **(G)** SAMHD1 tetramerization was examined in leukemic cells under the indicated conditions by protein crosslinking. **(H)** Protein levels of SAMHD1 in leukemic cells treated with purine metabolites. **(I-J)** Leukemic cells were electroporated with dATP and SAMHD1 tetramerization was examined by protein crosslinking (I) and by native PAGE (J). **(K)** Survival analysis of AML patients was performed based on RRM2 and SAMHD1 expression levels (GSE37642). **(L)** Leukemic cells were treated with Ara-C combined with 1-methyladenosine (1-MA) (10  $\mu$ M) or N6-methyladenosine (N6-MA) (10  $\mu$ M). Viability was accessed 24 h post-treatment (n=3). **(M)** MOLM-13 and Ara-C-resistant MOLM-13 cells (MOLM-13R) were treated with Ara-C, with or without 1-MA. Viability was assessed 48 h post treatment (n=3). **(N)** SAMHD1 tetramerization was examined in cells treated with 1-MA, Ara-C, or Ara-C combined with 1-MA by protein crosslinking. **(O)** MOLM-13 leukemic mice were subjected to indicated treatments, followed by survival assessment (n=7). All data are represented as mean  $\pm$  SD. Quantification is provided for each gel image. \*,  $p \leq 0.05$ ; \*\*,  $p \leq 0.01$ ; \*\*\*,  $p \leq 0.001$ ; \*\*\*\*,  $p \leq 0.0001$ .

**Table S1. 24-h and 48-h relative viability of leukemic cells treated with Ara-C in combination with the indicated metabolites**

| 24h                                         |                    |
|---------------------------------------------|--------------------|
| Metabolites                                 | Relative Viability |
| 2'-Deoxycytidine                            | 1.6437             |
| Tryptamine                                  | 1.6412             |
| 5-Methyl-2'-deoxycytidine                   | 1.5489             |
| Deoxycorticosterone acetate                 | 1.4516             |
| Canrenone                                   | 1.3805             |
| Quinolinic acid                             | 1.3796             |
| Adenine                                     | 1.3788             |
| SDMA                                        | 1.3771             |
| 3-Hydroxybenzoic acid                       | 1.3686             |
| Phenoxyacetic acid                          | 1.3644             |
| Azelaic acid                                | 1.3619             |
| DL-Homocysteine thiolactone (hydrochloride) | 1.3619             |
| Diethyl phosphate                           | 1.3525             |
| Thyroxine sulfate                           | 1.3449             |
| Deoxycorticosterone                         | 1.3449             |
| p-Hydroxycinnamic acid                      | 1.3441             |
| 21-Hydroxypregnenolone                      | 1.3441             |
| 3-Amino-4-methylpentanoic acid              | 1.3432             |
| (E/Z)-4-Hydroxytamoxifen                    | 1.3415             |
| 11beta-Hydroxyprogesterone                  | 1.3255             |
| Gamma-Linolenic acid                        | 1.3246             |
| Ac-Ala-OH                                   | 1.3238             |
| D-Ribonolactone                             | 1.3170             |
| Epiandrosterone                             | 1.3170             |
| Cortisone                                   | 1.3119             |
| Cortodoxone                                 | 1.3060             |
| Adenosine                                   | 1.3009             |
| Uridine 5'-monophosphate                    | 1.2992             |
| Liothyronine                                | 1.2925             |
| Inosine                                     | 1.2899             |
| Urolithin A                                 | 1.2882             |
| Adenosine monophosphate                     | 1.2823             |
| Dichlorisone acetate                        | 1.2671             |
| 2-(2-Methylbenzamido)acetic acid            | 1.2561             |
| Pregnenolone                                | 1.2535             |
| D-Desthiobiotin                             | 1.2518             |
| 4,4-Dimethoxy-2-butanone                    | 1.2501             |
| Desloratadine                               | 1.2290             |
| Androsterone                                | 1.2256             |

|                                             |        |
|---------------------------------------------|--------|
| 5'-Deoxyadenosine                           | 1.2230 |
| Progesterone                                | 1.2230 |
| Retinoic acid                               | 1.2214 |
| Coniferyl alcohol                           | 1.2180 |
| (R)-pyrrolidine-2-carboxylic acid           | 1.2095 |
| NADH (disodium salt)                        | 1.2053 |
| Mandelic acid                               | 1.2044 |
| L-SelenoMethionine                          | 1.2027 |
| Taurine                                     | 1.2010 |
| 2,6-Dimethoxybenzoic acid                   | 1.1977 |
| L-Glutamic acid                             | 1.1960 |
| N-Acetyl-L-methionine                       | 1.1951 |
| Aflatoxin B1                                | 1.1943 |
| Corticosterone                              | 1.1850 |
| Aminomalonic acid                           | 1.1841 |
| (-)-(S)-Equol                               | 1.1833 |
| Etiocholanolone                             | 1.1833 |
| Indole                                      | 1.1799 |
| Docetaxel                                   | 1.1790 |
| Fluticasone (propionate)                    | 1.1765 |
| 5'-Methylthioadenosine                      | 1.1757 |
| Acetyl Coenzyme A (trisodium)               | 1.1757 |
| NAD <sup>+</sup>                            | 1.1740 |
| Cytidine                                    | 1.1723 |
| 10-Undecenoic acid                          | 1.1706 |
| Flavin adenine dinucleotide (disodium salt) | 1.1646 |
| NADPH (tetrasodium salt)                    | 1.1630 |
| Hypoxanthine                                | 1.1621 |
| N-Acetylglycine                             | 1.1613 |
| Uridine triphosphate                        | 1.1613 |
| Substance P                                 | 1.1596 |
| Isohomovanillic acid                        | 1.1596 |
| Chenodeoxycholic Acid                       | 1.1596 |
| Palmitic acid                               | 1.1596 |
| Prednisolone                                | 1.1570 |
| Hydrocortisone                              | 1.1570 |
| Ursodeoxycholic acid                        | 1.1528 |
| 1,3-Dimethyluric acid                       | 1.1511 |
| 2,6-Dihydroxyacetophenone                   | 1.1503 |
| 3-Hydroxypicolinic acid                     | 1.1494 |
| 4-Aminobenzoic acid                         | 1.1486 |
| Pantethine                                  | 1.1477 |
| Oxoadipic acid                              | 1.1477 |

|                                              |        |
|----------------------------------------------|--------|
| 3-Amino-2-piperidinone                       | 1.1452 |
| Indole-3-carboxylic acid                     | 1.1443 |
| Estradiol                                    | 1.1443 |
| D-Panthenol                                  | 1.1426 |
| Guanosine 5'-triphosphate (trisodium salt)   | 1.1418 |
| 3-Indolepropionic acid                       | 1.1401 |
| Arachidonic acid                             | 1.1401 |
| D-Mannose                                    | 1.1393 |
| 2-Methylbenzoxazole                          | 1.1384 |
| D-Alanine                                    | 1.1359 |
| Histamine                                    | 1.1350 |
| (S)-b-aminoisobutyric acid                   | 1.1342 |
| Methoxyacetic acid                           | 1.1333 |
| 2',4'-Dihydroxyacetophenone                  | 1.1316 |
| D-Arabitol                                   | 1.1299 |
| Adenosine 5'-diphosphate                     | 1.1299 |
| DL-O-Phosphoserine                           | 1.1283 |
| Isorhamnetin                                 | 1.1274 |
| Oxalic Acid                                  | 1.1266 |
| 4-Hydroxy-3-methylbenzoic acid               | 1.1249 |
| Dehydroepiandrosterone sulfate (sodium salt) | 1.1249 |
| Arachidic acid                               | 1.1240 |
| L-Hydroxyproline                             | 1.1240 |
| 2-Methylbenzaldehyde                         | 1.1215 |
| Triacetin                                    | 1.1198 |
| 2-Hydroxyhexanoic acid                       | 1.1198 |
| Dihydrodaidzein                              | 1.1172 |
| Vanilpyruvic acid                            | 1.1164 |
| Myricetin                                    | 1.1156 |
| Docosaehaenoic Acid                          | 1.1147 |
| Cytidine 5'-monophosphate                    | 1.1147 |
| Malic acid                                   | 1.1139 |
| Trimethylamine N-oxide                       | 1.1130 |
| Isomaltose                                   | 1.1122 |
| L-Glutamine                                  | 1.1113 |
| 3,3'-Diiodo-L-thyronine                      | 1.1096 |
| $\alpha$ -Pyridone                           | 1.1096 |
| 4,6-Dioxoheptanoic acid                      | 1.1062 |
| L-Arginine                                   | 1.1062 |
| Nicotinamide riboside (chloride)             | 1.1046 |
| alpha-D-glucose                              | 1.1003 |
| Ergothioneine                                | 1.1003 |
| Coproporphyrin III                           | 1.0995 |

