

| Met_ID  | New Annotation                              | Source                                  | Family                              | PubChem   | HMDB        | ChEBI  | KEGG   | LM ID        |
|---------|---------------------------------------------|-----------------------------------------|-------------------------------------|-----------|-------------|--------|--------|--------------|
| Met_001 | Sphinganine                                 | Endogenous                              | Sphingolipid/Sphinganine            | 91486     | HMDB0000269 | 16566  | C00836 | LMSP01020001 |
| Met_002 | Piperine                                    | Exogenous                               | Alkaloid                            | 638024    | HMDB0029377 | 28821  | C03882 | NA           |
| Met_003 | Cer(t18:1(6OH)/17:0(2OH))                   | Endogenous                              | Sphingolipid/Ceramide               | NA        | NA          | NA     | NA     | LMSP02010192 |
| Met_004 | Aripiprazole                                | Exogenous - Drug                        | N-arylpiperazine                    | 60795     | HMDB0005042 | 31236  | C12564 | NA           |
| Met_005 | Pentadecanoylcarnitine                      | Endogenous                              | Fatty acyl/Fatty acyl carnitines    | 123132011 | HMDB0062517 | 131886 | NA     | NA           |
| Met_006 | PE(21:0/0:0)                                | Endogenous                              | Glycerolphospholipid/Glyceroph      | 52925145  | NA          | 138536 | NA     | LMGP02050026 |
| Met_007 | Sphingosine                                 | Endogenous                              | Sphingolipid/Sphinganine            | 5280335   | HMDB0000252 | 16393  | C00319 | LMSP01010001 |
| Met_008 | DG(17:1(9Z)/17:1(9Z)/0:0)                   | Endogenous                              | Glycerolipid/Diacylglycerol         | 9543689   | NA          | NA     | NA     | LMGL02010021 |
| Met_009 | 2-(2-Ethoxyethoxy)ethanol                   | Exogenous - Exosome                     | Solvent                             | 8146      | NA          | NA     | NA     | NA           |
| Met_010 | Phenolic phthiocerol                        | Exogenous - Epitope                     | Fatty acyl/Fatty Alcohol            | 45266796  | NA          | 59237  | NA     | LMFA05000691 |
| Met_011 | O-Decanoyl-L-carnitine                      | Endogenous                              | Fatty acyl/Fatty acyl carnitines    | 11953821  | HMDB0000651 | 28717  | C03299 | LMFA07070006 |
| Met_012 | Cer(t18:1(6OH)/21:0(2OH))                   | Endogenous                              | Sphingolipid/Ceramide               | NA        | NA          | NA     | NA     | LMSP02010188 |
| Met_013 | 5-Methyl-1H-benzimidazole                   | Exogenous - Exosome                     | Imidazole                           | 11979     | NA          | 40205  | NA     | NA           |
| Met_014 | Cer(t18:1(6OH)/15:0(2OH))                   | Endogenous                              | Sphingolipid/Ceramide               | NA        | NA          | NA     | NA     | LMSP02010194 |
| Met_015 | 3,5-Di-O-methyl-8-prenylafzelechin-4beta-ol | Exogenous                               | Polyketide/Flavonoid                | 44257167  | NA          | NA     | NA     | LMPK12020216 |
| Met_016 | 10-oxo-nonadecanoic acid                    |                                         | Fatty acyl/Fatty Acid               | 5312916   | NA          | 138422 | NA     | LMFA01060128 |
| Met_017 | PE(P-18:0/20:5(5Z,8Z,11Z,14Z,17Z))          | Endogenous                              | Glycerolphospholipid/Glyceroph      | 52925089  | HMDB0011387 | 170521 | NA     | LMGP02030056 |
| Met_018 | medorinone                                  | Exogenous - Drug (Cardiovascular Agent) | Naphthyridines                      | 5362132   | NA          | NA     | D04884 | NA           |
| Met_019 | Topostin B-553                              | Exogenous - Bacteria                    | Fatty acyl/N-acyl amine             | 10347618  | NA          | NA     | NA     | LMFA08020284 |
| Met_020 | N-palmitoyl serine                          | Endogenous                              | Fatty acyl/N-acyl amine/Endocan     | 6453686   | HMDB0242111 | 165558 | NA     | LMFA08020101 |
| Met_021 | PE(20:4(5Z,8Z,11Z,14Z)/0:0)                 | Endogenous                              | Glycerolphospholipid/Glyceroph      | 42607465  | HMDB0011517 | 64395  |        | LMGP02050009 |
| Met_022 | PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)         | Endogenous                              | Glycerolphospholipid/Glyceroph      | 10415542  | HMDB0010404 | 73873  | C04230 | LMGP01050056 |
| Met_023 | 11-Nor-9-carboxy-delta9-THC                 | Exogenous - Drug (THC metabolite)       |                                     | 108207    | HMDB0062770 | 77273  | NA     | NA           |
