**Приложение 5**

**Перечень метаболитов, полученных в ходе МС-анализа образцов немодельных организмов типа членистоногие на масс- спектрометре типа Leco**

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **№** | **Название метаболита  (производной)** | **Идентификатор  HMDB** | **Название  исходного  метаболита**  **(не измененного  силилированием)** | **Группы классификации  метаболитов** | **Интенсивность масс-спектрометрического сигнала метаболита** | | | | | | **Кластер** |
| **Холост.образец** | **-80°С** | **+20°С** | **+4°С** | **-20°С** | **-20°С (пере-**  **замо-**  **розка)** |
| 1 | 2,3,4-Trihydroxybutyric acid tetrakis(trimethylsilyl) deriv., (, (R\*,R\*)-) | HMDB0000613 | (2R,3R)-2,3,4-Trihydroxybutanoic acid | Carbohydrates and carbohydrate conjugates | 18502 | 356135 | 326182 | 361752 | 404900 | 381823 | 2 |
| 2 | N-acetyl-L-aspartic acid 1 | HMDB0000812 | (2S)-2-Acetamidobutanedioic acid | Amino acids, peptides, and analogues | 4099 | 497998 | 304901 | 399239 | 355921 | 479372 | 2 |
| 3 | Oleamide, TMS derivative | HMDB0002117 | (9Z)-Octadec-9-enamide | Fatty amides | 62210 | 1817914 | 2172666 | 1713026 | 6254351 | 2351843 | 2 |
| 4 | 9-Octadecenoic acid, (E)-, TMS derivative | HMDB0000573 | (E)-9-Octadecenoic acid | Fatty acids and conjugates | 2316466 | 43705743 | 35757447 | 33144292 | 34662665 | 48793895 | 2 |
| 5 | palmitoleic acid | HMDB0003229 | (Z)-Hexadec-9-enoic acid | Fatty acids and conjugates | 284907 | 2446727 | 1761193 | 1830049 | 2101215 | 2188051 | 2 |
| 6 | 1,2,3-Butanetriol, 3TMS derivative | HMDB0034778 | 1,2,3-Butanetriol | Alcohols and polyols | 14197 | 123406 | 128742 | 152073 | 98633 | 137571 | 2 |
| 7 | 1,2-Ethanediamine, N,N-diethyl-N'-methyl- | indefinite | 1,2-Ethanediamine, N,N-diethyl-N'-methyl- | Amines | 42218 | 2658080 | 1859484 | 1269540 | 2725225 | 2977080 | 2 |
| 8 | 1-Deoxypentitol, 4TMS derivative | HMDB0041486 | 1-Deoxypentitol | Alcohols and polyols | 15390 | 54530 | 48452 | 62776 | 64100 | 103234 | 2 |
| 9 | 1-Hexanamine, 2-ethyl-N-(2-ethylhexyl)-N-methyl- | indefinite | 1-Hexanamine, 2-ethyl-N-(2-ethylhexyl)-N-methyl- | Amines | 5468 | 441103 | 373920 | 387973 | 294257 | 370985 | 2 |
| 10 | Diethylene glycol, n-butyl ether, trimethylsilyl ether | HMDB0244918 | 2-(2-Butoxyethoxy)ethanol | Ethers | 69587 | 2303162 | 251649 | 172102 | 255448 | 1807573 | 1 |
| 11 | N-Acetyl-D-galactosamine 1 | HMDB0000853 | 2-(Acetylamino)-2-deoxy-β-D-galactopyranose | Carbohydrates and carbohydrate conjugates | 24026 | 3125734 | 1829471 | 1872363 | 2144439 | 2030862 | 2 |
| 12 | methionine sulfoxide 1 | HMDB0002005 | 2-Amino-4-(methanesulfinyl)butanoic acid | Amino acids, peptides, and analogues | 7199 | 322155 | 487223 | 292144 | 254447 | 443827 | 2 |
| 13 | O-Phosphorylethanolamine | HMDB0000224 | 2-Aminoethyl dihydrogen phosphate | Phosphate esters | 24778 | 433051 | 1144656 | 446822 | 1524587 | 2001206 | 3 |
| 14 | 2'-Deoxyadenosine, 3TMS derivative | HMDB0000101 | 2'-Deoxyadenosine | Purine 2'-deoxyribonucleosides | 176717 | 1459130 | 1652414 | 1110568 | 806794 | 1318841 | 2 |