|                                                    |        |
|----------------------------------------------------|--------|
| Crustecdysone                                      | 1.0978 |
| Isethionic acid                                    | 1.0969 |
| AICAR (phosphate)                                  | 1.0969 |
| 2-Furoic acid                                      | 1.0969 |
| Biocytin                                           | 1.0961 |
| Glycocholic acid                                   | 1.0952 |
| D-Sorbitol                                         | 1.0952 |
| m-Anisaldehyde                                     | 1.0944 |
| 2-Acetyl-3-ethylpyrazine                           | 1.0944 |
| 4-Hydroxybenzoic acid                              | 1.0944 |
| (-)-Aspartic acid                                  | 1.0944 |
| 2,4-Dihydroxybenzoic acid                          | 1.0927 |
| Benzophenone                                       | 1.0919 |
| Meglutol                                           | 1.0910 |
| Cinnamic acid                                      | 1.0910 |
| all-trans-Anhydro Retinol                          | 1.0902 |
| Perillartine                                       | 1.0893 |
| Bisphenol A                                        | 1.0885 |
| Lornoxicam                                         | 1.0868 |
| Dimethylmalonic acid                               | 1.0851 |
| 4-Hydroxyphenylacetic acid                         | 1.0842 |
| 4-Hydroxymethylpyrazole                            | 1.0842 |
| $\alpha$ -D-Glucose-1-phosphate (disodium hydrate) | 1.0842 |
| Squalene                                           | 1.0834 |
| (R,R)-(+)-Hydrobenzoin                             | 1.0825 |
| Sorbic acid                                        | 1.0825 |
| Menaquinone-4                                      | 1.0817 |
| Ethylmalonic acid                                  | 1.0809 |
| (S)-(+)-1,2-Propanediol                            | 1.0809 |
| 5 $\alpha$ -Pregnane-3,20-dione                    | 1.0809 |
| Vanillylmandelic acid                              | 1.0792 |
| Methyl 3-phenylpropanoate                          | 1.0783 |
| Dodecanedioic acid                                 | 1.0783 |
| Glucosamine                                        | 1.0775 |
| Taurolithocholic acid (sodium salt)                | 1.0758 |
| Nerol                                              | 1.0749 |
| Pimelic acid                                       | 1.0741 |
| SAH                                                | 1.0732 |
| Glycochenodeoxycholic acid                         | 1.0732 |
| Alanylphenylalanine                                | 1.0724 |
| L-Alanyl-L-leucine                                 | 1.0707 |
| Raffinose                                          | 1.0699 |
| D-(-)-Lactic acid                                  | 1.0699 |

|                                    |        |
|------------------------------------|--------|
| β-Alanine                          | 1.0699 |
| D-(+)-Cellobiose                   | 1.0690 |
| Cytidine-5'-triphosphate           | 1.0682 |
| 17α-Hydroxyprogesterone            | 1.0673 |
| Erucic acid                        | 1.0673 |
| Docosapentaenoic acid (22n-3)      | 1.0673 |
| (Ethoxymethyl)benzene              | 1.0656 |
| Glutathione oxidized               | 1.0656 |
| Hydrocinnamic acid                 | 1.0656 |
| Medroxyprogesterone acetate        | 1.0648 |
| L-Carnitine                        | 1.0631 |
| Palmitoylethanolamide              | 1.0622 |
| DL-Norvaline                       | 1.0622 |
| Valdecoxib                         | 1.0622 |
| Royal Jelly acid                   | 1.0614 |
| Phloretin                          | 1.0614 |
| L-Azetidine-2-carboxylic acid      | 1.0614 |
| Melatonin                          | 1.0605 |
| Ferulic acid                       | 1.0605 |
| γ-Aminobutyric acid                | 1.0605 |
| p-Tolualdehyde                     | 1.0597 |
| 2,6-Dibromophenol                  | 1.0597 |
| Lipoic acid                        | 1.0588 |
| L-Tartaric acid                    | 1.0588 |
| L-Methionine                       | 1.0588 |
| L-Cysteine                         | 1.0580 |
| N-Acetyl-L-phenylalanine           | 1.0572 |
| 2'-Deoxyadenosine-5'-monophosphate | 1.0563 |
| Hydroxyacetone                     | 1.0555 |
| Acetylcysteine                     | 1.0546 |
| Daidzein                           | 1.0538 |
| Thymine                            | 1.0538 |
| 4-Aminohippuric acid               | 1.0529 |
| Hydroxyphenyllactic acid           | 1.0529 |
| H-Abu-OH                           | 1.0529 |
| Pyrogallol                         | 1.0521 |
| p-Anisic acid                      | 1.0521 |
| Maltose                            | 1.0521 |
| 2-(4-Methoxyphenyl)acetic acid     | 1.0512 |
| L-Palmitoylcarnitine (chloride)    | 1.0512 |
| L-Arabinitol                       | 1.0504 |
| Ethoxyacetic acid                  | 1.0504 |
| Creosol                            | 1.0495 |

|                                               |        |
|-----------------------------------------------|--------|
| 3-(3-Hydroxyphenyl)propionic acid             | 1.0495 |
| Zeaxanthin                                    | 1.0495 |
| 2'-Deoxyadenosine-5'-triphosphate (trisodium) | 1.0495 |
| 11-Beta-hydroxyandrostenedione                | 1.0487 |
| 2-hydroxymethyl benzoic acid                  | 1.0478 |
| D-(+)-Glucono-1,5-lactone                     | 1.0478 |
| Methyl p-tert-butylphenylacetate              | 1.0478 |
| LysoPC(14:0/0:0)                              | 1.0478 |
| L-Lactic acid                                 | 1.0462 |
| Hippuric acid                                 | 1.0462 |
| Folinic acid                                  | 1.0453 |
| (-)-Fucose                                    | 1.0453 |
| Levulinic acid                                | 1.0453 |
| Oleoylethanolamide                            | 1.0453 |
| Ursocholic acid                               | 1.0445 |
| Indole-3-acetamide                            | 1.0436 |
| Terephthalic acid                             | 1.0436 |
| 5-Methoxyindole-3-acetic acid                 | 1.0436 |
| H-HoArg-OH                                    | 1.0436 |
| Taurochenodeoxycholic acid (sodium salt)      | 1.0428 |
| Fumaric acid                                  | 1.0428 |
| Cholesterol                                   | 1.0428 |
| Sucrose                                       | 1.0419 |
| Taurocholic acid                              | 1.0419 |
| Ethynyl Estradiol                             | 1.0411 |
| Citicoline                                    | 1.0411 |
| Oglufanide                                    | 1.0402 |
| Urocanic acid                                 | 1.0394 |
| Xylitol                                       | 1.0394 |
| Uracil                                        | 1.0385 |
| 2,6-Dihydroxybenzoic acid                     | 1.0385 |
| 2-O-Methylcytosine                            | 1.0385 |
| L-Thyroxine                                   | 1.0377 |
| Theophylline                                  | 1.0377 |
| L-Isoleucine                                  | 1.0377 |
| D-Kynurenine                                  | 1.0360 |
| 5-Aminosalicylic Acid                         | 1.0360 |
| 4-Pentenoic acid                              | 1.0360 |
| 2-Hydroxy-4-methylbenzaldehyde                | 1.0351 |
| 3-Methyluridine                               | 1.0343 |
| N-Oleoyl glycine                              | 1.0343 |
| Nerolidol                                     | 1.0326 |
| Heparan Sulfate                               | 1.0318 |

|                                      |        |
|--------------------------------------|--------|
| Cysteamine (hydrochloride)           | 1.0309 |
| Stearic acid                         | 1.0309 |
| Norepinephrine                       | 1.0301 |
| 3-Methoxybenzoic acid                | 1.0292 |
| Indole-2-carboxylic acid             | 1.0292 |
| $\alpha$ -Vitamin E                  | 1.0292 |
| 2-Piperidone                         | 1.0292 |
| N-Acetyl-L-tryptophan                | 1.0292 |
| (S)-2-Hydroxy-3-phenylpropanoic acid | 1.0284 |
| 4-Methyl-1-phenyl-2-pentanone        | 1.0284 |
| Xylose                               | 1.0284 |
| Thiamine (hydrochloride)             | 1.0284 |
| Adipic acid                          | 1.0267 |
| $\alpha$ -Lipoic Acid                | 1.0267 |
| 4-Methoxycinnamic acid               | 1.0267 |
| Octopamine (hydrochloride)           | 1.0267 |
| Dimethyl trisulfide                  | 1.0258 |
| (S)-Malic acid                       | 1.0258 |
| Aminoadipic acid                     | 1.0258 |
| L-Homocitrulline                     | 1.0258 |
| 3-Methyladipic acid                  | 1.0250 |
| 3-Methyl-L-histidine                 | 1.0250 |
| Selenomethionine                     | 1.0250 |
| Xanthosine                           | 1.0241 |
| N-Methylnicotinamide                 | 1.0241 |
| Mesitaldehyde                        | 1.0233 |
| 2-Hydroxy-2-methylbutanoic acid      | 1.0233 |
| Eicosapentaenoic Acid                | 1.0225 |
| Folic acid                           | 1.0225 |
| $\gamma$ -Cyclodextrin               | 1.0225 |
| 4-Methylbiphenyl                     | 1.0216 |
| 5,6-Dihydroxyindole                  | 1.0216 |
| Xanthine                             | 1.0216 |
| (-)-Menthol                          | 1.0208 |
| trans-Vaccenic acid                  | 1.0208 |
| O-Acetylserine                       | 1.0208 |
| L-Valine                             | 1.0208 |
| L-Alanine                            | 1.0208 |
| Undecanoic acid                      | 1.0199 |
| TFAP                                 | 1.0191 |
| Cyclo(his-pro) (TFA)                 | 1.0191 |
| Estriol                              | 1.0191 |
| 2-Methoxybenzoic acid                | 1.0182 |

|                                  |        |
|----------------------------------|--------|
| Vanillic acid                    | 1.0182 |
| Butylparaben                     | 1.0182 |
| 2-Methylacetophenone             | 1.0182 |
| 2-Ethylpyrazine                  | 1.0174 |
| 2-Acetonaphthone                 | 1.0174 |
| 2',4'-Dimethylacetophenone       | 1.0174 |
| Natamycin                        | 1.0174 |
| D-Mannitol                       | 1.0174 |
| 6-Mercaptopurine                 | 1.0157 |
| Hexadecanedioic acid             | 1.0157 |
| Diphenyl disulfide               | 1.0157 |
| N-Acetyl-D-glucosamine           | 1.0157 |
| 6-Thioguanine                    | 1.0140 |
| N2,N2-Dimethylguanosine          | 1.0140 |
| D-Leucine                        | 1.0140 |
| H-D-Trp-OH                       | 1.0140 |
| N4-Acetylcytidine                | 1.0140 |
| Coenzyme Q9                      | 1.0131 |
| 5-Methyluridine                  | 1.0131 |
| 7-Ketolithocholic acid           | 1.0114 |
| Eriodictyol                      | 1.0106 |
| 2-Naphthol                       | 1.0098 |
| Myristic acid                    | 1.0098 |
| Paraxanthine                     | 1.0098 |
| 5-Methylcytosine                 | 1.0098 |
| D-(+)-Phenyllactic acid          | 1.0089 |
| Pentadecanoic acid               | 1.0089 |
| 4-Carboxypyrazole                | 1.0089 |
| L-Gulono-1,4-lactone             | 1.0089 |
| 2-Methoxyestrone                 | 1.0081 |
| D-Glucuronic acid                | 1.0072 |
| 1-Methylguanosine                | 1.0047 |
| 5-Hydroxymethyluracil            | 1.0047 |
| 3,5-Dihydroxyacetophenone        | 1.0047 |
| Protoporphyrin IX                | 1.0038 |
| Deoxycholic acid                 | 1.0038 |
| 3-Methyl-2-oxobutanoic acid      | 1.0038 |
| Prostaglandin E2                 | 1.0038 |
| Sucralose                        | 1.0030 |
| Oxytocin (acetate)               | 1.0030 |
| Maltotetraose                    | 1.0030 |
| N-Acetylputrescine hydrochloride | 1.0021 |
| Coenzyme A                       | 1.0021 |