| Met_024 | O-octanoyl-R-carnitine                      | Endogenous                              | Fatty acyl/Fatty acyl carnitines    | 11953814  | HMDB0000791 | 18102  | C02838 | LMFA07070002 |
| Met_025 | N-oleoyl L-serine                           | Endogenous                              | Fatty acyl/Fatty N-acyl amine       | 44190514  | HMDB0242185 | 136614 | NA     | LMFA08020305 |
| Met_026 | N-oleoyl L-serine_b                         |                                         |                                     | 44190514  | NA          | NA     | NA     | NA           |
| Met_027 | Cohibin A                                   | Endogenous                              | Annonaceous acetogenins             | 131751147 | HMDB0031168 | 176705 | NA     | NA           |
| Met_028 | Aminopentol                                 | Exogenous - Exosome (Micotoxin)         |                                     | 21119850  | HMDB0248328 | 62519  | NA     | NA           |
| Met_029 | Cotinine                                    | Exogenous - Exosome (Tobacco)           | Alkaloid                            | 408       | HMDB0001046 | 127762 | NA     | NA           |
| Met_030 | Nicotine                                    | Exogenous - Exosome (Tobacco)           | Alkaloid                            | 89594     | HMDB0001934 | 17688  | C00745 | NA           |
| Met_031 | Dehydroaripiprazole                         | Exogenous - Drug (Antipsychotic)        | N-arylpiperazine                    | 10114519  | HMDB0250942 | NA     | NA     | NA           |
| Met_032 | 7-Dehydrodesmosterol                        | Endogenous                              | Sterol lipid/Cholesterol and deriva | 440558    | HMDB0003896 | 27910  | C05107 | LMST01010121 |
| Met_033 | Cer(d18:2(4E,14Z)/24:1(15Z))                | Endogenous                              | Sphingolipid/Ceramide               | 156960926 | HMDB0240680 | NA     | NA     | NA           |
| Met_034 | 2(3H)-Benzothiazolone                       | Exogenous - Exosome (Tobacco)           | Benzothiazole                       | 13625     | HMDB0249030 | 115196 | NA     | NA           |
| Met_035 | N-Isobutylhexacosanamide                    | Exogenous                               | Amide                               | NA        | NA          | NA     | NA     | NA           |
| Met_036 | Tryptophan P1                               | Exogenous - Exosome (Tobacco)           | Pyridoindole.                       | 5284474   | HMDB0029746 | NA     | C19306 | NA           |
| Met_037 | PE(18:1(9Z)/0:0)                            | Endogenous                              | Glycerolphospholipid/Glyceroph      | 53480925  | HMDB0011476 | 76088  | NA     | LMGP02050004 |
| Met_038 | Cer(t18:0/19:0(2OH))                        | Endogenous                              | Sphingolipid/Ceramide               | 91820041  | NA          | NA     | NA     | LMSP02030065 |
| Met_039 | 3-Deoxyvitamin D3                           | Endogenous                              | Sterol lipid/Vitamine D3 and deriv  | 24779628  | NA          | 137139 | NA     | NA           |
| Met_040 | Benzoylarginine nitroanilide                | Exogenous - Exosome                     | Aniline                             | 13494     | HMDB0249046 | 15766  | C04303 | NA           |
| Met_041 | 2-(12-Tridecyn-1-yl)furan                   | Exogenous - Exosome                     | Heteroarene                         | 6857797   | HMDB0030933 | 977231 | NA     | NA           |
| Met_042 | trans-2-Dodecenoylcarnitine                 | Endogenous                              | Fatty Acyl/Acylcarnitine            | 53481671  | HMDB0013326 | 89717  | NA     | NA           |
| Met_043 | Cer(d18:1/18:1(9Z))                         | Endogenous                              | Sphingolipid/Ceramide               | 5283563   | HMDB0004948 | 77996  | C00195 | LMSP02010003 |
| Met_044 | Torrubiellone B                             | Exogenous                               | Alkaloid                            | 54729461  | NA          | 70287  | NA     | NA           |
| Met_045 | 2-amino-8-oxo-9,10-epoxy-decanoic acid      | Exogenous                               | Fatty acyl/Fatty acid               | 16061039  | NA          | 165431 | C12027 | LMFA01060176 |
| Met_046 | TG(17:2(9Z,12Z)/17:2(9Z,12Z)/18:0)[iso3]    | Endogenous                              | Glycerolipid/Triradylglycerols      | 9544082   | NA          | NA     | NA     | LMGL03010117 |

|         |                                                                                                                    |                                              |                                 |           |             |        |        |                |
