Table S4 The secondary metabolites with differential fold of more than 2.0 between P-*B. sorokiniana* and W-*B. sorokiniana* strains.

|  |  |  |  |
| --- | --- | --- | --- |
| m/z | fold\_change(A/M) | qvalue | name |
| 59.05005715 | 2.210499358 | 2.72E-05 | NMF; N-Methylformamide; |
| 59.05005715 | 2.210499358 | 2.72E-05 | Haloacetate; |
| 59.05005715 | 2.210499358 | 2.72E-05 | Thiocyanate; Thiocyanic acid; |
| 59.05005715 | 2.210499358 | 2.72E-05 | Guanidine; Carbamidine; |
| 59.05018314 | 3.90380647 | 0.000106094 | NMF; N-Methylformamide; |
| 59.05018314 | 3.90380647 | 0.000106094 | Haloacetate; |
| 59.05018314 | 3.90380647 | 0.000106094 | Thiocyanate; Thiocyanic acid; |
| 59.05018314 | 3.90380647 | 0.000106094 | Guanidine; Carbamidine; |
| 61.02884676 | 3.607523393 | 9.98E-05 | Dihydroxyaluminum; |
| 61.02884676 | 3.607523393 | 9.98E-05 | HCO3-; Bicarbonate; Hydrogen carbonate; Acid carbonate; |
| 61.02884676 | 3.607523393 | 9.98E-05 | Nitromethane; |
| 61.02889247 | 2.86159278 | 0.002160986 | Dihydroxyaluminum; |
| 61.02889247 | 2.86159278 | 0.002160986 | HCO3-; Bicarbonate; Hydrogen carbonate; Acid carbonate; |
| 61.02889247 | 2.86159278 | 0.002160986 | Nitromethane; |
| 74.05888996 | 0.239497912 | 0.00084089 | Triacetylene; 1,3,5-Hexatriyne; |
| 74.05888996 | 0.239497912 | 0.00084089 | Calcium hydroxide; |
| 74.05888996 | 0.239497912 | 0.00084089 | Methyl acetate; Devoton; Tereton; |
| 74.05888996 | 0.239497912 | 0.00084089 | N-Methylurea; Methylurea; |
| 74.05888996 | 0.239497912 | 0.00084089 | Glyoxylate; Glyoxalate; Glyoxylic acid; |
| 74.05888996 | 0.239497912 | 0.00084089 | Ethylnitronate; |
| 74.06001987 | 2.511518292 | 0.003477976 | Triacetylene; 1,3,5-Hexatriyne; |
| 74.06001987 | 2.511518292 | 0.003477976 | Calcium hydroxide; |
| 74.06001987 | 2.511518292 | 0.003477976 | Methyl acetate; Devoton; Tereton; |
| 74.06001987 | 2.511518292 | 0.003477976 | N-Methylurea; Methylurea; |
| 74.06001987 | 2.511518292 | 0.003477976 | Glyoxylate; Glyoxalate; Glyoxylic acid; |
| 74.06001987 | 2.511518292 | 0.003477976 | Ethylnitronate; |
| 74.06020206 | 0.24939252 | 0.000627817 | Triacetylene; 1,3,5-Hexatriyne; |
| 74.06020206 | 0.24939252 | 0.000627817 | Calcium hydroxide; |
| 74.06020206 | 0.24939252 | 0.000627817 | Methyl acetate; Devoton; Tereton; |
| 74.06020206 | 0.24939252 | 0.000627817 | N-Methylurea; Methylurea; |
| 74.06020206 | 0.24939252 | 0.000627817 | Glyoxylate; Glyoxalate; Glyoxylic acid; |
| 74.06020206 | 0.24939252 | 0.000627817 | Ethylnitronate; |
| 99.04331724 | 0.06529797 | 8.82E-08 | Hymexazol; |
| 110.007172 | 0.471385487 | 0.001058094 | Dimethyl hydrogen phosphite; |
| 110.007172 | 0.471385487 | 0.001058094 | Formylphosphonate; Phosphonoformaldehyde; Formylphosphonic acid; |
| 128.1088343 | 0.408626653 | 0.000293652 | Thiouracil; 4-Hydroxy-2-pyrimidinethiol; |
| 128.1088343 | 0.408626653 | 0.000293652 | 4-Fluorocatechol; |
| 128.1088343 | 0.408626653 | 0.000293652 | 1-Methylparabanic acid; Imidazolidinetrione, methyl-; |
| 128.1088343 | 0.408626653 | 0.000293652 | Ammelide; 2,4-Dihydroxy-6-amino-1,3,5-triazine; |
| 128.1088343 | 0.408626653 | 0.000293652 | (R)-5,6-Dihydrothymine; (5R)-Dihydrothymine; |
| 128.1088343 | 0.408626653 | 0.000293652 | 4-Hydroxy-2,5-dimethylfuran-3(2H)-one; Dimethylhydroxy furanone; |
| 128.1088343 | 0.408626653 | 0.000293652 | Calcium oxalate; |
| 140.034334 | 6.625532791 | 1.83E-06 | (S)-2-Hydroxypropylphosphonate; |
| 140.034334 | 6.625532791 | 1.83E-06 | Phosphonoacetate; Phosphonoacetic acid; Fosfonet; |
| 152.030683 | 3.034908452 | 0.000272643 | 3-(Hydrohydroxyphosphoryl)pyruvate; (Hydroxyphosphinyl)pyruvate; |
| 157.0465796 | 0.258733539 | 1.26E-05 | Bromobenzene; |
| 183.9590821 | 0.429612286 | 0.000733849 | Arsonoacetate; |
| 201.1673583 | 15.90056658 | 1.19E-06 | 3-{[(2E)-4-Amino-4-oxobut-2-enoyl]amino}-L-alanine; |
| 215.0198416 | 2.696940037 | 0.000162921 | 4-Bromophenylacetate; 4-Bromophenylacetic acid; |
| 216.1228825 | 0.056160446 | 2.70E-09 | Sodium glucuronate; |
| 216.1228825 | 0.056160446 | 2.70E-09 | 4-Phospho-D-erythronate; 4-Phosphoerythronate; |
| 216.1228825 | 0.056160446 | 2.70E-09 | 2-C-Methyl-D-erythritol 4-phosphate; |
| 216.1228825 | 0.056160446 | 2.70E-09 | S-(1,2-Dichlorovinyl)-L-cysteine; DCVC; |
| 216.1228825 | 0.056160446 | 2.70E-09 | S-Methyl-3-phospho-1-thio-D-glycerate; |
| 216.1228825 | 0.056160446 | 2.70E-09 | 4-Carboxy-2-hydroxy-6-methoxy-6-oxohexa-2,4-dienoate; |
| 219.1701841 | 0.452186812 | 0.019082018 | N-Acetyl-D-mannosaminolactone; |
| 219.1701841 | 0.452186812 | 0.019082018 | 1D-1-Guanidino-1-deoxy-3-dehydro-scyllo-inositol; Amidino-3-keto-scyllo-inosamine; |
| 219.1701841 | 0.452186812 | 0.019082018 | 8-Methoxykynurenate; Xanthurenic acid 8-methyl ether; |
| 219.1701841 | 0.452186812 | 0.019082018 | N(omega)-Nitro-L-arginine; N(G)-Nitro-L-arginine; |
| 219.1701841 | 0.452186812 | 0.019082018 | 4-Amino-2-methyl-5-(phosphooxymethyl)pyrimidine; (4-Amino-2-methylpyrimidin-5-yl)methyl phosphate; 4-Amino-5-hydroxymethyl-2-methylpyrimidine phosphate; |
| 219.1711601 | 0.374537112 | 3.17E-05 | N-Acetyl-D-mannosaminolactone; |
| 219.1711601 | 0.374537112 | 3.17E-05 | 1D-1-Guanidino-1-deoxy-3-dehydro-scyllo-inositol; Amidino-3-keto-scyllo-inosamine; |
| 219.1711601 | 0.374537112 | 3.17E-05 | 8-Methoxykynurenate; Xanthurenic acid 8-methyl ether; |
| 219.1711601 | 0.374537112 | 3.17E-05 | N(omega)-Nitro-L-arginine; N(G)-Nitro-L-arginine; |
| 219.1711601 | 0.374537112 | 3.17E-05 | 4-Amino-2-methyl-5-(phosphooxymethyl)pyrimidine; (4-Amino-2-methylpyrimidin-5-yl)methyl phosphate; 4-Amino-5-hydroxymethyl-2-methylpyrimidine phosphate; |
| 219.1719471 | 0.465383537 | 6.03E-05 | N-Acetyl-D-mannosaminolactone; |
| 219.1719471 | 0.465383537 | 6.03E-05 | 1D-1-Guanidino-1-deoxy-3-dehydro-scyllo-inositol; Amidino-3-keto-scyllo-inosamine; |