|                                          |        |
|------------------------------------------|--------|
| Nudifloramide                            | 1.0021 |
| 4-Hydroxycoumarin                        | 1.0021 |
| Lactose                                  | 1.0021 |
| Dihydrocaffeic acid                      | 1.0021 |
| 3-Methyl-2-cyclopenten-1-one             | 1.0021 |
| 6-Biopterin                              | 1.0013 |
| Ascorbyl palmitate                       | 1.0013 |
| Ara-C                                    | 1.0000 |
| Dihydrouracil                            | 0.9996 |
| 2-Naphthoxyacetic acid                   | 0.9988 |
| 4,6-O-Ethylidene- $\alpha$ -D-glucose    | 0.9988 |
| 8-Hydroxyguanosine                       | 0.9979 |
| 1-Methylinosine                          | 0.9979 |
| Oleic acid                               | 0.9971 |
| Aceglutamide                             | 0.9971 |
| 4-Hydroxybenzyl alcohol                  | 0.9971 |
| L-Homocysteine                           | 0.9971 |
| Gamma-glutamylcysteine                   | 0.9971 |
| Guanidinosuccinic acid                   | 0.9962 |
| 3-Methylcrotonylglycine                  | 0.9954 |
| N-Acetyl-5-hydroxytryptamine             | 0.9954 |
| Succinic acid                            | 0.9937 |
| Spermidine                               | 0.9937 |
| 2'-Deoxyuridine                          | 0.9937 |
| Scyllo-Inositol                          | 0.9928 |
| Chondroitin (sulfate)                    | 0.9920 |
| N2-Methylguanosine                       | 0.9920 |
| Methyl anisate                           | 0.9920 |
| 5-Aminolevulinic acid (hydrochloride)    | 0.9894 |
| Tetrahydrobiopterin                      | 0.9886 |
| N1,N8-Diacetylspermidine (hydrochloride) | 0.9886 |
| Agmatine (sulfate)                       | 0.9886 |
| D-Pipecolinic acid                       | 0.9877 |
| p-Coumaric acid                          | 0.9869 |
| 17 $\alpha$ -Hydroxypregnenolone         | 0.9869 |
| 4-Methoxybenzaldehyde                    | 0.9869 |
| 2-Methylpentanedioic acid                | 0.9852 |
| Docosanoic acid                          | 0.9852 |
| Sarcosine                                | 0.9852 |
| 3-Hydroxycapric acid                     | 0.9835 |
| Pyrocatechuic acid                       | 0.9835 |
| Glycodeoxycholic Acid                    | 0.9835 |
| Vitamin K1                               | 0.9835 |

|                                     |        |
|-------------------------------------|--------|
| Dulcitol                            | 0.9827 |
| Pyridoxylamine                      | 0.9818 |
| 2'-O-Methyladenosine                | 0.9818 |
| Mevalonic acid (lithium salt)       | 0.9810 |
| Benzamide                           | 0.9810 |
| Glycoursodeoxycholic acid           | 0.9810 |
| i-Inositol                          | 0.9810 |
| Genistein                           | 0.9801 |
| Tauroursodeoxycholate               | 0.9801 |
| Glycine                             | 0.9793 |
| Octanoic acid                       | 0.9784 |
| Ethyl glucuronide                   | 0.9784 |
| 3-(Methylthio)propionic acid        | 0.9784 |
| 5 $\alpha$ -Cholestan-3 $\beta$ -ol | 0.9776 |
| Dehydrocholate (sodium)             | 0.9776 |
| Linalool                            | 0.9776 |
| 2-Phenylpropionic acid              | 0.9767 |
| 2-Hydroxy-3-methylbutanoic acid     | 0.9767 |
| N-Methylhydantoin                   | 0.9759 |
| 1-Hydroxypyrene                     | 0.9751 |
| 5,6-Dimethyl-1H-benzo[d]imidazole   | 0.9751 |
| Phenylpropionic acid                | 0.9751 |
| SY-640                              | 0.9751 |
| 1,2-Cyclohexanedione                | 0.9742 |
| Melanin                             | 0.9742 |
| Pyridoxal phosphate                 | 0.9742 |
| L-Homocystine                       | 0.9742 |
| Sulcatone                           | 0.9742 |
| Isovalerylcarnitine                 | 0.9734 |
| Creatinine                          | 0.9734 |
| Triolein                            | 0.9725 |
| 1-Hexadecanol                       | 0.9717 |
| 6-Hydroxynicotinic acid             | 0.9700 |
| Hypotaurine                         | 0.9700 |
| L-Alloisoleucine                    | 0.9700 |
| Benzylideneacetone                  | 0.9683 |
| 4-Ethylphenol                       | 0.9683 |
| 3-Indoleacetonitrile                | 0.9683 |
| Creatine                            | 0.9683 |
| Guanidine (hydrochloride)           | 0.9674 |
| Linoleic acid                       | 0.9666 |
| Isoprenaline (hydrochloride)        | 0.9657 |
| Orotic acid                         | 0.9657 |

|                                          |        |
|------------------------------------------|--------|
| Methyl Paraben                           | 0.9657 |
| Oxaloacetic acid                         | 0.9649 |
| 7-Methylguanosine                        | 0.9649 |
| Cholic acid                              | 0.9641 |
| Dodecanoylcarnitine                      | 0.9624 |
| 3,4-Dihydroxybenzeneacetic acid          | 0.9624 |
| 8-Hydroxy-2'-deoxyguanosine              | 0.9615 |
| Undecanedioic acid                       | 0.9607 |
| N-Acetyl-L-leucine                       | 0.9607 |
| Methyl cyclohexanecarboxylate            | 0.9598 |
| Phthalic acid mono-2-ethylhexyl ester    | 0.9590 |
| D-Glutamine                              | 0.9581 |
| N-Acetyl-L-tyrosine                      | 0.9581 |
| Cytosine                                 | 0.9564 |
| 2-Hydroxyphenylacetic acid               | 0.9556 |
| Hydrocortisone acetate                   | 0.9556 |
| 1,3-Dithiane                             | 0.9556 |
| L-Tryptophan                             | 0.9556 |
| L-Aspartic acid                          | 0.9556 |
| Spinacine                                | 0.9547 |
| Pyrroloquinoline quinone                 | 0.9547 |
| Guanosine 5'-diphosphate (disodium salt) | 0.9547 |
| Chlorogenic acid                         | 0.9539 |
| 7-Methylxanthine                         | 0.9539 |
| p-Toluic acid                            | 0.9530 |
| Guaiacol                                 | 0.9530 |
| NSC 16590                                | 0.9530 |
| Leucyl-phenylalanine                     | 0.9530 |
| Cholesteryl oleate                       | 0.9522 |
| 3-Hydroxyphenylacetic acid               | 0.9522 |
| 4-Amino-L-phenylalanine                  | 0.9522 |
| L-Norleucine                             | 0.9514 |
| L-Prolylglycine                          | 0.9505 |
| L-Pipecolic acid                         | 0.9505 |
| Palmitoleic acid                         | 0.9488 |
| Tyramine                                 | 0.9488 |
| 3-Hydroxyanthranilic acid                | 0.9488 |
| 5-Hydroxytryptophol                      | 0.9480 |
| Dimethyl sulfone                         | 0.9471 |
| trans-trans-Muconic acid                 | 0.9463 |
| Urea                                     | 0.9454 |
| 3-Chloro-L-tyrosine                      | 0.9454 |
| Ribitol                                  | 0.9446 |

|                                        |        |
|----------------------------------------|--------|
| β-Nicotinamide mononucleotide          | 0.9446 |
| Propofol                               | 0.9437 |
| L-Valyl-L-phenylalanine                | 0.9437 |
| D(-)-2-Aminobutyric acid               | 0.9437 |
| Homogentisic acid                      | 0.9429 |
| D-(+)-Trehalose                        | 0.9429 |
| 2-Phenylacetamide                      | 0.9429 |
| Niacin                                 | 0.9420 |
| Lauric acid                            | 0.9404 |
| L-Homoserine                           | 0.9404 |
| Oxypurinol                             | 0.9395 |
| Thymine                                | 0.9395 |
| DL-Tryptophan                          | 0.9387 |
| 3-Nitro-L-tyrosine                     | 0.9387 |
| 5-Aminovaleric acid                    | 0.9387 |
| 2,4-Dihydroxybenzaldehyde              | 0.9378 |
| DL-Asparagine                          | 0.9370 |
| 7,8-Dihydro-L-biopterin                | 0.9361 |
| 5-Hydroxymethyl-2-furancarboxylic acid | 0.9361 |
| DL-Homocystine                         | 0.9361 |
| Riboflavin (phosphate sodium)          | 0.9361 |
| [Leu5]-Enkephalin                      | 0.9361 |
| 2'-Deoxyadenosine                      | 0.9353 |
| meso-Erythritol                        | 0.9336 |
| β-cyano-L-Alanine                      | 0.9336 |
| p-Synephrine                           | 0.9336 |
| PCL 016                                | 0.9336 |
| 2,4-Di-tert-butylphenol                | 0.9327 |
| Uridine                                | 0.9310 |
| Imidazol-1-yl-acetic acid              | 0.9310 |
| Dimethyl fumarate                      | 0.9302 |
| D-Allothreonine                        | 0.9302 |
| Desaminotyrosine                       | 0.9302 |
| Isovaleric acid                        | 0.9293 |
| 5-Amino-3H-imidazole-4-Carboxamide     | 0.9285 |
| Urolithin B                            | 0.9285 |
| γ-Glu-Phe                              | 0.9277 |
| DL-Homocysteine                        | 0.9260 |
| L-Serine                               | 0.9260 |
| 2-Methylsuccinic acid                  | 0.9251 |
| Glycohyodeoxycholic acid               | 0.9251 |
| Dehydroascorbic acid                   | 0.9251 |
| 5-Hydroxytryptophan                    | 0.9243 |