|---------|--------------------------------------------------------------------------------------------------------------------|----------------------------------------------|---------------------------------|-----------|-------------|--------|--------|----------------|
| Met_047 | PG(22:0/12:0)                                                                                                      | Endogenous                                   | Glycerophospholipids/Glycerophc | 52927115  | NA          | 178666 | NA     | LMGP04010850   |
| Met_048 | N-palmitoyl threonine                                                                                              | Endogenous                                   | Fatty acyl/N-acyl amine/Endocan | 14239842  | HMDB0241933 | 165559 | NA     | LMFA08020107   |
| Met_049 | 7,8,7',8'-Tetrahydrozeaxanthin                                                                                     | Exogeonus - Exosome                          | Prenol Lipids/Isoprenoid        | 16061230  | NA          | NA     | NA     | LMPRO1070093   |
| Met_050 | 2,7,8,9-Tricyclazole                                                                                               | Exogeonus - Exosome (Pesticide)              |                                 | 39040     | HMDB0031809 | 81783  | C18492 | NA             |
| Met_051 | Decarbamoylsaxitoxin                                                                                               |                                              | Alkaloid                        | 14917396  | HMDB0038319 | NA     | NA     | NA             |
| Met_052 | 32,35-anhydrobacteriohopaneterol                                                                                   | Exogenous - Exosome (phycotoxin)             | Prenol Lipid/Hopanoid           | 42608329  | NA          | NA     | NA     | LMPRO4000022   |
| Met_053 | Luminide B                                                                                                         | Exogenous - Exosome (Bacteria)               | Cyclic peptide                  | 101582539 | NA          | NA     | NA     | NA             |
| Met_054 | Cer(t18:1(6OH)/20:0(2OH))                                                                                          | Endogenous                                   | Sphingolipid/Ceramide           | NA        |             |        |        | LMSP02010189   |
| Met_055 | 1-(14-methyl-pentadecanoyl)-2-{8-[3]-ladderane-octanyl}-sn-glycerol                                                |                                              | Glycerolipid/Diradylglycerol    | 24778510  | NA          | NA     | NA     | LMGL02070004   |
| Met_056 | MG(18:0/0:0/0:0)                                                                                                   | Endogenous                                   | Glycerolipid/Monoacylglycerol   | 24699     | HMDB0011131 | 526874 | NA     | LMGL01010003   |
| Met_057 | Medelamine A                                                                                                       | Exogenous - Exosome (Fungi)                  | Amine                           | 10353173  | NA          | NA     | NA     | NA             |
| Met_058 | 7-Methyl-2,6,9,12-tetraoxahexadecane                                                                               | Endogenous                                   | Dialkyl ether                   | 24838540  | HMDB0032181 | 169509 | NA     | NA             |
| Met_059 | TG(17:1(9Z)/17:2(9Z,12Z)/18:0)[iso6]                                                                               |                                              | Glycerolipid/Triradylglycerol   | 9544065   | NA          | NA     | NA     | LMGL03010099   |
| Met_060 | 1-Methylnicotinamide                                                                                               | Endogenous                                   | Nicotinamide                    | 457       | HMDB0000699 | 16797  | C02918 | NA             |
| Met_061 | Cholacalcioic acid                                                                                                 |                                              | Sterol Lipid/Secosteroid        | 9547281   | NA          | 137138 | NA     | LMST03020021   |
| Met_062 | Cer(m18:1(4E)/24:0)                                                                                                |                                              | Sphingolipids/Ceramide          | 73242199  | NA          | NA     | NA     | LMSP00000008   |
| Met_063 | 20-oxo-heneicosanoic acid                                                                                          |                                              | Fatty Acyl/Fatty Acid           | 5312924   | NA          | 165430 | NA     | LMFA01060136   |