| 219.1719471 | 0.465383537 | 6.03E-05 | 8-Methoxykynurenate; Xanthurenic acid 8-methyl ether; |
| 219.1719471 | 0.465383537 | 6.03E-05 | N(omega)-Nitro-L-arginine; N(G)-Nitro-L-arginine; |
| 219.1719471 | 0.465383537 | 6.03E-05 | 4-Amino-2-methyl-5-(phosphooxymethyl)pyrimidine; (4-Amino-2-methylpyrimidin-5-yl)methyl phosphate; 4-Amino-5-hydroxymethyl-2-methylpyrimidine phosphate; |
| 219.1804816 | 10.39957154 | 0.001383218 | Pantothenate; Pantothenic acid; (R)-Pantothenate; |
| 219.1804816 | 10.39957154 | 0.001383218 | N-Acetyl-D-mannosaminolactone; |
| 219.1804816 | 10.39957154 | 0.001383218 | 1D-1-Guanidino-1-deoxy-3-dehydro-scyllo-inositol; Amidino-3-keto-scyllo-inosamine; |
| 219.1804816 | 10.39957154 | 0.001383218 | 8-Methoxykynurenate; Xanthurenic acid 8-methyl ether; |
| 219.1804816 | 10.39957154 | 0.001383218 | N(omega)-Nitro-L-arginine; N(G)-Nitro-L-arginine; |
| 219.1804816 | 10.39957154 | 0.001383218 | 4-Amino-2-methyl-5-(phosphooxymethyl)pyrimidine; (4-Amino-2-methylpyrimidin-5-yl)methyl phosphate; 4-Amino-5-hydroxymethyl-2-methylpyrimidine phosphate; |
| 223.0637701 | 0.448588908 | 0.017514676 | 3,5-Dichlorobiphenyl; PCB 1 |
| 223.0637701 | 0.448588908 | 0.017514676 | 6-Bromo-2-naphthol; |
| 223.0637701 | 0.448588908 | 0.017514676 | Bromisovalum; Bromovalerylurea; |
| 226.182442 | 2.112185596 | 0.000973784 | Genipin; |
| 226.182442 | 2.112185596 | 0.000973784 | Carnosine; Nalpha-(beta-alanyl)-L-histidine; |
| 226.182442 | 2.112185596 | 0.000973784 | Porphobilinogen; |
| 226.182442 | 2.112185596 | 0.000973784 | Isochorismate; Isochorismic acid; |
| 226.182442 | 2.112185596 | 0.000973784 | 5,10-Dihydrophenazine-1-carboxylate; |
| 226.182442 | 2.112185596 | 0.000973784 | 1,3,7-Trimethyl-5-hydroxyisourate; |
| 226.182442 | 2.112185596 | 0.000973784 | Flurecol; |
| 228.1989014 | 2.060686488 | 0.000163818 | Glyphosate-isopropylammonium; |
| 228.1989014 | 2.060686488 | 0.000163818 | (S)-ATPA; |
| 228.1989014 | 2.060686488 | 0.000163818 | Deoxyguanidinoproclavaminic acid; Deoxyguanidinoproclavaminate; Deoxyamidinoproclavaminate; |
| 228.1989014 | 2.060686488 | 0.000163818 | Euxanthone; 1,7-Dihydroxyxanthone; |
| 228.1989014 | 2.060686488 | 0.000163818 | 2-Hydroxy-3-carboxy-6-oxo-7-methylocta-2,4-dienoate; |
| 228.1989014 | 2.060686488 | 0.000163818 | 4,4',6-Trimethylangelicin; |
| 228.1989014 | 2.060686488 | 0.000163818 | Deoxyuridine; 2-Deoxyuridine; 2'-Deoxyuridine; |
| 235.1658272 | 2.486773078 | 4.25E-05 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.1658272 | 2.486773078 | 4.25E-05 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 235.166982 | 0.395307273 | 0.000487349 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.166982 | 0.395307273 | 0.000487349 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 235.1673371 | 0.208939642 | 0.000267093 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.1673371 | 0.208939642 | 0.000267093 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 235.1675831 | 2.520066511 | 0.000144876 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.1675831 | 2.520066511 | 0.000144876 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 235.1675894 | 0.263581179 | 7.91E-07 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.1675894 | 0.263581179 | 7.91E-07 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 235.1890139 | 2.708783426 | 0.02994652 | N-Glycolyl-D-mannosaminolactone; Glycolyl-D-mannosaminolactone; |
| 235.1890139 | 2.708783426 | 0.02994652 | 3,4-Dihydro-7-methoxy-2-methylene-3-oxo-2H-1,4-benzoxazine-5-carboxylic acid; Benzoxazolinate; |
| 237.1772084 | 2.198064999 | 5.11E-06 | Biopterin; 2-Amino-6-(1,2-dihydroxypropyl)-4(1H)-pteridinone; |
| 237.1772084 | 2.198064999 | 5.11E-06 | Pyrido[3,4-c]psoralen; |
| 237.1772084 | 2.198064999 | 5.11E-06 | Dicrotophos; |
| 237.1772084 | 2.198064999 | 5.11E-06 | Glycolyl-D-mannosamine; N-Glycolyl-D-mannosamine; |
| 237.1841558 | 0.322277886 | 0.000268436 | Biopterin; 2-Amino-6-(1,2-dihydroxypropyl)-4(1H)-pteridinone; |
| 237.1841558 | 0.322277886 | 0.000268436 | Pyrido[3,4-c]psoralen; |
| 237.1841558 | 0.322277886 | 0.000268436 | Dicrotophos; |
| 237.1841558 | 0.322277886 | 0.000268436 | Glycolyl-D-mannosamine; N-Glycolyl-D-mannosamine; |
| 238.1831701 | 0.458064781 | 0.001890061 | SQ 2618 |
| 238.1831701 | 0.458064781 | 0.001890061 | Nitrofurantoin; |
| 238.1831701 | 0.458064781 | 0.001890061 | Xanthopterin-B 1-(7,8-Dihydro-2,4-dihydroxypteridin-6-yl)-2-hydroxypropan-1-one; |
| 238.1831701 | 0.458064781 | 0.001890061 | D-erythro-1-(Imidazol-4-yl)glycerol 3-phosphate; D-erythro-Imidazole-glycerol 3-phosphate; D-erythro-Imidazole-glycerol phosphate; |
| 238.1831701 | 0.458064781 | 0.001890061 | Ketodeoxyoctonic acid; Ketodeoxyoctulonic acid; 3-Deoxy-D-manno-oct-2-ulopyranosonic acid; |
| 247.099597 | 0.006116246 | 8.00E-06 | Isocil; |
| 247.099597 | 0.006116246 | 8.00E-06 | Eudistomin N; |
| 247.099597 | 0.006116246 | 8.00E-06 | Pyridoxal phosphate; Pyridoxal 5-phosphate; Pyridoxal 5'-phosphate; PLP; |
| 247.1177438 | 0.0042064 | 4.44E-05 | N-Phosphotaurocyamine; Taurocyamine phosphate; N(omega)-Phosphotaurocyamine; |
| 247.1177438 | 0.0042064 | 4.44E-05 | Isocil; |
| 247.1177438 | 0.0042064 | 4.44E-05 | Eudistomin N; |
| 247.1177438 | 0.0042064 | 4.44E-05 | Pyridoxal phosphate; Pyridoxal 5-phosphate; Pyridoxal 5'-phosphate; PLP; |
| 248.0981936 | 0.005059197 | 6.76E-14 | N-(3,4-Dichlorophenyl)-malonamate; |
| 248.0981936 | 0.005059197 | 6.76E-14 | DCI; Dichloroisoproterenol; |
| 248.1026393 | 0.005114366 | 1.14E-13 | N-(3,4-Dichlorophenyl)-malonamate; |
| 248.1026393 | 0.005114366 | 1.14E-13 | DCI; Dichloroisoproterenol; |
| 250.1814484 | 3.492175555 | 1.05E-06 | Diflunisal; |