| 15 | D-Erythro-Pentopyranose, 2-deoxy-1,3,4-tris-O-(trimethylsilyl)- | indefinite | 2-Deoxy-a-L-erythro pentopyranose | Oxanes | 13068 | 327423 | 291845 | 350693 | 390008 | 447823 | 2 |
| 16 | 2'-Deoxyinosine, tris(trimethylsilyl) derivative | HMDB0000071 | 2'-Deoxyinosine | Purine 2'-deoxyribonucleosides | 20265 | 895460 | 285885 | 155502 | 149887 | 239673 | 1 |
| 17 | Trimethylolpropane, 3TMS derivative | HMDB0259243 | 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol | Alcohols and polyols | 43405 | 500794 | 436180 | 456971 | 282394 | 1356897 | 2 |
| 18 | 2-Hexenoic acid, (E)-, TMS derivative | HMDB0302424 | 2-Hexenoic acid | Fatty acids and conjugates | 24668 | 1207835 | 981524 | 574506 | 1424623 | 1567412 | 2 |
| 19 | 2-keto-isovaleric acid 2 | HMDB0000019 | 2-Ketoisovaleric acid | Short-chain keto acids and derivatives | 5589 | 641050 | 550915 | 612643 | 341150 | 635595 | 2 |
| 20 | 2-Thiazolidinecarboxamide, 2-methyl- | HMDB0062599 | 2-methyl-1,3-thiazolidine-2-carboxamide | Amino acids, peptides, and analogues | 7857 | 1442524 | 710758 | 761320 | 1241991 | 759196 | 2 |
| 21 | 2-Methyl-1,3-propanediol, 2TMS derivative | indefinite | 2-Methylpropane-1,3-diol | Alcohols and polyols | 13983 | 39729 | 120728 | 93817 | 74220 | 126780 | 3 |
| 22 | 2-Oleoylglycerol, 2TMS derivative | HMDB0011537 | 2-Oleoylglycerol | Monoradylglycerols | 530844 | 2462352 | 1899534 | 2314798 | 1743441 | 2343003 | 2 |
| 23 | 1-O-Tetradecylglycerol 2,3-ditrimethylsilyl ether | indefinite | 3-(Tetradecyloxy)-1,2-propanediol | Monoradylglycerols | 5129 | 502368 | 400482 | 506985 | 378107 | 405440 | 2 |
| 24 | Cholest-5-en-3-ol (3ОІ)-, carbonochloridate | HMDB0000067 | 3-Cholesteryl chloroformate | Cholestane steroids | 1666 | 187575 | 133356 | 160223 | 169268 | 125009 | 2 |
| 25 | Propanoic acid, 2-methyl-3-[(trimethylsilyl)oxy]-, trimethylsilyl ester | HMDB0062640 | 3-Hydroxyisobutyric acid | Beta hydroxy acids and derivatives | 257498 | 2134893 | 2711477 | 6431218 | 1816976 | 3499983 | 2 |
| 26 | 3-Pyridinol, TMS derivative | indefinite | 3-Pyridinol | Hydroxypyridines | 13584 | 22880 | 377211 | 254977 | 291847 | 554660 | 3 |
| 27 | 4(5H)-Thiazolone, 2-imino- | indefinite | 4(5H)-Thiazolone, 2-amino- | Thiazolines | 18055 | 2047635 | 2936419 | 3298931 | 1279354 | 2911238 | 2 |
| 28 | Androst-4-en-3-one, 17-methoxy-, 3-methoxime, (17ОІ)- | HMDB0000053 | 4-Androstene-3,17-dione | Androstane steroids | 10206 | 335729 | 158360 | 118817 | 151846 | 251192 | 1 |
| 29 | 9,12-Octadecadienoic acid (Z,Z)-, TMS derivative | HMDB0247706 | 9,12-Octadecadienoic acid | Lineolic acids and derivatives | 901837 | 20296471 | 14848867 | 17342469 | 11599954 | 18383593 | 2 |
| 30 | Acetamide, TMS derivative | HMDB0031645 | Acetamide | Carboximidic acids | 2076897 | 381908038 | 314134828 | 403309890 | 285476736 | 343746308 | 2 |
| 31 | 1,2-Ethandimine, N,N'-ditrifluoroacetyl- | indefinite | acetamide, n,n'-1,2-ethanediylbis[2,2,2-trifluoro- | Carboxylic acid derivatives | 9947 | 927830 | 247670 | 687820 | 81300 | 242408 | 1 |
| 32 | adenine | HMDB0000034 | Adenine | Purines and purine derivatives | 40632 | 15597566 | 14298598 | 14096489 | 17101431 | 19546195 | 2 |