| Met_064 | N-Stearoyl Glutamic acid                                                                                           | Endogenous                                   | Fatty acyl/N-acyl amine/Endocan | 94481     | HMDB0241942 | 165566 | NA     | LMFA08020090   |
| Met_065 | N-(3-Hydroxy-9Z-octadecenoyl) glycine                                                                              | Exogenous                                    | Fatty acyl/N-acyl amine         | NA        | NA          | NA     | NA     | LMFA08020333   |
| Met_066 | N-arachidonylethanolamine                                                                                          | Endogenous                                   | Fatty acyl/ N-acyl ethanolamide | 5281969   | HMDB0004080 | 2700   | C11695 | LMFA08040001   |
| Met_067 | 3,5-Tetradecadiencarnitine                                                                                         | Endogenous                                   | Fatty Acyl/ Acylcarnitine       | 53481681  | HMDB0013331 | 89746  | NA     | NA             |
| Met_068 | TG(17:2(9Z,12Z)/17:2(9Z,12Z)/20:1(11Z))[iso3]                                                                      |                                              | Glycerolipid/Triradylglycerol   | 9544270   | NA          | NA     | NA     | LMGL03010306   |
| Met_069 | PE(18:0/18:3(6Z,9Z,12Z))                                                                                           | Endogenous                                   | Glycerolphospholipid/Glyceroph  | 52924329  | HMDB0008995 | NA     | C00350 | LMGP02010628   |
| Met_070 | Glycicyl Oleate                                                                                                    |                                              | NA                              | NA        | NA          | NA     | NA     | NA             |
| Met_071 | Trygliceride OPO                                                                                                   | Endogenous                                   | Glycerolipid/Triacylglycerol    | 13183955  | HMDB0049741 | 75846  | NA     | LMGL03010083   |
| Met_072 | 2-Geranylphenol                                                                                                    | Exogenous                                    | Monoterpenoid                   | 5280829   | NA          | 177421 | C05807 | NA             |
| Met_073 | Cer(m18:1(4E)/24:1(15Z))                                                                                           | Endogenous                                   | Sphingolipid/Ceramide           | 73242201  | NA          | NA     | NA     | LMSP00000010   |
| Met_074 | PE(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z))                                                                           | Endogenous                                   | Glycerolphospholipid/Glyceroph  | 52924409  | HMDB0009141 | 169166 | C00350 | LMGP02010708   |
| Met_075 | Patulin                                                                                                            | Exogenous - Exosome (Micotoxin - Antibiotic) | Furopyran                       | 4696      | HMDB0034299 | 74926  | C16748 | NA             |
| Met_076 | PE(18:1(9E)/18:1(9E))                                                                                              | Endogenous                                   | Glycerolphospholipid/Glyceroph  | 9546744   | NA          | 84844  | NA     | LMGP02010039   |
| Met_077 | Pelretin                                                                                                           | Exogenous - Exosome (Vitamin - Mineral)      |                                 | 6435504   | NA          | NA     | D05402 | NA             |
| Met_078 | 9-(3,5-dimethylfuran-2-yl)-nonanoic acid                                                                           | Exogenous                                    | Fatty Acyl/Fatty Acid           | 134812131 | NA          | NA     | NA     | LMFA01150016   |
| Met_079 | Tropeolin                                                                                                          | Exogenous - Food biomarker                   | Thiocyanate                     | 18170     | HMDB0034273 | 16017  | C02660 | NA             |
| Met_080 | cis-5-Tetradecenoylcarnitine                                                                                       | Endogenous                                   | Fatty acyl/N-acyl amine         | 22833575  | HMDB0002014 | 73060  | NA     | LMFA08020305   |
| Met_081 | Docosanamide                                                                                                       | Endogenous                                   | Fatty acyl/Primary amide        | 76468     | HMDB0000583 | 165591 | NA     | LMFA08010020   |