|                                              |        |
|----------------------------------------------|--------|
| Maltohexaose                                 | 0.9243 |
| 2'-Deoxyadenosine monohydrate                | 0.9234 |
| Kynurenic acid                               | 0.9209 |
| Maltotriose                                  | 0.9200 |
| 2-Oxovaleric acid                            | 0.9192 |
| Cyclohexaneacetic acid                       | 0.9192 |
| Nicotinamide                                 | 0.9192 |
| 1-Dodecanol                                  | 0.9183 |
| Glutaric acid                                | 0.9183 |
| N-Acetylhistamine                            | 0.9175 |
| Acetyl-L-carnitine (hydrochloride)           | 0.9175 |
| N-Acetyl-L-arginine                          | 0.9167 |
| Elaidic acid                                 | 0.9133 |
| L-Asparagine                                 | 0.9133 |
| Ellagic acid                                 | 0.9124 |
| L-Phenylalanine                              | 0.9124 |
| Suberic acid                                 | 0.9116 |
| 4-Methyl-2-oxopentanoic acid                 | 0.9116 |
| Phosphocreatine (disodium)                   | 0.9116 |
| 2-Methylcitric acid                          | 0.9107 |
| 3-Methylglutaric acid                        | 0.9107 |
| Norharmane                                   | 0.9107 |
| 3b-Hydroxy-5-cholenoic acid                  | 0.9099 |
| 2,5-Dihydroxybenzoic acid                    | 0.9099 |
| Purine                                       | 0.9099 |
| Antineoplaston A10                           | 0.9090 |
| D- $\alpha$ -Hydroxyglutaric acid (disodium) | 0.9090 |
| 4-Hydroxybenzyl cyanide                      | 0.9090 |
| 5-Methoxytryptophol                          | 0.9082 |
| Glycylglycine                                | 0.9082 |
| Tetrahydrothiophen-3-one                     | 0.9073 |
| 3-Hydroxyisobutyric acid                     | 0.9065 |
| 4-Acetamidobutanoic acid                     | 0.9065 |
| L-Alanyl-L-glutamine                         | 0.9065 |
| L-Kynurenine                                 | 0.9056 |
| Glyoxalic acid                               | 0.9056 |
| Beta-Cortol                                  | 0.9056 |
| Allantoin                                    | 0.9056 |
| Pseudouridine                                | 0.9048 |
| D-Serine                                     | 0.9048 |
| Oxytetracycline                              | 0.9040 |
| 5-Methyltetrahydrofolic acid                 | 0.9040 |
| Homovanillic acid                            | 0.9040 |

|                                            |        |
|--------------------------------------------|--------|
| FAPy-adenine                               | 0.9031 |
| 3-Methylbut-2-enoic acid                   | 0.9031 |
| L-Proline                                  | 0.9023 |
| Lecithin                                   | 0.9014 |
| Methylmalonic acid                         | 0.9014 |
| Glycolic acid                              | 0.9014 |
| Pyruvic acid                               | 0.9006 |
| 5-Hydroxy-2'-deoxyuridine                  | 0.9006 |
| L-Citrulline                               | 0.9006 |
| (Z)-Aconitic acid                          | 0.8997 |
| L-Cystathionine                            | 0.8997 |
| L-Histidine                                | 0.8989 |
| Hyodeoxycholic acid                        | 0.8980 |
| (S)-3-Hydroxybutanoic acid                 | 0.8980 |
| Uridine-5'-diphosphate disodium salt       | 0.8972 |
| 3-Hydroxyglutaric acid                     | 0.8963 |
| Delta-Tocopherol                           | 0.8955 |
| Nervonic acid                              | 0.8955 |
| Benzoic acid                               | 0.8955 |
| Phosphorylcholine                          | 0.8955 |
| 3-Indoleacetic acid                        | 0.8946 |
| Guanosine                                  | 0.8946 |
| N-Acetyl-L-aspartic acid                   | 0.8938 |
| 12-Hydroxydodecanoic acid                  | 0.8921 |
| 3,4-Dimethoxyphenylacetic acid             | 0.8913 |
| Phosphorylethanolamine                     | 0.8904 |
| Phenylephrine (hydrochloride)              | 0.8896 |
| 2,3,5-Trimethylpyrazine                    | 0.8887 |
| L-Ornithine                                | 0.8887 |
| Thymidine-5'-monophosphate (disodium) salt | 0.8887 |
| 3-Hydroxybutyric acid                      | 0.8887 |
| 2-(1H-Indol-3-yl)ethan-1-ol                | 0.8879 |
| Deoxycholic acid sodium salt               | 0.8879 |
| Phenylpyruvic acid                         | 0.8870 |
| Phosphonoacetic acid                       | 0.8870 |
| trans-Aconitic acid                        | 0.8853 |
| 3-Methyl-2-oxovaleric acid                 | 0.8845 |
| H-Tyr(3-I)-OH                              | 0.8845 |
| Citraconic acid                            | 0.8828 |
| C16-PAF                                    | 0.8828 |
| Thiamine pyrophosphate                     | 0.8828 |
| Cysteinylglycine (TFA)                     | 0.8811 |
| DL-3-Phenyllactic acid                     | 0.8794 |

|                                         |        |
|-----------------------------------------|--------|
| Pregnanediol                            | 0.8786 |
| Cyclic AMP                              | 0.8777 |
| Caffeic acid                            | 0.8769 |
| Nicotinuric acid                        | 0.8760 |
| H-Val-Tyr-OH                            | 0.8760 |
| (E)-Ferulic acid                        | 0.8752 |
| 3-Methylxanthine                        | 0.8752 |
| (R)-3-Hydroxybutanoic acid              | 0.8752 |
| 3,4-Dihydroxymandelic acid              | 0.8743 |
| DL-Glutamine                            | 0.8743 |
| L-DABA                                  | 0.8735 |
| 2,5-Furandicarboxylic acid              | 0.8735 |
| Octadecanal                             | 0.8726 |
| Uric acid                               | 0.8718 |
| Nicotinamide N-oxide                    | 0.8718 |
| Pipecolic acid                          | 0.8718 |
| L-Lysine                                | 0.8709 |
| 1-Methyl-L-histidine                    | 0.8684 |
| D-Cysteine                              | 0.8659 |
| L-Ascorbic acid 2-phosphate (trisodium) | 0.8659 |
| 2(5H)-Furanone                          | 0.8616 |
| Maltopentaose                           | 0.8616 |
| L-Dihydroorotic acid                    | 0.8599 |
| DPPC                                    | 0.8566 |
| Decanedioic acid                        | 0.8557 |
| 3-Hydroxyisovaleric acid                | 0.8557 |
| Spaglumatic Acid                        | 0.8557 |
| 1-Octanol                               | 0.8557 |
| Indolelactic acid                       | 0.8540 |
| γ-L-Glutamyl-L-alanine                  | 0.8489 |
| Butyrylcarnitine                        | 0.8489 |
| 3,5-Dihydroxybenzoic acid               | 0.8472 |
| 3-Hydroxyvaleric acid                   | 0.8472 |
| 25-Hydroxycholesterol                   | 0.8464 |
| L-Threonine                             | 0.8464 |
| Cholestenone                            | 0.8447 |
| Dinoprost                               | 0.8439 |
| 2-(2-Phenylacetamido)acetic acid        | 0.8430 |
| 5'-Guanylic acid (disodium salt)        | 0.8430 |
| sn-Glycerol 3-phosphate                 | 0.8413 |
| 1,4-Dimethoxybenzene                    | 0.8405 |
| H-Phe-Phe-OH                            | 0.8388 |
| Glycyl-L-valine                         | 0.8379 |

|                                         |        |
|-----------------------------------------|--------|
| Ergosterol                              | 0.8362 |
| D-Ribose(mixture of isomers)            | 0.8362 |
| N4-Acetylcytidine triphosphate (sodium) | 0.8354 |
| D-(-)-Quinic acid                       | 0.8329 |
| TRIA-662                                | 0.8320 |
| Methionine sulfoxide                    | 0.8320 |
| L-Carnosine                             | 0.8303 |
| 3-Amino-2-methylpropanoic acid          | 0.8286 |
| 1-Naphthol                              | 0.8261 |
| (2-Aminoethyl)phosphonic acid           | 0.8252 |
| 4-Pyridoxic acid                        | 0.8202 |
| 3-Methoxytyramine                       | 0.8185 |
| N-Methylsarcosine                       | 0.8176 |
| 1,5-Anhydrosorbitol                     | 0.8159 |
| 3-Hydroxyhippuric acid                  | 0.8134 |
| N-(5-Aminopentyl)acetamide              | 0.8100 |
| Adrenosterone                           | 0.8100 |
| L-Methionine sulfoxide                  | 0.8083 |
| 5,6-Dihydrouridine                      | 0.8007 |
| 2'-Deoxyguanosine                       | 0.7965 |
| Sphingomyelin                           | 0.7965 |
| N-Acetylornithine                       | 0.7922 |
| 1-Hydroxyoctadecane                     | 0.7905 |
| Pregnenolone monosulfate                | 0.7872 |
| 5-Hydroxyindole-3-acetic acid           | 0.7804 |
| Galactose 1-phosphate Potassium salt    | 0.7728 |
| Maleic Acid                             | 0.7677 |
| Cholesteryl palmitate                   | 0.7643 |
| 5,6-Dihydro-5-methyluracil              | 0.7592 |
| 1-Methyladenine                         | 0.7550 |
| H-Gly-Pro-OH                            | 0.7516 |
| Citric acid                             | 0.7491 |
| Nepsilon-Acetyl-L-lysine                | 0.7448 |
| 2-Hydroxyadipic acid                    | 0.7271 |
| 2'-Deoxyinosine                         | 0.7093 |
| Anserine                                | 0.7008 |
| 1-Methyluric acid                       | 0.6966 |
| Thymidine                               | 0.6873 |
| Phenylacetylglutamine                   | 0.6814 |
| 2,6-Diaminoheptanedioic acid            | 0.6788 |
| 1-Methyladenosine                       | 0.6763 |
| 4-Methylcatechol                        | 0.6238 |
| 4-Ethoxyphenol                          | 0.6170 |