| 250.1814484 | 3.492175555 | 1.05E-06 | 2-Hydroxy-6-oxo-6-(2-hydroxyphenoxy)-hexa-2,4-dienoate; |
| 250.1814484 | 3.492175555 | 1.05E-06 | Blue pigment; Nicotine blue; (E)-2,2',5,5'-Tetrahydroxy-6H,6'H-[3,3'-bipyridinylidene]-6,6'-dione; |
| 252.1633358 | 0.479467933 | 0.000495734 | Anatoxin a(s); Anatoxin-A(S); Phosphoric acid, mono[(5S)-2-amino-5-[(dimethylamino)methyl]-4,5-dihydro-1H-imidazol-1-yl] monomethyl ester; |
| 252.1633358 | 0.479467933 | 0.000495734 | 3,3'-Bipyridine-2,2',5,5',6,6'-hexol; |
| 262.2124165 | 3.198775385 | 0.004103626 | 5-Fluorouridine; |
| 262.2124165 | 3.198775385 | 0.004103626 | Ornaline; Nopalinic acid; |
| 262.2124165 | 3.198775385 | 0.004103626 | 2-Hydroxy-6-oxo-6-(2-carboxyphenyl)-hexa-2,4-dienoate; |
| 262.2124165 | 3.198775385 | 0.004103626 | Cinoxacin; |
| 262.2124165 | 3.198775385 | 0.004103626 | Bentazone-sodium; |
| 264.2303333 | 0.454213719 | 0.000525056 | Tulobuterol hydrochloride; |
| 264.2303333 | 0.454213719 | 0.000525056 | Bluensidine; |
| 264.2303333 | 0.454213719 | 0.000525056 | Frutinone A; |
| 264.2303333 | 0.454213719 | 0.000525056 | 1'-Acetoxyeugenol acetate; |
| 264.2303333 | 0.454213719 | 0.000525056 | 1-(4-Hydroxyphenylazo)-2-naphthol; 4'-OH-Sudan I; |
| 264.2303333 | 0.454213719 | 0.000525056 | Formyl-N-acetyl-5-methoxykynurenamine; |
| 264.2324825 | 0.160450745 | 4.72E-05 | Tulobuterol hydrochloride; |
| 264.2324825 | 0.160450745 | 4.72E-05 | Bluensidine; |
| 264.2324825 | 0.160450745 | 4.72E-05 | Frutinone A; |
| 264.2324825 | 0.160450745 | 4.72E-05 | 1'-Acetoxyeugenol acetate; |
| 264.2324825 | 0.160450745 | 4.72E-05 | 1-(4-Hydroxyphenylazo)-2-naphthol; 4'-OH-Sudan I; |
| 264.2324825 | 0.160450745 | 4.72E-05 | Formyl-N-acetyl-5-methoxykynurenamine; |
| 264.6630374 | 0.366699184 | 0.037006631 | Ozagrel hydrochloride; |
| 265.2261472 | 0.131968575 | 0.003144084 | 5'-Dehydroadenosine; |
| 265.2261472 | 0.131968575 | 0.003144084 | N6-Methyl-2'-deoxyadenosine; |
| 265.2261472 | 0.131968575 | 0.003144084 | Isoniazid alpha-ketoglutaric acid; |
| 265.2261472 | 0.131968575 | 0.003144084 | Streptozocin; Zanosar; |
| 265.2261472 | 0.131968575 | 0.003144084 | Anhydrolycorinone; |
| 266.1669171 | 0.121682697 | 0.003725147 | 5'-Oxoinosine; 5'-Dehydroinosine; |
| 266.1669171 | 0.121682697 | 0.003725147 | Dinex; |
| 267.1601528 | 2.05946737 | 0.000401706 | Chlorfenethol; |
| 267.1601528 | 2.05946737 | 0.000401706 | 4,4'-Methylene-bis-(2-chloroaniline); Methylenebis(chloroaniline); MOCA; |
| 267.1601528 | 2.05946737 | 0.000401706 | 2-(2-Carboxy-4-methylthiazol-5-yl)ethyl phosphate; 4-Methyl-5-[2-(phosphonooxy)ethyl]-1,3-thiazole-2-carboxylate; cThz-P; |
| 268.1048272 | 5.382326382 | 1.94E-05 | 2,6-Dichloroindophenol; 2,6-Dichlorophenolindophenol; DCIP; |
| 277.0858359 | 2.418521249 | 2.49E-05 | N'-Phosphoguanidinoethyl methyl phosphate; |
| 277.0858359 | 2.418521249 | 2.49E-05 | Aldoifosfamide; |
| 277.0917122 | 2.971036235 | 1.91E-05 | N'-Phosphoguanidinoethyl methyl phosphate; |
| 277.0917122 | 2.971036235 | 1.91E-05 | Aldoifosfamide; |
| 287.2138505 | 0.31202242 | 0.00011407 | Indoleglycerol phosphate; 1-C-(Indol-3-yl)glycerol 3-phosphate; (3-Indolyl)-glycerol phosphate; C1-(3-Indolyl)-glycerol 3-phosphate; (1S,2R)-1-C-(Indol-3-yl)glycerol 3-phosphate; Indole-3-glycerol phosphate; |
| 287.2138505 | 0.31202242 | 0.00011407 | Aurantinidin; |
| 292.2005372 | 0.167078495 | 3.89E-10 | 1,3-Dinitropyrene; |
| 292.2005372 | 0.167078495 | 3.89E-10 | EDTA; Ethylenediaminetetraacetic acid; Edetic acid; |
| 292.2005372 | 0.167078495 | 3.89E-10 | Hydroxyflutamide; |
| 296.2354548 | 0.404741608 | 0.001099177 | Phaseolic acid; |
| 296.2354548 | 0.404741608 | 0.001099177 | 3,3'-Dimethoxybenzidine-4,4'-diisocyanate; |
| 296.2354548 | 0.404741608 | 0.001099177 | Aspulvinone E; (5Z)-4-Hydroxy-3-(4-hydroxyphenyl)-5-[(4-hydroxyphenyl)methylene]-2(5H)-furanone; |
| 296.2354548 | 0.404741608 | 0.001099177 | Medinoterb acetate; |
| 296.2354548 | 0.404741608 | 0.001099177 | Dehypoxanthine futalosine; |
| 296.2354548 | 0.404741608 | 0.001099177 | 2-Methylaminoadenosine; |
| 306.246404 | 5.510886713 | 0.000331439 | Sertraline; |
| 306.246404 | 5.510886713 | 0.000331439 | 2-Protocatechoylphloroglucinolcarboxylate; 2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate; |
| 306.246404 | 5.510886713 | 0.000331439 | Kinobscurinone; 4,9-Dihydroxy-2-methyl-11H-benzo[b]fluorene-5,10,11-trione; |
| 306.246404 | 5.510886713 | 0.000331439 | (-)-Epigallocatechin; Epigallocatechol; |
| 306.246404 | 5.510886713 | 0.000331439 | 4-Carboxy-4'-sulfoazobenzene; |
| 306.246404 | 5.510886713 | 0.000331439 | 4-(beta-D-Ribofuranosyl)phenol 5'-phosphate; |
| 308.2173712 | 2.156380212 | 0.000171911 | dUMP; Deoxyuridylic acid; Deoxyuridine monophosphate; Deoxyuridine 5'-phosphate; 2'-Deoxyuridine 5'-phosphate; |
| 309.2150195 | 0.374734448 | 0.000351817 | Aplysinal; |
| 309.2150195 | 0.374734448 | 0.000351817 | p,p'-Methoxychlor olefin; 1,1-Dichloro-2,2-bis(p-methoxyphenyl)ethylene; 1,1-Bis(p-methoxyphenyl)-2,2-dichloroethylene; |
| 310.2041441 | 0.165531681 | 0.00076315 | Tricalcium phosphate; Calcium phosphate tribasic; Synthos; |
| 310.2314712 | 0.155197783 | 0.001376992 | Acromelic acid A; |
| 310.2314712 | 0.155197783 | 0.001376992 | 6-Demethylsterigmatocystin; |
| 322.1990135 | 25.31697826 | 3.85E-09 | CGH 246 |
| 322.1990135 | 25.31697826 | 3.85E-09 | Digallate; Digallic acid; |
| 322.1990135 | 25.31697826 | 3.85E-09 | dTMP; Thymidine 5'-phosphate; Deoxythymidine 5'-phosphate; Thymidylic acid; 5'-Thymidylic acid; Thymidine monophosphate; Deoxythymidylic acid; Thymidylate; |
| 322.1990135 | 25.31697826 | 3.85E-09 | Dinitramine; |
| 322.2028136 | 25.21572006 | 3.15E-10 | CGH 246 |
| 322.2028136 | 25.21572006 | 3.15E-10 | Digallate; Digallic acid; |