| Met_082 | Oxaloterpin E                                                                                                      | Exogenous - Exosome (Bacteria)               | Terpenoid                       | 24179109  | NA          | NA     | NA     | NA             |
| Met_083 | Calcimycin                                                                                                         | Exogenous - Exosome (Bacteria - Antibiotic)  | Aminobenzoic acid.              | 40486     | HMDB0249542 | 3305   | NA     | NA             |
| Met_084 | (3aR,4R,6S,6aS,9bR)-4-hydroxy-6,9-dimethyl-3-methylidene-4,5,6,6a,7,9b-hexahydro-3aH-azuleno[4,5-b]furan-2,8-dione |                                              |                                 | 38348159  | NA          | NA     | NA     | NA             |
| Met_085 | Albaflavenone                                                                                                      | Exogenous - Exosome (Bacteria - Antibiotic)  | Sesquiterpenoid                 | 25137938  | NA          | 51460  | C17954 | NA             |
| Met_086 | Aphidicol-16-ene                                                                                                   | Exogenous                                    | Prenol Lipid/Isoprenoid         | 15907363  | NA          | NA     | NA     | LMPRO104160001 |
| Met_087 | PS(O-18:0/0:0)                                                                                                     | Endogenous                                   | Glycerophospholipid/Glyceroph   | 52926302  | NA          | 72738  | NA     | LMGP03060002   |
| Met_088 | 2,4,6,8,10-dodecapentaenal                                                                                         | Endogenous                                   | Fatty Acyl/Fatty Aldehyde       | 5283362   | NA          | 137718 | NA     | LMFA06000073   |
| Met_089 | 4-[(2R)-2-(Aminomethyl)-2-(hydroxymethyl)-5-oxo-1-pyrrolidinyl]-3-(3-pentanylamino)benzoic acid                    |                                              | NA                              | NA        | NA          | NA     | NA     | NA             |
| Met_090 | 11-oxo-undeca-5,8-dienoic acid                                                                                     | Exogenous                                    | Fatty Acyl/Fatty Acid           | 134812119 | NA          | NA     | NA     | LMFA01060220   |
| Met_091 | Urauchimycin A                                                                                                     | Exogenous - Exosome (Bacteria)               | Lactone                         | 10343746  | NA          | NA     | NA     | NA             |
| Met_092 | 12-Hydroxy-19-[(2Z)-4-hydroxy-3-methyl-2-buten-1-yl                                                                |                                              | NA                              | NA        | NA          | NA     | NA     | NA             |
| Met_093 | Neryl acetate                                                                                                      | Exogenous - Plant metabolite                 | Acetate ester                   | 1549025   | HMDB0035157 | 141210 | C09861 | NA             |

|                |                                                                      |                                  |                                     |           |             |        |        |              |
|----------------|----------------------------------------------------------------------|----------------------------------|-------------------------------------|-----------|-------------|--------|--------|--------------|
| <b>Met_094</b> | Caproic acid                                                         | Endogenous                       | Fatty Acyl/Fatty acid               | 8892      | HMDB0000535 | 30776  | C01585 | LMFA01010006 |
| <b>Met_095</b> | 1,2,3,4-Tetrahydroisochinolin                                        | Endogenous                       | Isoquinoline                        | 7046      | HMDB0012489 | 114116 | NA     | NA           |
| <b>Met_096</b> | Deoxycholic Acid                                                     | Endogenous                       | Sterol Lipid/Bile acids and derivat | 222528    | HMDB0000626 | 28834  | C04483 | LMST04010040 |
| <b>Met_097</b> | Tricyclazole                                                         | Exogenous - Exposome (Fungicide) | Thiazole                            | 39040     | HMDB0031809 | 81783  | C18492 | NA           |
| <b>Met_098</b> | Cer(d18:0/16:0)                                                      | Endogenous                       | Sphingolipid/Ceramide               | 5283572   | HMDB0011760 | 67042  | NA     | LMSP02020001 |
| <b>Met_099</b> | Cer(d18:0/18:0)                                                      | Endogenous                       | Sphingolipid/Ceramide               | 5283573   | HMDB0011761 | 67033  | NA     | LMSP02020008 |