|                    |        |
|--------------------|--------|
| Kinetensin         | 0.5172 |
| N6-Methyladenosine | 0.2412 |

| 48h                                  |                    |
|--------------------------------------|--------------------|
| Metabolites                          | Relative Viability |
| N-Desmethyltamoxifen (hydrochloride) | 6.1549             |
| 2'-Deoxycytidine                     | 6.1420             |
| Pimelic acid                         | 6.1420             |
| Tryptamine                           | 6.0453             |
| 5-Methyl-2'-deoxycytidine            | 5.7134             |
| Adenine                              | 4.5082             |
| m-Anisaldehyde                       | 3.8959             |
| Canrenone                            | 3.7187             |
| Uridine triphosphate                 | 3.6961             |
| Oxypurinol                           | 3.6059             |
| Adenosine                            | 3.5576             |
| Retinoic acid                        | 3.4770             |
| L-Serine                             | 3.4641             |
| 5'-Methylthioadenosine               | 3.4158             |
| Adenosine monophosphate              | 3.3739             |
| Deoxycorticosterone acetate          | 3.1515             |
| 5'-Deoxyadenosine                    | 3.0839             |
| Inosine                              | 3.0742             |
| 2-(2-Methylbenzamido)acetic acid     | 2.8873             |
| all-trans-Anhydro Retinol            | 2.8358             |
| Mandelic acid                        | 2.7455             |
| 2'-Deoxyadenosine                    | 2.6360             |
| Hypoxanthine                         | 2.5941             |
| 21-Hydroxypregnenolone               | 2.5618             |
| Zeaxanthin                           | 2.5167             |
| 2'-Deoxyadenosine-5'-monophosphate   | 2.3911             |
| Squalene                             | 2.3492             |
| Ursodeoxycholic acid                 | 2.2525             |
| Deoxycorticosterone                  | 2.2203             |
| NAD+                                 | 2.1945             |
| Adenosine 5'-diphosphate             | 2.1655             |
| 2,6-Dihydroxybenzoic acid            | 2.1268             |
| Indole-2-carboxylic acid             | 2.1268             |
| Epiandrosterone                      | 2.1236             |
| Acetyl Coenzyme A (trisodium)        | 2.0849             |
| Progesterone                         | 2.0269             |
| Sorbic acid                          | 2.0205             |
| 4,4-Dimethoxy-2-butanone             | 2.0140             |

|                                             |        |
|---------------------------------------------|--------|
| 11beta-Hydroxyprogesterone                  | 1.9818 |
| Chlorogenic acid                            | 1.9594 |
| Fluticasone (propionate)                    | 1.9206 |
| Etiocholanolone                             | 1.9045 |
| Undecanoic acid                             | 1.8529 |
| Cytidine 5'-monophosphate                   | 1.8529 |
| p-Hydroxycinnamic acid                      | 1.8432 |
| 2-Naphthoxyacetic acid                      | 1.8336 |
| NADH (disodium salt)                        | 1.8303 |
| 5a-Pregnane-3,20-dione                      | 1.8078 |
| 2'-Deoxyadenosine monohydrate               | 1.7981 |
| Thymine                                     | 1.7981 |
| 3-Hydroxycapric acid                        | 1.7885 |
| Glycoursodeoxycholic acid                   | 1.7820 |
| Guaiacol                                    | 1.7627 |
| 5-Hydroxymethyl-2-furancarboxylic acid      | 1.7530 |
| 5,6-Dimethyl-1H-benzo[d]imidazole           | 1.7466 |
| Flavin adenine dinucleotide (disodium salt) | 1.7466 |
| Oxaloacetic acid                            | 1.7369 |
| Cortisone                                   | 1.7305 |
| AICAR (phosphate)                           | 1.7305 |
| Hydroxyphenyllactic acid                    | 1.7143 |
| (-)-Aspartic acid                           | 1.7143 |
| Prednisolone                                | 1.6821 |
| Spermidine                                  | 1.6724 |
| Palmitic acid                               | 1.6628 |
| Benzamide                                   | 1.6306 |
| Nicotinamide riboside (chloride)            | 1.6177 |
| Glycocholic acid                            | 1.6177 |
| 2'-O-Methyladenosine                        | 1.6080 |
| Folinic acid                                | 1.5951 |
| Sucralose                                   | 1.5854 |
| Cortodoxone                                 | 1.5822 |
| Taurochenodeoxycholic acid (sodium salt)    | 1.5822 |
| Benzophenone                                | 1.5726 |
| 1-Hexadecanol                               | 1.5726 |
| N-Acetyl-L-tryptophan                       | 1.5564 |
| N-Acetyl-D-glucosamine                      | 1.5468 |
| Methyl 3-phenylpropanoate                   | 1.5436 |
| 3-Hydroxybenzoic acid                       | 1.5403 |
| Royal Jelly acid                            | 1.5242 |
| 2-Phenylpropionic acid                      | 1.5178 |
| D-Cysteine                                  | 1.5178 |

|                                   |        |
|-----------------------------------|--------|
| L-Homocitrulline                  | 1.5178 |
| Coniferyl alcohol                 | 1.5017 |
| 2',4'-Dimethylacetophenone        | 1.4888 |
| 2-(4-Methoxyphenyl)acetic acid    | 1.4823 |
| 3,3'-Diiodo-L-thyronine           | 1.4791 |
| Raffinose                         | 1.4791 |
| Menaquinone-4                     | 1.4727 |
| Levulinic acid                    | 1.4694 |
| N4-Acetylcytidine                 | 1.4662 |
| Sucrose                           | 1.4630 |
| Taurocholic acid                  | 1.4630 |
| Octopamine (hydrochloride)        | 1.4565 |
| Hydroxyacetone                    | 1.4533 |
| Docosapentaenoic acid (22n-3)     | 1.4469 |
| Vanillic acid                     | 1.4469 |
| N-Acetyl-L-methionine             | 1.4437 |
| 2-Furoic acid                     | 1.4404 |
| 1-Hydroxypyrene                   | 1.4243 |
| Glyoxalic acid                    | 1.4211 |
| NADPH (tetrasodium salt)          | 1.4211 |
| 3-(3-Hydroxyphenyl)propionic acid | 1.4179 |
| 7-Ketolithocholic acid            | 1.4147 |
| 5-Methoxyindole-3-acetic acid     | 1.4114 |
| Fumaric acid                      | 1.4114 |
| Malic acid                        | 1.4082 |
| Desloratadine                     | 1.4050 |
| (S)-b-aminoisobutyric acid        | 1.4050 |
| Nerol                             | 1.4018 |
| p-Toluic acid                     | 1.3985 |
| 4,6-Dioxoheptanoic acid           | 1.3985 |
| Dihydrocaffeic acid               | 1.3921 |
| Arachidonic acid                  | 1.3921 |
| Oglufanide                        | 1.3857 |
| Vanillylmandelic acid             | 1.3857 |
| 4-Methylbiphenyl                  | 1.3824 |
| Dulcitol                          | 1.3792 |
| L-Pipecolic acid                  | 1.3792 |
| $\alpha$ -Lipoic Acid             | 1.3760 |
| Melatonin                         | 1.3695 |
| Hippuric acid                     | 1.3663 |
| Sulcatone                         | 1.3631 |
| Erucic acid                       | 1.3566 |
| L-Tartaric acid                   | 1.3534 |

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|----------------------------------------------------|--------|
| L-Carnitine                                        | 1.3502 |
| Azelaic acid                                       | 1.3470 |
| Ac-Ala-OH                                          | 1.3341 |
| 2-Methylbenzoxazole                                | 1.3341 |
| $\alpha$ -D-Glucose-1-phosphate (disodium hydrate) | 1.3341 |
| Lactose                                            | 1.3309 |
| 2-Acetonaphthone                                   | 1.3244 |
| Liothyronine                                       | 1.3212 |
| (-)-(S)-Equol                                      | 1.3148 |
| 4-Methoxycinnamic acid                             | 1.3148 |
| N-Acetyl-5-hydroxytryptamine                       | 1.3115 |
| Lornoxicam                                         | 1.3083 |
| 4-Pyridoxic acid                                   | 1.3051 |
| Pentadecanoic acid                                 | 1.3019 |
| 2-Hydroxyhexanoic acid                             | 1.2986 |
| 2,4-Dihydroxybenzaldehyde                          | 1.2954 |
| Biocytin                                           | 1.2922 |
| 2,4-Dihydroxybenzoic acid                          | 1.2858 |
| Spinacine                                          | 1.2793 |
| Cyclo(his-pro) (TFA)                               | 1.2729 |
| Acetylcysteine                                     | 1.2729 |
| SDMA                                               | 1.2632 |
| Mevalonic acid (lithium salt)                      | 1.2632 |
| DL-Homocysteine thiolactone (hydrochloride)        | 1.2600 |
| 2,6-Dimethoxybenzoic acid                          | 1.2600 |
| DL-O-Phosphoserine                                 | 1.2600 |
| Isorhamnetin                                       | 1.2568 |
| N-Oleoyl glycine                                   | 1.2535 |
| Corticosterone                                     | 1.2535 |
| L-Arabinitol                                       | 1.2471 |
| 5-Hydroxyindole-3-acetic acid                      | 1.2406 |
| Creosol                                            | 1.2342 |
| 3-Methyl-L-histidine                               | 1.2342 |
| L-Azetidine-2-carboxylic acid                      | 1.2310 |
| 1-Methyluric acid                                  | 1.2310 |
| Methyl p-tert-butylphenylacetate                   | 1.2278 |
| 5-Hydroxymethyluracil                              | 1.2245 |
| Cinnamic acid                                      | 1.2245 |
| 1,3-Dimethyluric acid                              | 1.2213 |
| Guanosine 5'-triphosphate (trisodium salt)         | 1.2213 |
| Trimethylamine N-oxide                             | 1.2149 |
| D-(-)-Lactic acid                                  | 1.2149 |
| 2-Methoxybenzoic acid                              | 1.2116 |