| 322.2028136 | 25.21572006 | 3.15E-10 | dTMP; Thymidine 5'-phosphate; Deoxythymidine 5'-phosphate; Thymidylic acid; 5'-Thymidylic acid; Thymidine monophosphate; Deoxythymidylic acid; Thymidylate; |
| 322.2028136 | 25.21572006 | 3.15E-10 | Dinitramine; |
| 327.2193115 | 0.25897763 | 0.000341255 | Fluazifop; |
| 327.2413277 | 0.125140194 | 0.001694587 | Fluazifop; |
| 327.2413277 | 0.125140194 | 0.001694587 | Robenacoxib; |
| 338.3362135 | 0.447194989 | 0.003872018 | Demethoxycurcumin; |
| 338.3362135 | 0.447194989 | 0.003872018 | Ustalic acid; |
| 338.3362135 | 0.447194989 | 0.003872018 | Aziridyl benzoquinone; Benzoquinone aziridine; |
| 338.3362135 | 0.447194989 | 0.003872018 | p-Coumaroyl quinic acid; trans-5-O-(4-Coumaroyl)-D-quinate; |
| 338.3362135 | 0.447194989 | 0.003872018 | 1-Peroxyferolide; |
| 338.3362135 | 0.447194989 | 0.003872018 | Jatrorrhizine; |
| 338.3362135 | 0.447194989 | 0.003872018 | Sodium caffeine benzoate; |
| 338.3362135 | 0.447194989 | 0.003872018 | Alamarine; |
| 339.3092401 | 0.499937974 | 0.000257396 | N,6-O-Disulfo-D-glucosamine; N2,6-Disulfo-D-glucosamine; |
| 339.3092401 | 0.499937974 | 0.000257396 | Vulgaxanthin-I; |
| 347.1787724 | 0.077520557 | 2.26E-06 | S-Seven; O-Ethyl O-2,4-dichlorophenyl thionobenzenephosphonate; EPBP; |
| 347.1787724 | 0.077520557 | 2.26E-06 | 2-Hydroxy-dAMP; |
| 352.3313801 | 0.147934293 | 6.55E-05 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3313801 | 0.147934293 | 6.55E-05 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3313801 | 0.147934293 | 6.55E-05 | Fortimicin KL |
| 352.3313801 | 0.147934293 | 6.55E-05 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3313801 | 0.147934293 | 6.55E-05 | Savinin; |
| 352.3313801 | 0.147934293 | 6.55E-05 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3313801 | 0.147934293 | 6.55E-05 | Berberastine; |
| 352.3315782 | 0.194007482 | 0.006430118 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3315782 | 0.194007482 | 0.006430118 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3315782 | 0.194007482 | 0.006430118 | Fortimicin KL |
| 352.3315782 | 0.194007482 | 0.006430118 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3315782 | 0.194007482 | 0.006430118 | Savinin; |
| 352.3315782 | 0.194007482 | 0.006430118 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3315782 | 0.194007482 | 0.006430118 | Berberastine; |
| 352.3318025 | 0.176981944 | 0.000279166 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3318025 | 0.176981944 | 0.000279166 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3318025 | 0.176981944 | 0.000279166 | Fortimicin KL |
| 352.3318025 | 0.176981944 | 0.000279166 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3318025 | 0.176981944 | 0.000279166 | Savinin; |
| 352.3318025 | 0.176981944 | 0.000279166 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3318025 | 0.176981944 | 0.000279166 | Berberastine; |
| 352.3319775 | 0.188120143 | 0.000224073 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3319775 | 0.188120143 | 0.000224073 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3319775 | 0.188120143 | 0.000224073 | Fortimicin KL |
| 352.3319775 | 0.188120143 | 0.000224073 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3319775 | 0.188120143 | 0.000224073 | Savinin; |
| 352.3319775 | 0.188120143 | 0.000224073 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3319775 | 0.188120143 | 0.000224073 | Berberastine; |
| 352.3322077 | 0.189559987 | 0.000181112 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3322077 | 0.189559987 | 0.000181112 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3322077 | 0.189559987 | 0.000181112 | Fortimicin KL |
| 352.3322077 | 0.189559987 | 0.000181112 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3322077 | 0.189559987 | 0.000181112 | Savinin; |
| 352.3322077 | 0.189559987 | 0.000181112 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3322077 | 0.189559987 | 0.000181112 | Berberastine; |
| 352.3339229 | 0.476563382 | 0.021699884 | Deacetylepithienamycin F; Deacetyl MM 1788 NA 2697 |
| 352.3339229 | 0.476563382 | 0.021699884 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3339229 | 0.476563382 | 0.021699884 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3339229 | 0.476563382 | 0.021699884 | Fortimicin KL |
| 352.3339229 | 0.476563382 | 0.021699884 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3339229 | 0.476563382 | 0.021699884 | Savinin; |
| 352.3339229 | 0.476563382 | 0.021699884 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3339229 | 0.476563382 | 0.021699884 | Berberastine; |
| 352.3394252 | 0.167136459 | 0.00030125 | Deacetylepithienamycin F; Deacetyl MM 1788 NA 2697 |
| 352.3394252 | 0.167136459 | 0.00030125 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3394252 | 0.167136459 | 0.00030125 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3394252 | 0.167136459 | 0.00030125 | Fortimicin KL |
| 352.3394252 | 0.167136459 | 0.00030125 | Sudan III; C.I. Solvent Red 2 |
| 352.3394252 | 0.167136459 | 0.00030125 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3394252 | 0.167136459 | 0.00030125 | Savinin; |
| 352.3394252 | 0.167136459 | 0.00030125 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3394252 | 0.167136459 | 0.00030125 | Berberastine; |
| 352.3417706 | 0.194138856 | 0.007235445 | Deacetylepithienamycin F; Deacetyl MM 1788 NA 2697 |
| 352.3417706 | 0.194138856 | 0.007235445 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3417706 | 0.194138856 | 0.007235445 | 4-Methylumbelliferone glucuronide; 4-Methylumbelliferyl glucuronide; |
| 352.3417706 | 0.194138856 | 0.007235445 | Fortimicin KL |
| 352.3417706 | 0.194138856 | 0.007235445 | Sudan III; C.I. Solvent Red 2 |
| 352.3417706 | 0.194138856 | 0.007235445 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3417706 | 0.194138856 | 0.007235445 | Savinin; |