| 33 | Adenosine, 4TMS derivative | HMDB0000050 | Adenosine | Purine nucleosides | 37319 | 6031980 | 7053532 | 8036641 | 7864534 | 8966660 | 2 |
| 34 | 2-Aminobutanoic acid, 2TMS derivative | HMDB0245013 | alpha-Aminobutyric acid | Amino acids, peptides, and analogues | 22804 | 2959688 | 2239891 | 1914234 | 1515575 | 1532558 | 2 |
| 35 | alpha-ketoglutaric acid | HMDB0000208 | alpha-Ketoglutaric acid | Gamma-keto acids and derivatives | 18612 | 209781 | 231223 | 206584 | 276039 | 296243 | 2 |
| 36 | alpha-ketoisocaproic acid 1 | HMDB0000695 | alpha-Ketoisocaproic acid | Short-chain keto acids and derivatives | 13329 | 1311866 | 858876 | 726857 | 648185 | 803082 | 2 |
| 37 | 1-Phenylethanol, TMS derivative | HMDB0032619 | alpha-Methylbenzyl alcohol | Benzene and substituted derivatives | 5503 | 275642 | 515621 | 606546 | 263283 | 290316 | 2 |
| 38 | Arachidonic acid, TMS derivative | HMDB0001043 | Arachidonic acid | Fatty acids and conjugates | 344152 | 17384136 | 12580053 | 14850381 | 7365560 | 17823351 | 2 |
| 39 | Arachidonoyl amide, N-(trimethylsilyl)- | indefinite | Arachidonoyl amide | Fatty amides | 35578 | 309903 | 362457 | 333151 | 680380 | 370178 | 2 |
| 40 | 4-Hydroxybenzeneacetic acid, 2TMS derivative | HMDB0000020 | Benzeneacetic acid, 4-hydroxy- | 1-hydroxy-2-unsubstituted benzenoids | 4915 | 950492 | 140508 | 154779 | 66508 | 192490 | 1 |
| 41 | Benzenesulfonamide, TMS derivative | HMDB0248984 | Benzenesulfonamide | Benzenesulfonamides | 28680 | 291832 | 269477 | 436591 | 404546 | 636256 | 2 |
| 42 | benzoic acid, 3,5-dimethyl-, trimethylsilyl ester | HMDB0246063 | Benzoic acid, 3,5-dimethyl- | Benzoic acids and derivatives | 5315 | 68093 | 47026 | 50356 | 45906 | 51143 | 2 |
| 43 | beta-Alanine 2 | HMDB0000056 | beta-Alanine | Amino acids, peptides, and analogues | 14367 | 281640 | 879204 | 469008 | 718809 | 1020803 | 3 |
| 44 | 3-Aminoisobutyric acid, 3TMS derivative | HMDB0003911 | beta-Aminoisobutyric acid | Amino acids, peptides, and analogues | 15660 | 838957 | 7294151 | 1112154 | 6970463 | 4502817 | 3 |
| 45 | Maltose, octakis(trimethylsilyl) ether, methyloxime (isomer 2) | HMDB0000163 | beta-Maltose | Carbohydrates and carbohydrate conjugates | 12253 | 1870826 | 1903474 | 1311863 | 1369416 | 2749666 | 2 |
| 46 | N-Acetyl-D-glucosamine, 4TMS derivative | HMDB0000803 | beta-N-Acetylglucosamine | Carbohydrates and carbohydrate conjugates | 14994 | 2475225 | 1228489 | 1371610 | 1906165 | 2217795 | 2 |
| 47 | Butyl 4,7,10,13,16,19-docosahexaenoate | indefinite | Butyl 4,7,10,13,16,19-docosahexaenoate | Fatty acid esters | 7539 | 182070 | 96569 | 142116 | 159310 | 131688 | 2 |
| 48 | Cadaverine, 4TMS derivative | HMDB0002322 | Cadaverine | Amines | 12496 | 398546 | 577805 | 620453 | 574208 | 1007742 | 2 |
| 49 | epsilon-Caprolactam | HMDB0062769 | Caprolactam | Caprolactams | 2427 | 49214 | 1324678 | 460724 | 368768 | 1760330 | 3 |
| 50 | 4-Cholesten-3-one 1 | HMDB0000921 | Cholest-4-en-3-one | Cholestane steroids | 786 | 494208 | 224067 | 144531 | 217179 | 360513 | 1 |
| 51 | Cortexolone 1 | HMDB0000015 | Cortodoxone | Hydroxysteroids | 165 | 249512 | 102361 | 70580 | 104171 | 177481 | 1 |