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|-----------------------------------|--------|
| Pyridoxylamine                    | 1.2116 |
| Taurine                           | 1.2116 |
| Tyramine                          | 1.1987 |
| 6-Biopterin                       | 1.1987 |
| PCL 016                           | 1.1891 |
| 2',4'-Dihydroxyacetophenone       | 1.1891 |
| $\alpha$ -Pyridone                | 1.1859 |
| 4-Aminobenzoic acid               | 1.1826 |
| 3-Amino-4-methylpentanoic acid    | 1.1826 |
| (2-Aminoethyl)phosphonic acid     | 1.1730 |
| 1-Dodecanol                       | 1.1665 |
| L-Lactic acid                     | 1.1665 |
| D-Leucine                         | 1.1665 |
| Oleylethanolamide                 | 1.1665 |
| Eicosapentaenoic Acid             | 1.1633 |
| Pregnenolone                      | 1.1633 |
| 2,6-Dibromophenol                 | 1.1569 |
| Phenylpropionic acid              | 1.1536 |
| Paraxanthine                      | 1.1504 |
| Methyl anisate                    | 1.1375 |
| Arachidic acid                    | 1.1375 |
| (S)-Malic acid                    | 1.1311 |
| 3-Methyl-2-oxobutanoic acid       | 1.1311 |
| (S)-(+)-1,2-Propanediol           | 1.1311 |
| Methyl Paraben                    | 1.1311 |
| 1,2-Cyclohexanedione              | 1.1279 |
| Chenodeoxycholic Acid             | 1.1279 |
| LysoPC(14:0/0:0)                  | 1.1279 |
| H-D-Trp-OH                        | 1.1214 |
| Mesitaldehyde                     | 1.1214 |
| N-Acetyl-L-leucine                | 1.1117 |
| L-SelenoMethionine                | 1.1117 |
| (R)-pyrrolidine-2-carboxylic acid | 1.1085 |
| Lauric acid                       | 1.1053 |
| 2,4-Di-tert-butylphenol           | 1.1021 |
| $\gamma$ -Cyclodextrin            | 1.1021 |
| Linoleic acid                     | 1.0956 |
| Elaidic acid                      | 1.0924 |
| 4-Pentenoic acid                  | 1.0924 |
| Glycyl-L-valine                   | 1.0892 |
| Estradiol                         | 1.0892 |
| Pregnenolone monosulfate          | 1.0892 |
| Androsterone                      | 1.0795 |

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|----------------------------------|--------|
| Adipic acid                      | 1.0795 |
| Diethyl phosphate                | 1.0731 |
| 2-Methylsuccinic acid            | 1.0699 |
| Docosaehaenoic Acid              | 1.0699 |
| 2-Hydroxyphenylacetic acid       | 1.0602 |
| Uracil                           | 1.0602 |
| 3-Hydroxypicolinic acid          | 1.0602 |
| Cysteamine (hydrochloride)       | 1.0570 |
| Diphenyl disulfide               | 1.0570 |
| Eriodictyol                      | 1.0570 |
| 2-Hydroxy-4-methylbenzaldehyde   | 1.0505 |
| SY-640                           | 1.0473 |
| 3-Methyladipic acid              | 1.0441 |
| 2-O-Methylcytosine               | 1.0408 |
| 7-Methylxanthine                 | 1.0408 |
| Cholestenone                     | 1.0408 |
| 11-Beta-hydroxyandrostenedione   | 1.0408 |
| Bisphenol A                      | 1.0408 |
| 2-Hydroxy-2-methylbutanoic acid  | 1.0376 |
| Cyclohexaneacetic acid           | 1.0312 |
| Tetrahydrobiopterin              | 1.0247 |
| Medroxyprogesterone acetate      | 1.0247 |
| Imidazol-1-yl-acetic acid        | 1.0247 |
| 4-Methoxybenzaldehyde            | 1.0215 |
| 2-Methylbenzaldehyde             | 1.0215 |
| N-Acetylputrescine hydrochloride | 1.0183 |
| Nudifloramide                    | 1.0183 |
| D-Alanine                        | 1.0183 |
| 2-Oxovaleric acid                | 1.0151 |
| 3-Methyl-2-oxovaleric acid       | 1.0151 |
| 1-Hydroxyoctadecane              | 1.0086 |
| Oxalic Acid                      | 1.0054 |
| Orotic acid                      | 1.0054 |
| 3-Methylxanthine                 | 1.0054 |
| 5'-Guanylic acid (disodium salt) | 1.0022 |
| Dinoprost                        | 1.0022 |
| Ara-C                            | 1.0000 |
| 2,6-Dihydroxyacetophenone        | 0.9990 |
| Crustecdysone                    | 0.9893 |
| 5,6-Dihydroxyindole              | 0.9893 |
| alpha-D-glucose                  | 0.9893 |
| D-Sorbitol                       | 0.9893 |
| Histamine                        | 0.9893 |

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|----------------------------------|--------|
| Aminomalonic acid                | 0.9893 |
| Isethionic acid                  | 0.9861 |
| 2-Acetyl-3-ethylpyrazine         | 0.9861 |
| C16-PAF                          | 0.9861 |
| Uridine 5'-monophosphate         | 0.9828 |
| 2-Ethylpyrazine                  | 0.9828 |
| 8-Hydroxy-2'-deoxyguanosine      | 0.9828 |
| D-Glucuronic acid                | 0.9828 |
| D-Arabitol                       | 0.9828 |
| Cytidine                         | 0.9828 |
| Oxytetracycline                  | 0.9796 |
| Xanthine                         | 0.9796 |
| L-Hydroxyproline                 | 0.9796 |
| N-Acetyl-L-phenylalanine         | 0.9764 |
| Uridine                          | 0.9732 |
| L-Citrulline                     | 0.9732 |
| Lithocholic acid                 | 0.9700 |
| Phenoxyacetic acid               | 0.9700 |
| 2-Phenylacetamide                | 0.9667 |
| D-(+)-Phenyllactic acid          | 0.9667 |
| Valdecocix                       | 0.9667 |
| Dimethylmalonic acid             | 0.9635 |
| DL-Mevalonolactone               | 0.9635 |
| Methoxyacetic acid               | 0.9603 |
| DL-Asparagine                    | 0.9603 |
| H-Phe-Phe-OH                     | 0.9603 |
| 1-Octanol                        | 0.9571 |
| DPPC                             | 0.9571 |
| Dichlorisone acetate             | 0.9571 |
| Citicoline                       | 0.9506 |
| Xylose                           | 0.9506 |
| Phosphocreatine (disodium)       | 0.9474 |
| 4-Hydroxycoumarin                | 0.9410 |
| Isoprenaline (hydrochloride)     | 0.9377 |
| D-Pipecolinic acid               | 0.9377 |
| 1,4-Dimethoxybenzene             | 0.9377 |
| 4-Hydroxybenzyl cyanide          | 0.9377 |
| 12-Hydroxydodecanoic acid        | 0.9345 |
| Melanin                          | 0.9345 |
| 17 $\alpha$ -Hydroxyprogesterone | 0.9313 |
| (R,R)-(+)-Hydrobenzoin           | 0.9313 |
| Dodecanedioic acid               | 0.9313 |
| L-Tryptophan                     | 0.9313 |

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|---------------------------------------|--------|
| Oxoadipic acid                        | 0.9313 |
| D-Panthenol                           | 0.9281 |
| Guanidine (hydrochloride)             | 0.9281 |
| TRIA-662                              | 0.9281 |
| Genistein                             | 0.9248 |
| (E)-Ferulic acid                      | 0.9248 |
| L-Alanyl-L-leucine                    | 0.9248 |
| Adrenosterone                         | 0.9155 |
| Nervonic acid                         | 0.9152 |
| Cyclic AMP                            | 0.9152 |
| FAPy-adenine                          | 0.9152 |
| Indolelactic acid                     | 0.9152 |
| Octadecanal                           | 0.9120 |
| Gamma-Linolenic acid                  | 0.9087 |
| Quinolinic acid                       | 0.9087 |
| 10-Undecenoic acid                    | 0.9087 |
| N-Acetyl-L-arginine                   | 0.9055 |
| 2-Naphthol                            | 0.9055 |
| 3,5-Dihydroxyacetophenone             | 0.9055 |
| 7-Methylguanosine                     | 0.9023 |
| L-Glutamic acid                       | 0.9000 |
| 3-Hydroxyphenylacetic acid            | 0.8991 |
| 2-(1H-Indol-3-yl)ethan-1-ol           | 0.8991 |
| N-Acetyl-L-tyrosine                   | 0.8991 |
| 2'-Deoxyguanosine                     | 0.8991 |
| Prostaglandin E2                      | 0.8991 |
| Undecanedioic acid                    | 0.8958 |
| Kinetensin                            | 0.8926 |
| D-Mannose                             | 0.8926 |
| Palmitoleic acid                      | 0.8926 |
| 3-Methylbut-2-enoic acid              | 0.8926 |
| 6-Hydroxynicotinic acid               | 0.8926 |
| Triolein                              | 0.8894 |
| 3-Indolepropionic acid                | 0.8894 |
| 6-Thioguanine                         | 0.8894 |
| Thymine                               | 0.8894 |
| 3-Hydroxyhippuric acid                | 0.8894 |
| Phthalic acid mono-2-ethylhexyl ester | 0.8862 |
| Phenylephrine (hydrochloride)         | 0.8733 |
| 2-hydroxymethyl benzoic acid          | 0.8733 |
| p-Synephrine                          | 0.8701 |
| D-(+)-Cellobiose                      | 0.8668 |
| L-Methionine sulfoxide                | 0.8668 |