| 352.3417706 | 0.194138856 | 0.007235445 | Coumestrol diacetate; 3,9-Diacetoxy-6H-benzofuro[3,2-c][1]benzopyran-6-one; |
| 352.3417706 | 0.194138856 | 0.007235445 | Berberastine; |
| 352.344104 | 0.207813934 | 0.001261428 | Deacetylepithienamycin F; Deacetyl MM 1788 NA 2697 |
| 352.344104 | 0.207813934 | 0.001261428 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.344104 | 0.207813934 | 0.001261428 | Fortimicin KL |
| 352.344104 | 0.207813934 | 0.001261428 | Sudan III; C.I. Solvent Red 2 |
| 352.344104 | 0.207813934 | 0.001261428 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.344104 | 0.207813934 | 0.001261428 | Savinin; |
| 352.344104 | 0.207813934 | 0.001261428 | Berberastine; |
| 352.3659789 | 0.119920786 | 0.000940899 | 7-Hydroxymethyl-12-methylbenz[a]anthracene sulfate; |
| 352.3659789 | 0.119920786 | 0.000940899 | Deacetylepithienamycin F; Deacetyl MM 1788 NA 2697 |
| 352.3659789 | 0.119920786 | 0.000940899 | 8-(1,1-Dimethylallyl)-3-methylgalangin; 8-(1,1-DMA)-3-methylgalangin; |
| 352.3659789 | 0.119920786 | 0.000940899 | Fortimicin KL |
| 352.3659789 | 0.119920786 | 0.000940899 | Sudan III; C.I. Solvent Red 2 |
| 352.3659789 | 0.119920786 | 0.000940899 | Estra-1,3,5(10)-triene-3,17beta-diol 3-phosphate; Estra-1,3,5(10)-triene-3,17beta-diol 3-(dihydrogen phosphate); 17beta-Estradiol 3-phosphate; |
| 352.3659789 | 0.119920786 | 0.000940899 | Savinin; |
| 352.3659789 | 0.119920786 | 0.000940899 | Berberastine; |
| 352.3659789 | 0.119920786 | 0.000940899 | Benzylpenicilloic acid; |
| 353.3064626 | 0.373569548 | 5.69E-07 | Rugosinone; 1,3-Dioxolo[4,5-g]isoquinolin-5-yl(2-hydroxy-3,4-dimethoxyphenyl)methanone; |
| 353.3064626 | 0.373569548 | 5.69E-07 | Boc-Asn-OPhNO |
| 353.3386155 | 0.1047911 | 4.26E-05 | Fortimicin AO; |
| 353.3386155 | 0.1047911 | 4.26E-05 | Rugosinone; 1,3-Dioxolo[4,5-g]isoquinolin-5-yl(2-hydroxy-3,4-dimethoxyphenyl)methanone; |
| 353.3386155 | 0.1047911 | 4.26E-05 | Dihydrozeatin riboside; |
| 353.3386155 | 0.1047911 | 4.26E-05 | B 823-0 |
| 353.3386155 | 0.1047911 | 4.26E-05 | Boc-Asn-OPhNO |
| 353.3396625 | 0.179673612 | 1.33E-08 | Fortimicin AO; |
| 353.3396625 | 0.179673612 | 1.33E-08 | Rugosinone; 1,3-Dioxolo[4,5-g]isoquinolin-5-yl(2-hydroxy-3,4-dimethoxyphenyl)methanone; |
| 353.3396625 | 0.179673612 | 1.33E-08 | Dihydrozeatin riboside; |
| 353.3396625 | 0.179673612 | 1.33E-08 | B 823-0 |
| 353.3396625 | 0.179673612 | 1.33E-08 | Boc-Asn-OPhNO |
| 353.3411685 | 0.277419864 | 0.015357171 | Fortimicin AO; |
| 353.3411685 | 0.277419864 | 0.015357171 | Rugosinone; 1,3-Dioxolo[4,5-g]isoquinolin-5-yl(2-hydroxy-3,4-dimethoxyphenyl)methanone; |
| 353.3411685 | 0.277419864 | 0.015357171 | Dihydrozeatin riboside; |
| 353.3411685 | 0.277419864 | 0.015357171 | B 823-0 |
| 353.3411685 | 0.277419864 | 0.015357171 | Boc-Asn-OPhNO |
| 353.3423108 | 0.177905399 | 1.72E-08 | Fortimicin AO; |
| 353.3423108 | 0.177905399 | 1.72E-08 | Rugosinone; 1,3-Dioxolo[4,5-g]isoquinolin-5-yl(2-hydroxy-3,4-dimethoxyphenyl)methanone; |
| 353.3423108 | 0.177905399 | 1.72E-08 | Dihydrozeatin riboside; |
| 353.3423108 | 0.177905399 | 1.72E-08 | B 823-0 |
| 353.3423108 | 0.177905399 | 1.72E-08 | Boc-Asn-OPhNO |
| 357.3293018 | 0.160122983 | 2.82E-06 | Bakankoside; |
| 357.3293018 | 0.160122983 | 2.82E-06 | Tolrestat; |
| 357.3293018 | 0.160122983 | 2.82E-06 | cyclo-Dopa 5-O-glucoside; |
| 357.3293018 | 0.160122983 | 2.82E-06 | Protoviolaceinic acid; Protoviolaceinate; |
| 357.3293018 | 0.160122983 | 2.82E-06 | Cyhalofop-butyl; |
| 358.311737 | 0.063462354 | 6.70E-09 | N1-(5-Phospho-alpha-D-ribosyl)-5,6-dimethylbenzimidazole; alpha-Ribazole 5'-phosphate; |
| 358.311737 | 0.063462354 | 6.70E-09 | Cellobionate; Cellobionic acid; 4-O-beta-D-Glucopyranosyl-D-gluconate; |
| 358.311737 | 0.063462354 | 6.70E-09 | Sweroside; |
| 358.311737 | 0.063462354 | 6.70E-09 | Coumeroic acid; |
| 358.311737 | 0.063462354 | 6.70E-09 | Versiconal; |
| 358.311737 | 0.063462354 | 6.70E-09 | Chryso-obtusin; |
| 358.311737 | 0.063462354 | 6.70E-09 | 202-79 PN 202-79 |
| 360.3583934 | 2.112729756 | 6.69E-05 | 8-Epideoxyloganic acid; |
| 360.3583934 | 2.112729756 | 6.69E-05 | Metofluthrin; |
| 360.3583934 | 2.112729756 | 6.69E-05 | Acalyphin; |
| 360.3583934 | 2.112729756 | 6.69E-05 | (-)-Lariciresinol; |
| 360.3583934 | 2.112729756 | 6.69E-05 | Versiconol; |
| 360.3583934 | 2.112729756 | 6.69E-05 | 3-Methoxytyramine-betaxanthin; |
| 360.3583934 | 2.112729756 | 6.69E-05 | 2,3-Dihydro-2-(4-hydroxyphenyl)-5,6,7,8-tetramethoxy-4H-1-benzopyran-4-one; |
| 366.3685 | 0.021638638 | 0.001618043 | 20,21,21-Trifluoro-3-methoxy-19-nor-17alpha-pregna-1,3,5(10),20-tetraen-17-ol; 17-(Trifluorovinyl)-3-(methyl ether)-17beta-estradiol; |
| 366.3685 | 0.021638638 | 0.001618043 | Diacetoxyscirpenol; |
| 366.3685 | 0.021638638 | 0.001618043 | Glycyrol; Neoglycyrol; |
| 366.3685 | 0.021638638 | 0.001618043 | Fortimicin KK |
| 366.3685 | 0.021638638 | 0.001618043 | Tetracenomycin F |
| 369.3479905 | 0.399080989 | 0.003116808 | Amidosulfuron; |
| 369.3479905 | 0.399080989 | 0.003116808 | Fleroxacin; |
| 369.3479905 | 0.399080989 | 0.003116808 | U5048 trans-3,4-Dichloro-N-methyl-N-[2-(1-pyrrolidinyl)cyclohexyl]-benzeneacetamide; |
| 369.3479905 | 0.399080989 | 0.003116808 | Corpaine; |
| 369.3553739 | 3.064932313 | 0.000936816 | Amidosulfuron; |
| 369.3553739 | 3.064932313 | 0.000936816 | Fleroxacin; |
| 369.3553739 | 3.064932313 | 0.000936816 | U5048 trans-3,4-Dichloro-N-methyl-N-[2-(1-pyrrolidinyl)cyclohexyl]-benzeneacetamide; |
| 369.3553739 | 3.064932313 | 0.000936816 | Corpaine; |
| 369.3562564 | 0.430306828 | 0.006828382 | Amidosulfuron; |
| 369.3562564 | 0.430306828 | 0.006828382 | Fleroxacin; |
| 369.3562564 | 0.430306828 | 0.006828382 | U5048 trans-3,4-Dichloro-N-methyl-N-[2-(1-pyrrolidinyl)cyclohexyl]-benzeneacetamide; |