| 52 | creatine degr | HMDB0000064 | Creatine | Amino acids, peptides, and analogues | 23683 | 1283978 | 1137491 | 1141555 | 1567207 | 1783197 | 2 |
| 53 | d-Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)- | HMDB0000143 | D-​Galactopyranose | Carbohydrates and carbohydrate conjugates | 101 | 93586 | 87836 | 99591 | 104928 | 84390 | 2 |
| 54 | D-Glucose, 5TMS derivative | HMDB0000122 | D-​Glucopyranose | Carbohydrates and carbohydrate conjugates | 345825 | 10170656 | 12104150 | 15878116 | 16624465 | 9159986 | 2 |
| 55 | Mannonic acid, lactone - 4TMS derivative | HMDB0242119 | D-​Mannonic acid | Medium-chain hydroxy acids and derivatives | 25831 | 543159 | 580870 | 453890 | 494171 | 837950 | 2 |
| 56 | Arabinitol, 5TMS derivative | HMDB0000568 | D-Arabinitol | Carbohydrates and carbohydrate conjugates | 86623 | 1278988 | 703158 | 1156292 | 1338270 | 1083707 | 2 |
| 57 | D-Arabinose, tetrakis(trimethylsilyl) ether, ethyloxime (isomer 2) | HMDB0029942 | D-Arabinopyranose | Carbohydrates and carbohydrate conjugates | 358361 | 31984529 | 30575958 | 33193425 | 38179438 | 18297451 | 2 |
| 58 | 2'-deoxyguanosine 1 | HMDB0000085 | Deoxyguanosine | Purine 2'-deoxyribonucleosides | 2642 | 365595 | 483337 | 266166 | 179164 | 356933 | 2 |
| 59 | D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, O-methyloxime | HMDB0000660 | D-Fructose | Carbohydrates and carbohydrate conjugates | 256086 | 23201582 | 9963047 | 16235847 | 22810791 | 12019671 | 2 |
| 60 | D-galacturonic acid 1 | indefinite | D-Galactopyranuronic acid | Carbohydrates and carbohydrate conjugates | 18241 | 984627 | 811559 | 755451 | 1626120 | 816883 | 2 |
| 61 | D-Glucitol, 6TMS derivative | indefinite | D-Glucitol | Carbohydrates and carbohydrate conjugates | 237337 | 3132871 | 1640735 | 3544417 | 3939275 | 2070905 | 2 |
| 62 | D-Gluconic acid, 6TMS derivative | HMDB0000625 | D-Gluconic acid | Carbohydrates and carbohydrate conjugates | 34039 | 3258982 | 1428381 | 975945 | 1858814 | 1975688 | 1 |
| 63 | Diethanolamine, 3TMS derivative | HMDB0004437 | Diethanolamine | Amines | 8494 | 263424 | 198939 | 180532 | 234952 | 345055 | 2 |
| 64 | Cystathionine, 4TMS derivative | indefinite | DL-Cystathionine | Amino acids, peptides, and analogues | 18754 | 252574 | 517600 | 466597 | 485979 | 576787 | 3 |
| 65 | glutamic acid | HMDB0060475 | DL-Glutamic acid | Amino acids, peptides, and analogues | 203985 | 50310129 | 40523065 | 44282000 | 52677917 | 55257905 | 2 |
| 66 | ornithine 1 | HMDB0000214 | D-Ornithine | Amino acids, peptides, and analogues | 214737 | 5002970 | 4101097 | 4346991 | 5957521 | 8327672 | 2 |
| 67 | D-Ribofuranose, 1,2,3,5-tetrakis-O-(trimethylsilyl)- | HMDB0000283 | D-Ribofuranose | Carbohydrates and carbohydrate conjugates | 9045 | 309164 | 175525 | 254324 | 201687 | 343477 | 2 |
| 68 | D-Threitol, 4TMS derivative | HMDB0004136 | D-Threitol | Carbohydrates and carbohydrate conjugates | 55489 | 457413 | 277047 | 390011 | 430097 | 767537 | 2 |
| 69 | D-Trehalose, 7TMS derivative | HMDB0000975 | D-Trehalose | Carbohydrates and carbohydrate conjugates | 88184 | 27285457 | 11561649 | 17995950 | 6439662 | 10724406 | 1 |