| <b>Met_100</b> | Cer(d18:1/20:0)                                                      | Endogenous                       | Sphingolipid/Ceramide               | 5283566   | HMDB0004951 | 72962  | C00195 | LMSP02010007 |
| <b>Met_101</b> | Cer(d18:2/26:0(2OH))                                                 | Endogenous                       | Sphingolipid/Ceramide               | NA        | NA          | NA     | NA     | LMSP02020065 |
| <b>Met_102</b> | Cer(d18:1/16:0)                                                      | Endogenous                       | Sphingolipid/Ceramide               | 5283564   | HMDB0004949 | 72959  | C00195 | LMSP02010004 |
| <b>Met_103</b> | (2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(4Z,7Z,10Z,12E,16Z,1 | NA                               | NA                                  | NA        | NA          | NA     | NA     | NA           |
| <b>Met_104</b> | Oleic acid                                                           | Endogenous                       | Fatty Acyl/Unsaturated fatty acid   | 445639    | HMDB0000207 | 16196  | C00712 | LMFA01030002 |
| <b>Met_105</b> | Palmitoleic acid                                                     | Endogenous                       | Fatty acyl/Fatty acid               | 5312427   | HMDB0003229 | 28716  | C08362 | LMFA01030056 |
| <b>Met_106</b> | 11(Z)-Eicosenoic acid                                                | Endogenous                       | Fatty Acyl/Unsaturated fatty acid   | 5282768   | HMDB0002231 | 32425  | C16526 | LMFA01030085 |
| <b>Met_107</b> | Cer(d18:1/17:0)                                                      | Endogenous                       | Sphingolipid/Ceramide               | 44584335  | HMDB0240678 | 86513  | NA     | LMSP02010020 |
| <b>Met_108</b> | Mayolene-18                                                          | Exogenous                        | Fatty Acyl/Unsaturated fatty acid   | 52922006  | NA          | 165679 | NA     | LMFA07090147 |
| <b>Met_109</b> | Histidylaspartic acid                                                | Exogenous                        | Dipeptide                           | 7020094   | HMDB0028881 | 73925  | NA     | NA           |
| <b>Met_110</b> | Cer(d15:2(4E,6E)/20:0)                                               | Exogenous                        | Sphingolipid/Ceramide               | 70698947  | NA          | NA     | NA     | LMSP02010060 |
| <b>Met_111</b> | PE(18:2(9Z,12Z)/0:0)                                                 | Endogenous                       | Glycerolphospholipid/Glyceroph      | 52925130  | HMDB0011507 | 83058  | NA     | LMGP02050011 |
| <b>Met_112</b> | Fukiic acid                                                          | Exogenous                        | Phenylpropanoic acid                | 161871    | HMDB0029496 | 166659 | NA     | NA           |
| <b>Met_113</b> | Undecylic acid                                                       | Endogenous                       | Fatty Acyl/Fatty Acid               | 8180      | HMDB0000947 | 32368  | C17715 | LMFA01010011 |
| <b>Met_114</b> | Temanogrel                                                           | Exogenous                        | Benzamide                           | 11604525  | HMDB0258797 | 177604 | D09976 | NA           |
| <b>Met_115</b> | 9'-carboxy-gamma-tocotrienol                                         | Endogenous                       | Monoterpenoid                       | 53481537  | HMDB0012869 | 174955 | NA     | NA           |
| <b>Met_116</b> | 4-vinylphenol sulfate                                                | Exogenous                        | Sulfuric ester                      | 6426766   | HMDB0062775 | 82931  | NA     | NA           |
| <b>Met_117</b> | Protulactone A                                                       | Exogenous                        | Polyketide                          | 132489970 | NA          | NA     | NA     | NA           |
| <b>Met_118</b> | 7-heptadecynoic acid                                                 | Exogenous                        | Fatty Acyl/Unsaturated fatty acid   | 5312622   | NA          | 187284 | NA     | LMFA01030483 |
| <b>Met_119</b> | 2-methyl-2-dodecenoic acid                                           | Exogenous                        | Fatty Acyl/Unsaturated fatty acid   | 5282655   | NA          | 176863 | NA     | LMFA01020107 |
| <b>Met_120</b> | 5-Hydroxy-1-(4-hydroxyphenyl)-3-decanone                             | Exogenous                        | Fatty Acyl/Unsaturated fatty acid   | 70679005  | NA          | 70740  | NA     | LMFA01050502 |
| <b>Met_121</b> | 2,4-dimethyl-5-vinylthiazole                                         | Exogenous                        | Thiazole                            | 5362563   | HMDB0037285 | 173374 | NA     | NA           |