| 369.3562564 | 0.430306828 | 0.006828382 | Corpaine; |
| 370.2787995 | 3.194018669 | 0.000139623 | 1,2-beta-D-Glucuronosyl-D-glucuronate; (1->2)-beta-D-Glucuronosyl-D-glucuronate; |
| 370.2787995 | 3.194018669 | 0.000139623 | Eudistomin C; |
| 370.2787995 | 3.194018669 | 0.000139623 | Fraxin; |
| 370.28552 | 2.531277377 | 3.51E-05 | 1,2-beta-D-Glucuronosyl-D-glucuronate; (1->2)-beta-D-Glucuronosyl-D-glucuronate; |
| 370.28552 | 2.531277377 | 3.51E-05 | Eudistomin C; |
| 370.28552 | 2.531277377 | 3.51E-05 | Fraxin; |
| 381.1008657 | 0.194254968 | 0.001376992 | Teflubenzuron; |
| 383.2757305 | 74.56897174 | 1.52E-09 | WIN5495 5-(5-(2,6-Dichloro-4-(4,5-dihydro-2-oxazoly)phenoxy)pentyl)-3-methylisoxazole; |
| 383.3300376 | 2.315916071 | 0.001934645 | Tetraphenylarsonium; |
| 383.3300376 | 2.315916071 | 0.001934645 | Pantoprazole; |
| 383.3300376 | 2.315916071 | 0.001934645 | Lilaline; |
| 383.3300376 | 2.315916071 | 0.001934645 | Fluazifop butyl; |
| 383.3300376 | 2.315916071 | 0.001934645 | beta-D-Mannosyl-1,4-N-acetyl-D-glucosamine; 4-O-beta-D-Mannopyranosyl-N-acetyl-D-glucosamine; |
| 383.3306034 | 2.028397196 | 3.98E-05 | Tetraphenylarsonium; |
| 383.3306034 | 2.028397196 | 3.98E-05 | Pantoprazole; |
| 383.3306034 | 2.028397196 | 3.98E-05 | Lilaline; |
| 383.3306034 | 2.028397196 | 3.98E-05 | Fluazifop butyl; |
| 383.3306034 | 2.028397196 | 3.98E-05 | beta-D-Mannosyl-1,4-N-acetyl-D-glucosamine; 4-O-beta-D-Mannopyranosyl-N-acetyl-D-glucosamine; |
| 383.333511 | 0.307217797 | 0.000742286 | Tetraphenylarsonium; |
| 383.333511 | 0.307217797 | 0.000742286 | Pantoprazole; |
| 383.333511 | 0.307217797 | 0.000742286 | Lilaline; |
| 383.333511 | 0.307217797 | 0.000742286 | Fluazifop butyl; |
| 383.333511 | 0.307217797 | 0.000742286 | beta-D-Mannosyl-1,4-N-acetyl-D-glucosamine; 4-O-beta-D-Mannopyranosyl-N-acetyl-D-glucosamine; |
| 384.1157665 | 3.072873615 | 9.87E-06 | Carfentrazone; |
| 386.271607 | 7.033676508 | 6.31E-07 | O-Feruloylgalactarate; O-Feruloylgalactaric acid; 2'-(E)-O-Feruloylgalactaric acid; |
| 386.271607 | 7.033676508 | 6.31E-07 | Glutathioselenol; GSSeH; |
| 386.2799348 | 8.462670061 | 1.48E-05 | O-Feruloylgalactarate; O-Feruloylgalactaric acid; 2'-(E)-O-Feruloylgalactaric acid; |
| 386.2799348 | 8.462670061 | 1.48E-05 | Glutathioselenol; GSSeH; |
| 387.2176706 | 0.016527947 | 1.27E-08 | Sulfentrazone; F628 |
| 387.2176706 | 0.016527947 | 1.27E-08 | dCDP; 2'-Deoxycytidine diphosphate; 2'-Deoxycytidine 5'-diphosphate; |
| 389.2167524 | 0.006054334 | 4.16E-06 | Acetyl adenylate; 5'-Acetylphosphoadenosine; |
| 389.2167524 | 0.006054334 | 4.16E-06 | N-Acetylneuraminate 9-phosphate; |
| 389.2351681 | 0.00080758 | 2.18E-07 | Acetyl adenylate; 5'-Acetylphosphoadenosine; |
| 389.2351681 | 0.00080758 | 2.18E-07 | N-Acetylneuraminate 9-phosphate; |
| 389.401407 | 4.411178077 | 1.07E-05 | Cilazaprilat; (1S,9S)-9-((S)-1-Carboxy-3-phenylpropylamino)-10-oxo-4,6,7,8,9,10-hexahydro-1H-pyridazino[1,2-a][1,2]diazepine-1-carboxylic acid; |
| 389.401407 | 4.411178077 | 1.07E-05 | Balofloxacin; |
| 389.401407 | 4.411178077 | 1.07E-05 | Senaetnine; |
| 389.401407 | 4.411178077 | 1.07E-05 | 2-Methylbutyl glucosinolate; |
| 389.401407 | 4.411178077 | 1.07E-05 | Cefprozil; Cefprozil anhydrous; |
| 389.401407 | 4.411178077 | 1.07E-05 | (+/-)-6-Acetonyldihydrosanguinarine; 6-Acetonyl-5,6-dihydrosanguinarine; (+/-)-8-Acetonyldihydrosanguinarine; |
| 390.2392029 | 0.002172377 | 1.22E-06 | O-Carbamoyladenylate; |
| 391.2840124 | 0.274448189 | 2.97E-05 | trans-Permethrin; |
| 393.3131059 | 3.06220842 | 0.001451978 | 6-Methylthioguanosine monophosphate; |
| 396.3306809 | 35.55479309 | 4.43E-08 | Nogalaviketone; Methyl 5,7-dihydroxy-2-methyl-4,6,11-trioxo-3,4,6,11-tetrahydrotetracene-1-carboxylate; |
| 396.3306809 | 35.55479309 | 4.43E-08 | Sulfazecin; SQ 2644 |
| 397.3299068 | 18.68663489 | 1.77E-08 | 4-Keto-anhydrotetracycline; 4-Ketoanhydrotetracycline; 4-Keto-ATC; 4-Dedimethylamino-4-oxo-anhydrotetracycline; |
| 398.3392184 | 31.43788961 | 3.44E-08 | Nogalavinone; Nogalamycinone; |
| 398.3392184 | 31.43788961 | 3.44E-08 | Melarsoprol; |
| 398.3392184 | 31.43788961 | 3.44E-08 | 4-Amino-anhydrotetracycline; 4-Amino-ATC; 4-Dedimethyl-6-dehydro-anhydrotetracycline; |
| 401.2738058 | 11.44453318 | 2.94E-07 | Salbostatin 6'-phosphate; |
| 403.2800982 | 10.80544711 | 6.52E-07 | Pyrazoxyfen; |
| 403.2800982 | 10.80544711 | 6.52E-07 | Propionyladenylate; Propionyl-adenosine monophosphate; |
| 403.2800982 | 10.80544711 | 6.52E-07 | 6-(alpha-D-Glucosaminyl)-1D-myo-inositol 1,2-cyclic phosphate; |
| 403.2843495 | 11.95048819 | 1.13E-06 | Pyrazoxyfen; |
| 403.2843495 | 11.95048819 | 1.13E-06 | Propionyladenylate; Propionyl-adenosine monophosphate; |
| 403.2843495 | 11.95048819 | 1.13E-06 | 6-(alpha-D-Glucosaminyl)-1D-myo-inositol 1,2-cyclic phosphate; |
| 404.3201419 | 0.334449866 | 7.04E-05 | Aluminoparaaminosalicylate calcium; Alumino-p-aminosalicylic acid calcium salt; |
| 404.3201419 | 0.334449866 | 7.04E-05 | Scandoside methyl ester; |
| 404.3201419 | 0.334449866 | 7.04E-05 | 3-O-(3,6-Anhydro-alpha-D-galactopyranosyl)-D-galactose 4-O-sulfate; |
| 405.2650413 | 15.37887066 | 4.64E-09 | Spectinomycin dihydrochloride; |
| 406.1815039 | 82.29434873 | 3.26E-09 | Diclosulam; |
| 406.1885862 | 82.00820098 | 3.74E-09 | Diclosulam; |
| 406.3236628 | 0.414432472 | 0.002668361 | CGS 718 |
| 406.3236628 | 0.414432472 | 0.002668361 | Lancerin; 4-C-Glucosyl-1,3,7-trihydroxyxanthone; |
| 412.3181927 | 62.73640686 | 2.91E-08 | Cyflufenamid; |
| 412.3228785 | 141.9570282 | 2.66E-08 | Cyflufenamid; |
| 417.2219131 | 43.92593544 | 7.96E-09 | 2'-Deoxy-5-hydroxymethylcytidine-5'-diphosphate; |
| 418.2369435 | 5.383441799 | 0.000344042 | Metosulam; |