| 70 | О±-D-Xylopyranose, 4TMS derivative | HMDB0000098 | D-Xylopyranose | Carbohydrates and carbohydrate conjugates | 6729 | 1226647 | 1605230 | 1256577 | 1974267 | 1131646 | 2 |
| 71 | Cholest-5-en-3-ol, (3О±)-, TMS derivative | HMDB0251842 | Epicholesterol | Cholestane steroids | 963 | 12236 | 20886 | 13880 | 19667 | 24722 | 2 |
| 72 | (Z)-Docos-13-enamide, N-TMS | HMDB0244507 | Erucamide | Fatty amides | 651319 | 7658310 | 15984470 | 14207083 | 21595926 | 19732786 | 3 |
| 73 | Ethanolamine, 2TMS derivative | HMDB0000149 | Ethanolamine | Amines | 26243 | 1488656 | 374152 | 4298262 | 384779 | 152808 | 1 |
| 74 | fructose-6-phosphate | HMDB0000124 | Fructose, 6-(dihydrogen phosphate) | Carbohydrates and carbohydrate conjugates | 1962 | 40476 | 14585 | 17345 | 33386 | 27904 | 1 |
| 75 | 2-Butenedioic acid, (E)-, 2TMS derivative | HMDB0000134 | Fumaric acid | Dicarboxylic acids and derivatives | 43146 | 6173113 | 8059996 | 8880581 | 5108859 | 8320694 | 2 |
| 76 | Galactinol, nonakis(trimethylsilyl) ether | HMDB0005826 | Galactinol | Carbohydrates and carbohydrate conjugates | 4325 | 568685 | 1193011 | 349407 | 2994840 | 2167144 | 3 |
| 77 | Pentanedioic acid, 2-(methoxyimino)-, bis(trimethylsilyl) ester | HMDB0000661 | Glutaric acid | Dicarboxylic acids and derivatives | 19106 | 3503702 | 3750720 | 3528213 | 4457869 | 4963482 | 2 |
| 78 | Glyceric acid, 3TMS derivative | HMDB0000139 | Glyceric acid | Carbohydrates and carbohydrate conjugates | 169371 | 6234722 | 5676593 | 5397050 | 4504673 | 6709794 | 2 |
| 79 | Glycerol, 3TMS derivative | HMDB0000131 | Glycerol | Carbohydrates and carbohydrate conjugates | 5768813 | 71267406 | 74311706 | 84423470 | 63575313 | 75724469 | 2 |
| 80 | 1-Monoacetin, 2O-TMS | indefinite | Glycerol 1-monoacetate | Monoradylglycerols | 81222 | 633905 | 549649 | 947302 | 482908 | 582038 | 2 |
| 81 | Glycine, 3TMS derivative | HMDB0000123 | Glycine | Amino acids, peptides, and analogues | 1243456 | 62097603 | 82415428 | 61434786 | 67428338 | 82307625 | 2 |
| 82 | Glycolic acid, 2TMS derivative | HMDB0000115 | Glycolic acid | Alpha hydroxy acids and derivatives | 1099112 | 3865159 | 3751838 | 4309935 | 3753271 | 5150905 | 2 |
| 83 | N,9-bis(Trimethylsilyl)-6-[(trimethylsilyl)oxy]-9H-purin-2-amine | HMDB0000132 | Guanine | Purines and purine derivatives |  | 111226 | 102921 | 152665 | 56990 | 152580 | 2 |
| 84 | 9H-Purin-2-amine, N-(trimethylsilyl)-6-[(trimethylsilyl)oxy]-9-[2,3,5-tris-O-(trimethylsilyl)-ОІ-D-ribofuranosyl]- | HMDB0000133 | Guanosine | Purine nucleosides | 24079 | 956883 | 1289556 | 1301838 | 941543 | 1983500 | 2 |
| 85 | Heptadecanoic acid, TMS derivative | HMDB0002259 | Heptadecanoic acid | Fatty acids and conjugates | 5092 | 437418 | 323452 | 316583 | 256194 | 359578 | 2 |
| 86 | Hexanedioic acid, 2TMS derivative | HMDB0000448 | Hexanedioic acid | Fatty acids and conjugates | 90294 | 407431 | 442909 | 570360 | 370165 | 594513 | 2 |
| 87 | L-Hydroxyproline, (E)-, 3TMS derivative | HMDB0000725 | Hydroxyproline | Amino acids, peptides, and analogues | 37001 | 4074139 | 4673386 | 4386648 | 2396481 | 4974937 | 2 |