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|---------------------------------|--------|
| Suberic acid                    | 0.8604 |
| 3-Methoxytyramine               | 0.8604 |
| N-Acetylglycine                 | 0.8604 |
| 3-Hydroxyvaleric acid           | 0.8604 |
| Purine                          | 0.8572 |
| Homovanillic acid               | 0.8572 |
| Isomaltose                      | 0.8572 |
| Pantethine                      | 0.8539 |
| H-Gly-Pro-OH                    | 0.8539 |
| 5-Aminosalicylic Acid           | 0.8456 |
| Pyruvic acid                    | 0.8449 |
| Uric acid                       | 0.8443 |
| (-)-Menthol                     | 0.8443 |
| Delta-Tocopherol                | 0.8411 |
| Tetrahydrothiophen-3-one        | 0.8411 |
| Terephthalic acid               | 0.8378 |
| Caffeic acid                    | 0.8378 |
| i-Inositol                      | 0.8378 |
| L-Palmitoylcarnitine (chloride) | 0.8378 |
| 1-Methyl-L-histidine            | 0.8378 |
| Cholic acid                     | 0.8346 |
| 5-Hydroxytryptophan             | 0.8317 |
| O-Acetylserine                  | 0.8314 |
| 2(5H)-Furanone                  | 0.8282 |
| H-Val-Tyr-OH                    | 0.8282 |
| L-Gulono-1,4-lactone            | 0.8282 |
| Phosphorylethanolamine          | 0.8249 |
| Cytosine                        | 0.8217 |
| Alanylphenylalanine             | 0.8217 |
| L-Valyl-L-phenylalanine         | 0.8185 |
| Isovaleric acid                 | 0.8185 |
| 5-Methyltetrahydrofolic acid    | 0.8153 |
| L-Methionine                    | 0.8088 |
| Kynurenic acid                  | 0.8056 |
| Nepsilon-Acetyl-L-lysine        | 0.8056 |
| 3-Methoxybenzoic acid           | 0.8024 |
| N-Methylnicotinamide            | 0.8024 |
| Sphingomyelin                   | 0.8024 |
| p-Tolualdehyde                  | 0.7992 |
| Cysteinylglycine (TFA)          | 0.7992 |
| Desaminotyrosine                | 0.7959 |
| Daidzein                        | 0.7959 |
| Phenylpyruvic acid              | 0.7959 |

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|-------------------------------------|--------|
| 4-Aminohippuric acid                | 0.7927 |
| Maltotetraose                       | 0.7927 |
| L-Kynurenine                        | 0.7895 |
| D-Desthiobiotin                     | 0.7872 |
| L-Isoleucine                        | 0.7863 |
| Perillartine                        | 0.7798 |
| 3-Chloro-L-tyrosine                 | 0.7798 |
| Phloretin                           | 0.7776 |
| L-Dihydroorotic acid                | 0.7766 |
| 2-Piperidone                        | 0.7766 |
| Sarcosine                           | 0.7734 |
| Decanedioic acid                    | 0.7702 |
| 2,5-Furandicarboxylic acid          | 0.7702 |
| Lecithin                            | 0.7669 |
| 2-Methylcitric acid                 | 0.7669 |
| DL-3-Phenyllactic acid              | 0.7669 |
| 4-Amino-L-phenylalanine             | 0.7669 |
| H-HoArg-OH                          | 0.7669 |
| Indole-3-acetamide                  | 0.7628 |
| Methylmalonic acid                  | 0.7605 |
| D(-)-2-Aminobutyric acid            | 0.7605 |
| Ergothioneine                       | 0.7602 |
| meso-Erythritol                     | 0.7576 |
| (Ethoxymethyl)benzene               | 0.7573 |
| Taurolithocholic acid (sodium salt) | 0.7573 |
| Hydrocinnamic acid                  | 0.7573 |
| Octanoic acid                       | 0.7547 |
| Triacetin                           | 0.7541 |
| Nicotinuric acid                    | 0.7541 |
| Cholesterol                         | 0.7541 |
| L-Thyroxine                         | 0.7508 |
| Pyrocatechuic acid                  | 0.7508 |
| Citraconic acid                     | 0.7476 |
| (Z)-Aconitic acid                   | 0.7476 |
| L-Histidine                         | 0.7476 |
| 2'-Deoxyinosine                     | 0.7476 |
| Scyllo-Inositol                     | 0.7463 |
| DL-Norvaline                        | 0.7444 |
| Gamma-glutamylcysteine              | 0.7444 |
| Ascorbyl palmitate                  | 0.7412 |
| 3-Hydroxyisobutyric acid            | 0.7399 |
| L-DABA                              | 0.7376 |
| Deoxycholic acid sodium salt        | 0.7354 |

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|--------------------------------|--------|
| 3,5-Dihydroxybenzoic acid      | 0.7299 |
| Nicotinamide N-oxide           | 0.7270 |
| (S)-3-Hydroxybutanoic acid     | 0.7254 |
| 5-Hydroxytryptophol            | 0.7250 |
| L-Homocysteine                 | 0.7250 |
| D-Ribose(mixture of isomers)   | 0.7231 |
| Dihydrodaidzein                | 0.7218 |
| 3-Hydroxyisovaleric acid       | 0.7218 |
| 2,3,5-Trimethylpyrazine        | 0.7218 |
| 4-Ethylphenol                  | 0.7218 |
| N-Acetylmethionine             | 0.7212 |
| Pyridoxal phosphate            | 0.7196 |
| Ellagic acid                   | 0.7186 |
| L-Arginine                     | 0.7186 |
| Glycolic acid                  | 0.7154 |
| 4-Hydroxy-3-methylbenzoic acid | 0.7122 |
| 3-Indoleacetonitrile           | 0.7086 |
| 3,4-Dimethoxyphenylacetic acid | 0.7070 |
| D-Mannitol                     | 0.7067 |
| 4-Hydroxyphenylacetic acid     | 0.7064 |
| γ-Aminobutyric acid            | 0.7057 |
| Ethyl glucuronide              | 0.7057 |
| Beta-Cortol                    | 0.7025 |
| L-Glutamine                    | 0.7025 |
| Glycylglycine                  | 0.7025 |
| 4-Hydroxymethylpyrazole        | 0.7012 |
| p-Anisic acid                  | 0.7006 |
| trans-Vaccenic acid            | 0.6993 |
| Butylparaben                   | 0.6993 |
| Urocanic acid                  | 0.6960 |
| Spaglumic Acid                 | 0.6931 |
| 3-Nitro-L-tyrosine             | 0.6928 |
| Thiamine (hydrochloride)       | 0.6919 |
| L-Cystathionine                | 0.6915 |
| Ethoxyacetic acid              | 0.6915 |
| TFAP                           | 0.6893 |
| Anserine                       | 0.6880 |
| N-Acetylhistamine              | 0.6864 |
| L-Homoserine                   | 0.6864 |
| 3-Indoleacetic acid            | 0.6848 |
| Isovalerylcarnitine            | 0.6838 |
| Ethylmalonic acid              | 0.6799 |
| Urea                           | 0.6793 |

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|-----------------------------------------------|--------|
| Vanilpyruvic acid                             | 0.6790 |
| Glycohyodeoxycholic acid                      | 0.6786 |
| Thyroxine sulfate                             | 0.6761 |
| Hyodeoxycholic acid                           | 0.6761 |
| L-Proline                                     | 0.6761 |
| 5,6-Dihydro-5-methyluracil                    | 0.6757 |
| 5-Amino-3H-imidazole-4-Carboxamide            | 0.6741 |
| L-Ascorbic acid 2-phosphate (trisodium)       | 0.6732 |
| 4,6-O-Ethylidene- $\alpha$ -D-glucose         | 0.6728 |
| 4-Carboxypyrazole                             | 0.6719 |
| Linalool                                      | 0.6706 |
| Theophylline                                  | 0.6699 |
| Pseudouridine                                 | 0.6696 |
| L-Valine                                      | 0.6690 |
| Creatinine                                    | 0.6674 |
| 3-Methylglutaric acid                         | 0.6670 |
| Cholesteryl palmitate                         | 0.6638 |
| Cholesteryl oleate                            | 0.6622 |
| Pregnanediol                                  | 0.6616 |
| 4-Methyl-1-phenyl-2-pentanone                 | 0.6603 |
| Folic acid                                    | 0.6593 |
| Phosphorylcholine                             | 0.6587 |
| Allantoin                                     | 0.6580 |
| 5,6-Dihydrouridine                            | 0.6554 |
| Glycochenodeoxycholic acid                    | 0.6532 |
| H-Tyr(3-I)-OH                                 | 0.6516 |
| $\alpha$ -Vitamin E                           | 0.6509 |
| Tauroursodeoxycholate                         | 0.6506 |
| Ferulic acid                                  | 0.6503 |
| Methyl cyclohexanecarboxylate                 | 0.6467 |
| L-Alloisoleucine                              | 0.6458 |
| 2,5-Dihydroxybenzoic acid                     | 0.6448 |
| N6-Methyladenosine                            | 0.6442 |
| 4-Methyl-2-oxopentanoic acid                  | 0.6438 |
| 3b-Hydroxy-5-cholenoic acid                   | 0.6435 |
| N-Methylhydantoin                             | 0.6390 |
| Nicotinamide                                  | 0.6390 |
| Lipoic acid                                   | 0.6368 |
| DL-Glutamine                                  | 0.6368 |
| 1,5-Anhydrosorbitol                           | 0.6342 |
| 2'-Deoxyadenosine-5'-triphosphate (trisodium) | 0.6329 |
| Nerolidol                                     | 0.6313 |
| Glutathione oxidized                          | 0.6293 |