| 418.2369435 | 5.383441799 | 0.000344042 | Flucarbazone-sodium; |
| 418.7599292 | 7.310926791 | 1.93E-05 | Tefluthrin; |
| 419.4184489 | 5.319819816 | 4.06E-05 | Zopolrestat; |
| 419.4184489 | 5.319819816 | 4.06E-05 | NBMPR; 4-Nitrobenzylthioinosine; |
| 419.4184489 | 5.319819816 | 4.06E-05 | Prosulfuron; |
| 419.4184489 | 5.319819816 | 4.06E-05 | Jadomycin A; Jadomycin B aglycon; |
| 419.8840535 | 13.96616729 | 3.39E-06 | Esfenvalerate; |
| 419.8953665 | 39.17507754 | 2.85E-07 | Esfenvalerate; |
| 420.0402986 | 11.11378245 | 1.60E-05 | 6,6'-Dibromoindigotin; 6,6'-Dibromoindigo; Tyrian purple; |
| 420.0515933 | 122.2348929 | 3.15E-07 | D-myo-Inositol 1,4,5-trisphosphate; 1D-myo-Inositol 1,4,5-trisphosphate; Inositol 1,4,5-trisphosphate; Ins(1,4,5)P |
| 420.0515933 | 122.2348929 | 3.15E-07 | 6,6'-Dibromoindigotin; 6,6'-Dibromoindigo; Tyrian purple; |
| 425.2613271 | 4.310512203 | 1.94E-05 | 1,2,3,4,6,7,8-Heptachlorodibenzodioxin; 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin; 1,2,3,4,6,7,8-HpCDD; PCDD 7 |
| 434.2441172 | 9.251402705 | 3.44E-07 | Cyfluthrin; |
| 435.2462413 | 0.031080867 | 2.55E-08 | Chlorohyssopifolin A; |
| 435.2578062 | 0.017203569 | 3.79E-08 | Chlorohyssopifolin A; |
| 438.3787042 | 7.198798705 | 0.002891026 | sec-o-Glucosylhamaudol; |
| 451.3169417 | 0.136109363 | 3.38E-08 | 5'-Benzoylphosphoadenosine; |
| 451.3229417 | 0.129515444 | 1.17E-08 | 5'-Benzoylphosphoadenosine; |
| 453.3343012 | 0.36755731 | 0.000439875 | Bispyribac-sodium; |
| 453.3343271 | 0.391930867 | 0.002389206 | Bispyribac-sodium; |
| 453.3433925 | 0.335886763 | 0.005966875 | Bispyribac-sodium; |
| 453.356551 | 0.454409244 | 7.76E-05 | Bispyribac-sodium; |
| 454.2641691 | 0.021440194 | 3.42E-12 | 1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole; 1-(5'-Phosphoribosyl)-4-(N-succinocarboxamide)-5-aminoimidazole; 5'-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole; (S)-2-[5-Amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamido]succinate; |
| 454.2641691 | 0.021440194 | 3.42E-12 | 3,4-Bis(7-chloroindol-3-yl)pyrrole-2,5-dicarboxylate; Dichlorochromopyrrolate; |
| 454.2641691 | 0.021440194 | 3.42E-12 | Primisulfuron; |
| 454.3454107 | 0.266347417 | 0.000207658 | Kinamycin D; |
| 454.3454107 | 0.266347417 | 0.000207658 | Primisulfuron; |
| 456.2968954 | 0.005084963 | 1.70E-14 | FMN; Riboflavin-5-phosphate; Flavin mononucleotide; |
| 456.3184319 | 0.020009135 | 1.15E-06 | FMN; Riboflavin-5-phosphate; Flavin mononucleotide; |
| 456.3198524 | 0.033844027 | 6.38E-09 | FMN; Riboflavin-5-phosphate; Flavin mononucleotide; |
| 457.9904393 | 32.63673894 | 0.00028939 | LY-20276 2-[2-(5-Chloro-1H-indol-3-yl)ethyl]-3-[3-(1-methylethoxy)phenyl]-4(3H)-quinazolinone; |
| 457.9904393 | 32.63673894 | 0.00028939 | Azimilide; |
| 460.2291129 | 2.659763055 | 2.47E-05 | CDP-N-methylethanolamine; |
| 464.3091377 | 4.58110961 | 7.40E-05 | L 73582 |
| 469.3244661 | 2.146741526 | 0.002043389 | 2-(alpha-Hydroxyethyl)thiamine diphosphate; 2-Hydroxyethyl-ThPP; |
| 470.2789929 | 0.00264337 | 3.13E-09 | Dicloxacillin; |
| 470.2909839 | 0.033691977 | 1.74E-07 | Dicloxacillin; |
| 471.5008673 | 9.58E-05 | 9.16E-07 | Cefmetazole; |
| 471.5008673 | 9.58E-05 | 9.16E-07 | Puromycin; |
| 471.5008673 | 9.58E-05 | 9.16E-07 | GW 074 |
| 471.6779172 | 0.000378123 | 1.72E-08 | Terfenadine; |
| 472.5249331 | 0.00030422 | 1.10E-06 | Bryophyllin A; |
| 472.5249331 | 0.00030422 | 1.10E-06 | C1'-C9-Glycosylated UWM |
| 473.2852699 | 0.010905472 | 2.64E-09 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.2862562 | 0.000222652 | 2.90E-06 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.3016131 | 0.000260196 | 1.04E-06 | Compound WIN VIII; 5-(5-(2,6-Dichloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-(hydroxyethyloxymethyleneoxymethyl)isoxazole; |
| 473.3016131 | 0.000260196 | 1.04E-06 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.3177664 | 0.002890409 | 1.88E-11 | Compound WIN VIII; 5-(5-(2,6-Dichloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-(hydroxyethyloxymethyleneoxymethyl)isoxazole; |
| 473.3177664 | 0.002890409 | 1.88E-11 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.3204422 | 0.014005619 | 1.12E-06 | Compound WIN VIII; 5-(5-(2,6-Dichloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-(hydroxyethyloxymethyleneoxymethyl)isoxazole; |
| 473.3204422 | 0.014005619 | 1.12E-06 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.326136 | 0.022944997 | 1.02E-07 | Compound WIN VIII; 5-(5-(2,6-Dichloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-(hydroxyethyloxymethyleneoxymethyl)isoxazole; |
| 473.326136 | 0.022944997 | 1.02E-07 | CMP-N-trimethyl-2-aminoethylphosphonate; CMP-2-trimethylaminoethylphosphonate; |
| 473.525788 | 4.59E-05 | 5.18E-09 | Senampeline A; |
| 473.525788 | 4.59E-05 | 5.18E-09 | OA-6129 B |
| 474.1740632 | 0.001438835 | 1.02E-07 | Adenylylselenate; Adenosine-5'-phosphoselenate; |
| 474.183261 | 0.001019158 | 6.22E-08 | Adenylylselenate; Adenosine-5'-phosphoselenate; |
| 474.3337805 | 0.007664676 | 1.20E-07 | Chicoric acid; |
| 474.5351857 | 0.00017 | 4.01E-06 | Robustaol A; |
| 474.5351857 | 0.00017 | 4.01E-06 | Picrasin A; Nigakilactone G; |
| 474.5351857 | 0.00017 | 4.01E-06 | Sildenafil; |
| 474.5351857 | 0.00017 | 4.01E-06 | Amastatin; |
| 474.5428457 | 0.000246691 | 4.48E-06 | Robustaol A; |
| 474.5428457 | 0.000246691 | 4.48E-06 | Picrasin A; Nigakilactone G; |
| 474.5428457 | 0.000246691 | 4.48E-06 | Sildenafil; |
| 474.5428457 | 0.000246691 | 4.48E-06 | Amastatin; |
| 474.5428457 | 0.000246691 | 4.48E-06 | Diterpenoid EF-D; 12-Deoxy-phorbol-13-alpha-methylbutyrate-20-acetate; |
| 477.259332 | 0.014475207 | 2.93E-11 | CDP-glycerol; |
| 477.2759757 | 0.016539055 | 9.34E-08 | CDP-glycerol; |
| 477.2881227 | 0.041372276 | 2.45E-09 | CDP-glycerol; |