| 88 | inosine | HMDB0000195 | Inosine | Purine nucleosides | 53590 | 789857 | 990493 | 629967 | 527661 | 905465 | 2 |
| 89 | Myo-Inositol, 6TMS derivative | HMDB0000211 | Inositol | Alcohols and polyols | 642502 | 64816611 | 70005621 | 61069949 | 95583447 | 67457493 | 2 |
| 90 | Isonicotinic Acid, TMS derivative | HMDB0060665 | Isonicotinic acid | Pyridinecarboxylic acids and derivatives | 3200 | 50769 | 27721 | 25855 | 25979 | 30474 | 1 |
| 91 | Alanine, 2TMS derivative | HMDB0000161 | L-​Alanine | Amino acids, peptides, and analogues |  | 346539 | 339719 | 413492 | 285624 | 396888 | 2 |
| 92 | L-Lysine, 4TMS derivative | HMDB0000182 | L-​Lysine | Amino acids, peptides, and analogues | 136653 | 18115566 | 14126400 | 10796273 | 20681969 | 21484549 | 2 |
| 93 | Lactic Acid, 2TMS derivative | HMDB0000190 | Lactic acid | Alpha hydroxy acids and derivatives | 27627 | 378464 | 1085959 | 869097 | 538890 | 655385 | 3 |
| 94 | ОІ-Lactose, 8TMS derivative | HMDB0041627 | Lactose | Carbohydrates and carbohydrate conjugates | 6079 | 2603264 | 2290996 | 558977 | 1039462 | 1820121 | 1 |
| 95 | Asparagine, 3TMS derivative | HMDB0000168 | L-Asparagine | Amino acids, peptides, and analogues | 19277 | 1425310 | 2001529 | 1450704 | 1832981 | 2240014 | 2 |
| 96 | Dodecyl acrylate | indefinite | Lauryl acrylate | Fatty alcohol esters | 14802 | 213793 | 160333 | 229878 | 179922 | 175571 | 2 |
| 97 | L-Cysteine, 3TMS derivative | HMDB0000574 | L-Cysteine | Amino acids, peptides, and analogues | 3086 | 458818 | 350417 | 399803 | 295958 | 316601 | 2 |
| 98 | L-Glutamic acid, 3TMS derivative | HMDB0000148 | L-Glutamic acid | Amino acids, peptides, and analogues | 425 | 28106 | 25682 | 26667 | 30618 | 33563 | 2 |
| 99 | glutamine 2 | HMDB0000641 | L-Glutamine | Amino acids, peptides, and analogues | 28285 | 1812962 | 1248467 | 1610597 | 1499581 | 1213381 | 2 |
| 100 | О±-Linolenic acid, TMS derivative | HMDB0001388 | Linolenic acid | Lineolic acids and derivatives | 55733 | 1660796 | 1037709 | 1270973 | 1010723 | 1217915 | 2 |
| 101 | Isoleucine, 2TMS derivative | HMDB0000172 | L-Isoleucine | Amino acids, peptides, and analogues | 165273 | 30511111 | 21041521 | 21570760 | 18954388 | 19383719 | 2 |
| 102 | Leucine, 2TMS derivative | HMDB0000687 | L-Leucine | Amino acids, peptides, and analogues | 329037 | 80094499 | 56984025 | 58183121 | 48183082 | 56631561 | 2 |
| 103 | l-Norvaline, N-ethoxycarbonyl-, isobutyl ester | indefinite | l-Norvaline, N-ethoxycarbonyl-, isobutyl ester | Amino acids, peptides, and analogues | 8124 | 472973 | 857360 | 1139525 | 405834 | 562629 | 2 |
| 104 | Phenylalanine, 2TMS derivative | HMDB0000159 | L-Phenylalanine | Amino acids, peptides, and analogues | 52239 | 12636929 | 9121071 | 8453272 | 7643650 | 8910205 | 2 |
| 105 | L-Proline, 2TMS derivative | HMDB0000162 | L-Proline | Amino acids, peptides, and analogues | 256218 | 67784587 | 48580525 | 51683092 | 36335525 | 46613306 | 2 |
| 106 | serine 1 | HMDB0000187 | L-Serine | Amino acids, peptides, and analogues | 534702 | 42869616 | 34930525 | 38938489 | 30990525 | 37652999 | 2 |
| 107 | taurine | HMDB0000251 | l-Taurine | Organosulfonic acids and derivatives | 9393 | 2314226 | 13332478 | 11892583 | 14687040 | 25628654 | 3 |