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| 3,4-Dihydroxybenzeneacetic acid      | 0.6290 |
| SAH                                  | 0.6274 |
| Myristic acid                        | 0.6274 |
| Norharmane                           | 0.6252 |
| 1,3-Dithiane                         | 0.6248 |
| L-Aspartic acid                      | 0.6203 |
| Isohomovanillic acid                 | 0.6187 |
| 5-Methoxytryptophol                  | 0.6181 |
| Citric acid                          | 0.6181 |
| D-(+)-Glucono-1,5-lactone            | 0.6136 |
| Deoxycholic acid                     | 0.6129 |
| $\beta$ -Alanine                     | 0.6074 |
| Cytidine-5'-triphosphate             | 0.6068 |
| L-Ornithine                          | 0.6065 |
| (S)-2-Hydroxy-3-phenylpropanoic acid | 0.6049 |
| 3-Hydroxyglutaric acid               | 0.6049 |
| Pipecolic acid                       | 0.6049 |
| Leucyl-phenylalanine                 | 0.6013 |
| L-Norleucine                         | 0.6000 |
| 5-Aminovaleric acid                  | 0.5968 |
| 3-Amino-2-piperidinone               | 0.5955 |
| Maltose                              | 0.5904 |
| N-(5-Aminopentyl)acetamide           | 0.5897 |
| Succinic acid                        | 0.5894 |
| D-(+)-Trehalose                      | 0.5871 |
| Phenylacetylglutamine                | 0.5868 |
| L-Cysteine                           | 0.5865 |
| Chondroitin (sulfate)                | 0.5862 |
| 5-Hydroxy-2'-deoxyuridine            | 0.5817 |
| L-Threonine                          | 0.5813 |
| 3,4-Dihydroxymandelic acid           | 0.5807 |
| Methionine sulfoxide                 | 0.5788 |
| DL-Homocysteine                      | 0.5781 |
| Oleic acid                           | 0.5775 |
| 3-Methyluridine                      | 0.5759 |
| 4-Hydroxybenzoic acid                | 0.5759 |
| Coproporphyrin III                   | 0.5710 |
| sn-Glycerol 3-phosphate              | 0.5678 |
| NSC 16590                            | 0.5659 |
| 5-Methylcytosine                     | 0.5655 |
| 2-Methylacetophenone                 | 0.5646 |
| Creatine                             | 0.5626 |
| DL-Tryptophan                        | 0.5617 |

|                                              |        |
|----------------------------------------------|--------|
| Dehydrocholate (sodium)                      | 0.5601 |
| 4-Acetamidobutanoic acid                     | 0.5581 |
| Natamycin                                    | 0.5575 |
| 3-Methylcrotonylglycine                      | 0.5552 |
| Pyrogallol                                   | 0.5549 |
| Aminoadipic acid                             | 0.5539 |
| Homogentisic acid                            | 0.5504 |
| Myricetin                                    | 0.5488 |
| 3-Hydroxyanthranilic acid                    | 0.5485 |
| Glutaric acid                                | 0.5481 |
| Thiamine pyrophosphate                       | 0.5468 |
| Maleic Acid                                  | 0.5462 |
| Indole                                       | 0.5452 |
| 5-Aminolevulinic acid (hydrochloride)        | 0.5436 |
| Dihydrouracil                                | 0.5427 |
| Xanthosine                                   | 0.5420 |
| H-Abu-OH                                     | 0.5388 |
| Guanosine 5'-diphosphate (disodium salt)     | 0.5365 |
| Maltotriose                                  | 0.5362 |
| Butyrylcarnitine                             | 0.5349 |
| Propofol                                     | 0.5311 |
| 7,8-Dihydro-L-biopterin                      | 0.5291 |
| Dimethyl fumarate                            | 0.5285 |
| 6-Mercaptopurine                             | 0.5272 |
| 1-Methyladenosine                            | 0.5265 |
| Heparan Sulfate                              | 0.5230 |
| Benzylideneacetone                           | 0.5224 |
| D-Serine                                     | 0.5220 |
| 2,6-Diaminoheptanedioic acid                 | 0.5220 |
| Maltohexaose                                 | 0.5195 |
| Hypotaurine                                  | 0.5156 |
| Stearic acid                                 | 0.5117 |
| Dimethyl sulfone                             | 0.5117 |
| 5-Methyluridine                              | 0.5114 |
| Glycodeoxycholic Acid                        | 0.5114 |
| Dehydroepiandrosterone sulfate (sodium salt) | 0.5095 |
| 3-(Methylthio)propionic acid                 | 0.5091 |
| (R)-3-Hydroxybutanoic acid                   | 0.5066 |
| Ergosterol                                   | 0.5040 |
| Acetyl-L-carnitine (hydrochloride)           | 0.5040 |
| 2-Methylpentanedioic acid                    | 0.5014 |
| L-Alanyl-L-glutamine                         | 0.4963 |
| L-Carnosine                                  | 0.4956 |

|                                              |        |
|----------------------------------------------|--------|
| 8-Hydroxyguanosine                           | 0.4937 |
| D-Glutamine                                  | 0.4924 |
| L-Asparagine                                 | 0.4921 |
| 3-Hydroxybutyric acid                        | 0.4905 |
| Riboflavin (phosphate sodium)                | 0.4898 |
| $\beta$ -Nicotinamide mononucleotide         | 0.4872 |
| N2,N2-Dimethylguanosine                      | 0.4866 |
| Selenomethionine                             | 0.4863 |
| Glycine                                      | 0.4859 |
| Niacin                                       | 0.4837 |
| trans-Aconitic acid                          | 0.4824 |
| DL-Homocystine                               | 0.4795 |
| (-)-Fucose                                   | 0.4756 |
| Xylitol                                      | 0.4750 |
| 2-Hydroxyadipic acid                         | 0.4747 |
| Meglutol                                     | 0.4743 |
| 2'-Deoxyuridine                              | 0.4743 |
| Phosphonoacetic acid                         | 0.4718 |
| Substance P                                  | 0.4692 |
| L-Alanine                                    | 0.4682 |
| L-Prolylglycine                              | 0.4640 |
| Benzoic acid                                 | 0.4602 |
| L-Lysine                                     | 0.4563 |
| Ribitol                                      | 0.4550 |
| Galactose 1-phosphate Potassium salt         | 0.4531 |
| Glucosamine                                  | 0.4518 |
| 2-Hydroxy-3-methylbutanoic acid              | 0.4508 |
| $\gamma$ -L-Glutamyl-L-alanine               | 0.4492 |
| Thymidine                                    | 0.4489 |
| D- $\alpha$ -Hydroxyglutaric acid (disodium) | 0.4479 |
| 4-Hydroxybenzyl alcohol                      | 0.4473 |
| L-Phenylalanine                              | 0.4460 |
| Thymidine-5'-monophosphate (disodium) salt   | 0.4434 |
| L-(+)-Arabinose                              | 0.4408 |
| trans-trans-Muconic acid                     | 0.4379 |
| Agmatine (sulfate)                           | 0.4305 |
| Hexadecanedioic acid                         | 0.4296 |
| 3-Amino-2-methylpropanoic acid               | 0.4292 |
| [Leu5]-Enkephalin                            | 0.4205 |
| N-Acetyl-L-aspartic acid                     | 0.4202 |
| p-Coumaric acid                              | 0.4202 |
| L-Homocystine                                | 0.4180 |
| 2-Methoxyestrone                             | 0.4163 |

|                                          |        |
|------------------------------------------|--------|
| Hydrocortisone acetate                   | 0.4157 |
| Guanosine                                | 0.4144 |
| D-Allothreonine                          | 0.4031 |
| N4-Acetylcytidine triphosphate (sodium)  | 0.4022 |
| Dimethyl trisulfide                      | 0.4012 |
| $\gamma$ -Glu-Phe                        | 0.3983 |
| N-Methylsarcosine                        | 0.3947 |
| Uridine-5'-diphosphate disodium salt     | 0.3906 |
| D-Ribonolactone                          | 0.3815 |
| D-(-)-Quinic acid                        | 0.3809 |
| Guanidinosuccinic acid                   | 0.3802 |
| Coenzyme A                               | 0.3786 |
| Norepinephrine                           | 0.3728 |
| Antineoplaston A10                       | 0.3657 |
| N2-Methylguanosine                       | 0.3654 |
| Aceglutamide                             | 0.3596 |
| D-Kynurenine                             | 0.3587 |
| 1-Methylinosine                          | 0.3467 |
| Urolithin B                              | 0.3422 |
| $\beta$ -cyano-L-Alanine                 | 0.3387 |
| Pyrroloquinoline quinone                 | 0.3384 |
| 1-Methylguanosine                        | 0.3271 |
| N1,N8-Diacetylspermidine (hydrochloride) | 0.3219 |
| Dodecanoylcarnitine                      | 0.3190 |
| 4-Methylcatechol                         | 0.3155 |
| Coenzyme Q9                              | 0.3090 |
| Ursocholic acid                          | 0.3055 |
| Maltopentaose                            | 0.2952 |
| 17 $\alpha$ -Hydroxypregnenolone         | 0.2775 |
| Docosanoic acid                          | 0.2681 |
| Dehydroascorbic acid                     | 0.2671 |
| 1-Naphthol                               | 0.2194 |
| 5 $\alpha$ -Cholestan-3 $\beta$ -ol      | 0.2156 |