| 482.3953727 | 12.3438521 | 2.41E-08 | Isosilybin; |
| 482.3953727 | 12.3438521 | 2.41E-08 | N-[(7,8-Dihydropterin-6-yl)methyl]-4-(beta-D-ribofuranosyl)aniline 5'-phosphate; |
| 482.3953727 | 12.3438521 | 2.41E-08 | Catalposide; |
| 482.3953727 | 12.3438521 | 2.41E-08 | Cycloprothrin; |
| 483.277979 | 0.052850398 | 8.79E-10 | (2,3-Dihydroxybenzoyl)adenylate; |
| 488.2752689 | 0.016567393 | 3.96E-07 | CDP-choline; Cytidine 5'-diphosphocholine; Citicoline; |
| 488.2938187 | 0.471400053 | 1.72E-05 | CDP-choline; Cytidine 5'-diphosphocholine; Citicoline; |
| 488.3679844 | 0.341467893 | 0.000659214 | O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate; alpha-L-Dihydrostreptosyl-(1->4)-streptidine 6-phosphate; |
| 488.3679844 | 0.341467893 | 0.000659214 | CDP-choline; Cytidine 5'-diphosphocholine; Citicoline; |
| 488.3679844 | 0.341467893 | 0.000659214 | Flupyrsulfuron-methyl sodium; |
| 488.372547 | 0.315011539 | 0.000421996 | O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate; alpha-L-Dihydrostreptosyl-(1->4)-streptidine 6-phosphate; |
| 488.372547 | 0.315011539 | 0.000421996 | Flupyrsulfuron-methyl sodium; |
| 490.3172837 | 0.099163882 | 1.26E-06 | L-2-Aminoadipate adenylate; 5-Adenylyl-2-aminoadipate; alpha-Aminoadipoyl-C6-AMP; |
| 492.2892662 | 0.018294726 | 1.23E-07 | L-Threonylcarbamoyladenylate; L-Threonylcarbamoyl-AMP; TC-AMP; |
| 494.2479278 | 0.002443245 | 7.76E-13 | Pyriprole; |
| 494.2542474 | 0.011174923 | 8.37E-09 | Pyriprole; |
| 494.2611375 | 0.011633266 | 3.67E-09 | Pyriprole; |
| 495.2697993 | 0.006094277 | 1.33E-07 | Isopentenyladenosine-5'-diphosphate; Isopentenyl-ADP; N6-(Dimethylallyl)adenosine 5'-diphosphate; |
| 495.2846025 | 0.018081522 | 1.81E-07 | Isopentenyladenosine-5'-diphosphate; Isopentenyl-ADP; N6-(Dimethylallyl)adenosine 5'-diphosphate; |
| 495.304364 | 0.047276594 | 2.75E-07 | Isopentenyladenosine-5'-diphosphate; Isopentenyl-ADP; N6-(Dimethylallyl)adenosine 5'-diphosphate; |
| 499.4162821 | 0.328514047 | 0.000635376 | 5-O-(Indol-3-ylacetyl-myo-inositol) D-galactoside; |
| 507.2942595 | 0.007323505 | 7.08E-06 | 2'-Phosphoadenylylsulfate; |
| 511.333994 | 3.098743256 | 0.00040417 | Pyridoxalphosphate-6-azophenyl-2',4'-disulfonic acid; PPADS; |
| 511.333994 | 3.098743256 | 0.00040417 | trans-Zeatin riboside diphosphate; |
| 514.2800627 | 0.055150927 | 1.72E-07 | 6-(Dibromomethylene)-17beta-hydroxy-androst-4-en-3-one propionate; |
| 514.2800627 | 0.055150927 | 1.72E-07 | dTDP-4-oxo-2,3,6-trideoxy-D-glucose; dTDP-[(2R,6R)-tetrahydro-6-methyl-5-oxo-2H-pyran-2-yl] ester; dTDP-4-dehydro-2,3,6-trideoxy-alpha-D-hexopyranose; |
| 514.2906834 | 0.050445088 | 2.26E-06 | 6-(Dibromomethylene)-17beta-hydroxy-androst-4-en-3-one propionate; |
| 514.2906834 | 0.050445088 | 2.26E-06 | dTDP-4-oxo-2,3,6-trideoxy-D-glucose; dTDP-[(2R,6R)-tetrahydro-6-methyl-5-oxo-2H-pyran-2-yl] ester; dTDP-4-dehydro-2,3,6-trideoxy-alpha-D-hexopyranose; |
| 515.2317218 | 0.003147581 | 2.60E-12 | (2S)-Lactyl-2-diphospho-5'-guanosine; |
| 515.2388188 | 0.002462723 | 4.26E-12 | (2S)-Lactyl-2-diphospho-5'-guanosine; |
| 535.2751714 | 0.010610284 | 4.47E-07 | UDP-L-Ara4N; UDP-4-amino-4-deoxy-L-arabinose; UDP-4-amino-4-deoxy-beta-L-arabinopyranose; |
| 536.2820445 | 0.023171643 | 2.03E-07 | UDP-L-arabinofuranose; UDP-beta-L-arabinofuranose; |
| 537.533717 | 2.563812935 | 0.000151908 | Ambenonium; |
| 544.349797 | 1510.915044 | 3.29E-09 | dTDP-3-O-methyl-4-oxo-2,6-dideoxy-L-mannose; dTDP-4-keto-3-O-methyl-2,6-dideoxy-L-mannose; |
| 545.3561475 | 370.5072676 | 1.38E-09 | dTDP-L-vancosamine; dTDP-beta-L-vancosamine; |
| 547.2847453 | 0.034881127 | 1.28E-05 | CDP-4-dehydro-6-deoxy-D-glucose; |
| 547.318256 | 3.400104424 | 1.87E-05 | CDP-4-dehydro-6-deoxy-D-glucose; |
| 547.318256 | 3.400104424 | 1.87E-05 | dTDP-3-amino-3,6-dideoxy-alpha-D-galactopyranose; |
| 547.3271053 | 5.376679859 | 1.33E-05 | CDP-4-dehydro-6-deoxy-D-glucose; |
| 547.3271053 | 5.376679859 | 1.33E-05 | dTDP-3-amino-3,6-dideoxy-alpha-D-galactopyranose; |
| 559.4333783 | 0.428821815 | 0.000763889 | dTDP-beta-L-evernosamine; dTDP-3-amino-2,3,6-trideoxy-3-C-methyl-4-O-methyl-beta-L-arabino-hexopyranose; |
| 559.4400367 | 0.472303271 | 0.001474006 | dTDP-beta-L-evernosamine; dTDP-3-amino-2,3,6-trideoxy-3-C-methyl-4-O-methyl-beta-L-arabino-hexopyranose; |
| 568.5581229 | 0.028928558 | 0.004303802 | SN38 glucuronide; SN-38G; |
| 568.558326 | 0.037910428 | 0.005608763 | SN38 glucuronide; SN-38G; |
| 568.5674177 | 0.021665986 | 0.002384514 | SN38 glucuronide; SN-38G; |
| 568.5674177 | 0.021665986 | 0.002384514 | Lappaol D; |
| 568.5676179 | 0.019426892 | 0.008264349 | SN38 glucuronide; SN-38G; |
| 568.5676179 | 0.019426892 | 0.008264349 | Lappaol D; |
| 575.2535924 | 0.039601969 | 8.63E-07 | Isopentenyladenosine-5'-triphosphate; Isopentenyl-ATP; N6-(Dimethylallyl)adenosine 5'-triphosphate; |
| 587.3127161 | 2.639480057 | 5.53E-06 | GDP-4-keto-6-L-deoxygalactose; |
| 588.3004078 | 0.064357874 | 6.20E-08 | GDP-4-amino-4,6-dideoxy-alpha-D-mannose; GDP-alpha-D-perosamine; |
| 589.2934892 | 0.065001781 | 8.47E-07 | UDP-2-acetamido-2,6-dideoxy-beta-L-arabino-hexos-4-ulose; UDP-2-acetamido-2,6-dideoxy-beta-L-arabino-hex-4-ulose; |
| 589.2934892 | 0.065001781 | 8.47E-07 | ADP-mannose; APD-D-mannose; |
| 589.3089499 | 0.065913718 | 7.05E-06 | UDP-2-acetamido-2,6-dideoxy-beta-L-arabino-hexos-4-ulose; UDP-2-acetamido-2,6-dideoxy-beta-L-arabino-hex-4-ulose; |
| 589.3089499 | 0.065913718 | 7.05E-06 | ADP-mannose; APD-D-mannose; |
| 664.4519673 | 0.391117024 | 0.000320869 | NAD+; NAD; Nicotinamide adenine dinucleotide; DPN; Diphosphopyridine nucleotide; Nadide; beta-NAD+; |
| 664.4577619 | 2.485487055 | 0.000543616 | NAD+; NAD; Nicotinamide adenine dinucleotide; DPN; Diphosphopyridine nucleotide; Nadide; beta-NAD+; |