| 108 | L-Threonine, 3TMS derivative | HMDB0000167 | L-Threonine | Amino acids, peptides, and analogues | 137904 | 22656144 | 14515885 | 15128758 | 14200342 | 19480009 | 2 |
| 109 | Tryptophan, 3TMS derivative | HMDB0000929 | L-Tryptophan | Indolyl carboxylic acids and derivatives | 6861 | 7265516 | 5815456 | 5223243 | 5292778 | 6022217 | 2 |
| 110 | L-Tyrosine, 3TMS derivative | HMDB0000158 | L-Tyrosine | Amino acids, peptides, and analogues | 97109 | 30062659 | 19280777 | 20375522 | 15747095 | 19602347 | 2 |
| 111 | Valine, 2TMS derivative | HMDB0000883 | L-Valine | Amino acids, peptides, and analogues | 991649 | 155791091 | 139627230 | 176466364 | 129698590 | 146598186 | 2 |
| 112 | l-Valine, n-propargyloxycarbonyl-, decyl ester | indefinite | l-Valine, n-propargyloxycarbonyl-, decyl ester | Amino acids, peptides, and analogues | 134902 | 1536307 | 1101784 | 1727799 | 1068370 | 1668915 | 2 |
| 113 | Malic acid, 3TMS derivative | HMDB0000156 | Malic acid | Beta hydroxy acids and derivatives | 171994 | 23542060 | 15564232 | 18413642 | 20131464 | 20333957 | 2 |
| 114 | D-Mannose, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, O-methyloxime, 6-[bis(trimethylsilyl) phosphate] | HMDB0001078 | Mannose 6-phosphate | Carbohydrates and carbohydrate conjugates | 76772 | 3955226 | 1553951 | 1746057 | 4866750 | 2324464 | 2 |
| 115 | Methyl О±-N-acetyl-D-galactosamine, 3TMS derivative | indefinite | Methyl 2-acetamido-2-deoxy-α-D-galactopyranoside | Carbohydrates and carbohydrate conjugates | 269 | 381740 | 117019 | 224553 | 100594 | 280174 | 1 |
| 116 | Methyl galactoside (1S,2R,3S,4R,5R)-, 4TMS derivative | indefinite | Methyl galactoside | Carbohydrates and carbohydrate conjugates | 11461 | 1577474 | 5092410 | 2668420 | 2068173 | 6339846 | 3 |
| 117 | 1,2-Benzenedicarboxylic acid, monobutyl ester | HMDB0013247 | Monobutyl phthalate | Benzoic acids and derivatives | 173320 | 885636 | 1325718 | 1633436 | 1088330 | 1586828 | 2 |
| 118 | Myo-Inositol, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, bis(trimethylsilyl) phosphate | indefinite | myo-Inositol-1-phosphate | Alcohols and polyols | 4104 | 392078 | 408632 | 309084 | 696358 | 912599 | 2 |
| 119 | Niacin, TMS derivative | HMDB0001488 | Nicotinic acid | Pyridinecarboxylic acids and derivatives | 15363 | 1804378 | 1657624 | 1564566 | 1605396 | 2047525 | 2 |
| 120 | 2,3-Nonanedione | indefinite | Nonane-2,3-dione | Carbonyl compounds | 2890 | 404475 | 120138 | 185234 | 65415 | 138902 | 1 |
| 121 | 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-1,3-bis(trimethylsilyl)-, trimethylsilyl ester | HMDB0000226 | Orotic acid | Pyrimidines and pyrimidine derivatives | 4145 | 20315 | 19892 | 25291 | 21056 | 27855 | 2 |
| 122 | Pantothenic acid tritms | HMDB0000210 | Pantothenic acid | Alcohols and polyols | 24386 | 3250727 | 2486687 | 1917629 | 1472894 | 2815800 | 2 |
| 123 | Pentanoic acid, 2-(methoxyimino)-3-methyl-, trimethylsilyl ester | HMDB0000892 | Pentanoic acid | Fatty acids and conjugates | 12399 | 1341683 | 2181227 | 2357347 | 1399955 | 1920685 | 2 |
| 124 | Phosphoric acid, bis(trimethylsilyl)monomethyl ester | HMDB0001429 | Phosphate | Non-metal phosphates | 32005 | 3189707 | 21080288 | 28008302 | 12071673 | 19318383 | 3 |
| 125 | 2-Propenoic acid, 2-[(trimethylsilyl)oxy]-, anhydride with bis(trimethylsilyl) hydrogen phosphate | HMDB0000263 | Phosphoenolpyruvic acid | Phosphate esters | 23358 | 961834 | 686498 | 566106 | 1179420 | 903546 | 2 |
| 126 | Phosphoric acid, bis(trimethylsilyl) 2,3-bis[(trimethylsilyl)oxy]propyl ester | HMDB0001429 | Phosphoric acid | Non-metal phosphates | 57002 | 7710409 | 6177603 | 8854902 | 6569520 | 7588642 | 2 |
| 127 | Pyroglutamic acid, TMS derivative | HMDB0000267 | Pidolic acid | Amino acids, peptides, and analogues | 1401 | 148661 | 151970 | 160590 | 216324 | 235552 | 2 |
| 128 | Propanedioic acid, 2TMS derivative | HMDB0000691 | Propanedioic acid | Dicarboxylic acids and derivatives | 79255 | 863153 | 918434 | 931172 | 1004612 | 848436 | 2 |
| 129 | Pyridine, 1,2-dihydro-1-phenyl- | indefinite | Pyridine, 1,2-dihydro-1-phenyl- | Amines | 14645 | 397843 | 699084 | 1107527 | 846103 | 338505 | 2 |
| 130 | Ribonic acid, 2,3,4,5-tetrakis-O-(trimethylsilyl)-, trimethylsilyl ester | HMDB0000867 | Ribonic acid | Carbohydrates and carbohydrate conjugates | 18167 | 281532 | 381364 | 337735 | 364875 | 539674 | 2 |
| 131 | D-Altro-2-Heptulose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, O-methyloxime, 7-[bis(trimethylsilyl) phosphate] | indefinite | Sedoheptulose 7-phosphate | Carbohydrates and carbohydrate conjugates | 18054 | 908664 | 467474 | 491116 | 1468332 | 863749 | 2 |
| 132 | Eicosapentaenoic Acid, TMS derivative | HMDB0001999 | Timnodonic acid | Fatty acids and conjugates | 131946 | 6780460 | 4686044 | 5293409 | 3991085 | 6611706 | 2 |
| 133 | Triethylene glycol, 2TMS derivative | HMDB0259193 | Triethylene glycol | Ethers | 184994 | 1344871 | 846753 | 1174578 | 666806 | 2211061 | 2 |
| 134 | Tromethamine, 4TMS derivative | HMDB0240288 | Tromethamine | Amines | 281481 | 2552692 | 779639 | 1110786 | 686087 | 769076 | 1 |
| 135 | Tyramine, 3TMS derivative | HMDB0000306 | Tyramine | Phenethylamines | 5400 | 421039 | 218667 | 208107 | 487180 | 516087 | 2 |
| 136 | Uracil, 2TMS derivative | HMDB0000300 | Uracil | Pyrimidines and pyrimidine derivatives | 87433 | 15857390 | 9361515 | 9108884 | 7063057 | 7742606 | 1 |
| 137 | urea | HMDB0000294 | Urea | Ureas | 326600 | 7643135 | 9232972 | 8538432 | 7660932 | 7325736 | 2 |
| 138 | Uridine, 3TMS derivative | HMDB0000296 | Uridine | Pyrimidine nucleosides | 14023 | 10278906 | 3799384 | 4643659 | 4415747 | 5175869 | 1 |
| 139 | urocanic acid 1 | indefinite | Urocanic acid | Imidazoles | 13332 | 99983 | 143002 | 102266 | 47822 | 107633 | 2 |
| 140 | xanthine | HMDB0000292 | Xanthine | Purines and purine derivatives | 35881 | 13406321 | 1673724 | 1396759 | 1345864 | 1211768 | 1 |
| 141 | xanthosine | HMDB0000299 | Xanthosine | Purine nucleosides | 66749 | 928886 | 618947 | 782903 | 806572 | 1387351 | 2 |
| 142 | ribose-5-phosphate 2 | HMDB0001548 | α-D-Ribose-5-phosphate | Carbohydrates and carbohydrate conjugates | 2412 | 192710 | 98622 | 102399 | 106483 | 161509 | 2 |