## Sheet1
| Table S2. Associations between annotated metabolites and BMIz, with combined dataset of boys and girls and sex-stratified. Regression models identifying annotated metabolites (p=550) linearly associated with BMIz. Models ran for the entire cohort (n=206), as well as for boys (n=98) and girls (n=108). All models were adjusted for sex, age, and puberty onset (Model 1), along with additional phenotypic measures to identify metabolites that drive the association with BMIz including HOMA-CP (Model 2), MUAMA (Model 3), MUAFA (Model 4), WHtR (Model 5) and TR+SS (Model 6). Unadjusted p-value<0.05 highlighted in red. FDR<0.10 highlighted in green. Metabolites with FDR<0.10 in Model 1 listed first. AC, acylcarnitine; BCAA, branched chain amino acid; BMIz, BMI z-score; Cer, ceramide; DG, diglyceride; DHEA, dehydroepiandrosterone; DiC, dicarboxylic group; diOH, di-hydroxyl group; FA, fatty acid; FDR, false discovery rate; HOMA-CP, homeostatic model assessment of insulin resistance using C-peptide; keto, ketone; LysoPA, lysophosphatidic acid; LysoPC, lysophosphatidylcholine; LysoPE, lysophosphatidylethanolamine; MUAFA, mid-upper arm fat area; MUAMA, mid-upper arm muscle area; OH, hydroxyl group; PA, phosphatidic acid; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PG, phosphatidylglycerol; PI, phosphatidylinositol; PS, phosphatidylserine; SM, sphingomyelin; StdErr, standard error; TCA, tricarboxylic acid; TG, triglyceride; TR+SS, total subcutaneous adiposity; WHtR, waist to height ratio. | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 | Unnamed: 4 | Unnamed: 5 | Unnamed: 6 | Unnamed: 7 | Unnamed: 8 | Unnamed: 9 | Unnamed: 10 | Unnamed: 11 | Unnamed: 12 | Unnamed: 13 | Unnamed: 14 | Unnamed: 15 | Unnamed: 16 | Unnamed: 17 | Unnamed: 18 | Unnamed: 19 | Unnamed: 20 | Unnamed: 21 | Unnamed: 22 | Unnamed: 23 | Unnamed: 24 | Unnamed: 25 | Unnamed: 26 | Unnamed: 27 | Unnamed: 28 | Unnamed: 29 | Unnamed: 30 | Unnamed: 31 | Unnamed: 32 | Unnamed: 33 | Unnamed: 34 | Unnamed: 35 | Unnamed: 36 | Unnamed: 37 | Unnamed: 38 | Unnamed: 39 | Unnamed: 40 | Unnamed: 41 | Unnamed: 42 | Unnamed: 43 | Unnamed: 44 | Unnamed: 45 | Unnamed: 46 | Unnamed: 47 | Unnamed: 48 | Unnamed: 49 | Unnamed: 50 | Unnamed: 51 | Unnamed: 52 | Unnamed: 53 | Unnamed: 54 | Unnamed: 55 | Unnamed: 56 | Unnamed: 57 | Unnamed: 58 | Unnamed: 59 | Unnamed: 60 | Unnamed: 61 | Unnamed: 62 | Unnamed: 63 | Unnamed: 64 | Unnamed: 65 | Unnamed: 66 | Unnamed: 67 | Unnamed: 68 | Unnamed: 69 | Unnamed: 70 | Unnamed: 71 | Unnamed: 72 | Unnamed: 73 | Unnamed: 74 | Unnamed: 75 | Unnamed: 76 | Unnamed: 77 | Unnamed: 78 | Unnamed: 79 | Unnamed: 80 | Unnamed: 81 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metabolite | Neutral Mass | Retention Time | Super Pathway | Sub Pathway | Model 1: Including sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | Model 2: Including HOMA-CP, sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | Model 3: Including MUAMA, sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | v | Model 4: Including MUAFA, sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | Model 5: Including WHtR, sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | Model 6: Including TR+SS, sex, age, puberty onset | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN |
| NaN | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN | NaN | All | NaN | NaN | NaN | Boys | NaN | NaN | NaN | Girls | NaN | NaN | NaN |
| NaN | NaN | NaN | NaN | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | NaN | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR | Beta Coefficient | StdErr | Unadjusted p-value | FDR |
| N-acetylglycine | 117.043 | 0.884938 | Amino Acid | Acetyl Amino Acid | -0.2456 | 0.0889 | 0.005745 | 0.0705 | -0.1413 | 0.123 | 0.250663 | 0.5535 | -0.3573 | 0.1271 | 0.00494 | 0.0979 | NaN | -0.1135 | 0.0871 | 0.192389 | 0.548 | -0.0142 | 0.1114 | 0.898649 | 0.9613 | -0.2206 | 0.1297 | 0.08906 | 0.5595 | NaN | -0.0952 | 0.0643 | 0.138784 | 0.6296 | -0.0252 | 0.0873 | 0.772589 | 0.8997 | -0.1855 | 0.0932 | 0.046469 | 0.3772 | NaN | 0.0061 | 0.0489 | 0.9 | 0.9579 | 0.0384 | 0.0673 | 0.568719 | 0.7754 | -0.0156 | 0.0708 | 0.825793 | 0.9994 | NaN | 0.041 | 0.0393 | 0.295928 | 0.9708 | 0.0781 | 0.0557 | 0.160879 | 0.8793 | -0.0046 | 0.0554 | 0.93383 | 0.9967 | NaN | 0.0238 | 0.0487 | 0.624592 | 0.8641 | 0.0301 | 0.0667 | 0.652228 | 0.8353 | 0.0271 | 0.0716 | 0.705663 | 0.9666 |
| isovalerylcarnitine | 245.1626 | 4.58061 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.3198 | 0.0812 | 0.000082 | 0.0028 | 0.3499 | 0.1185 | 0.003157 | 0.0917 | 0.2843 | 0.1121 | 0.011209 | 0.1749 | NaN | 0.2565 | 0.0767 | 0.000831 | 0.025 | 0.2347 | 0.1087 | 0.030859 | 0.3624 | 0.2325 | 0.1069 | 0.029676 | 0.3979 | NaN | 0.1866 | 0.0586 | 0.00146 | 0.0448 | 0.2136 | 0.0849 | 0.011893 | 0.2845 | 0.1504 | 0.0816 | 0.065222 | 0.4338 | NaN | 0.0448 | 0.0459 | 0.329158 | 0.6375 | 0.0295 | 0.0699 | 0.672605 | 0.8457 | 0.069 | 0.0603 | 0.253158 | 0.9622 | NaN | 0.0543 | 0.0365 | 0.136022 | 0.9708 | 0.0952 | 0.0559 | 0.088376 | 0.7622 | 0.0159 | 0.0481 | 0.740066 | 0.9967 | NaN | 0.0288 | 0.0458 | 0.529146 | 0.8373 | 0.0093 | 0.0698 | 0.893806 | 0.9587 | 0.0529 | 0.0608 | 0.384663 | 0.8324 |
| isoleucine | 131.0954 | 1.502874 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.3132 | 0.082 | 0.000133 | 0.0043 | 0.4195 | 0.1019 | 0.000038 | 0.0093 | 0.1539 | 0.1319 | 0.243262 | 0.6109 | NaN | 0.2724 | 0.0765 | 0.000369 | 0.02 | 0.3175 | 0.0942 | 0.00075 | 0.0744 | 0.1403 | 0.1238 | 0.257001 | 0.6818 | NaN | 0.1945 | 0.0588 | 0.000934 | 0.0344 | 0.2334 | 0.0763 | 0.002233 | 0.173 | 0.1286 | 0.0932 | 0.167758 | 0.5664 | NaN | 0.0328 | 0.0463 | 0.479608 | 0.7505 | 0.0346 | 0.0655 | 0.597498 | 0.7872 | 0.0523 | 0.0683 | 0.443593 | 0.9735 | NaN | 0.004 | 0.0373 | 0.914552 | 0.9722 | 0.0309 | 0.0537 | 0.565125 | 0.9977 | -0.0381 | 0.0541 | 0.481096 | 0.9967 | NaN | 0.0539 | 0.0456 | 0.237864 | 0.7516 | 0.0525 | 0.0642 | 0.413156 | 0.7051 | 0.0732 | 0.0681 | 0.282786 | 0.7999 |
| leucine | 131.0951 | 1.596301 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.1858 | 0.082 | 0.023485 | 0.1752 | 0.3478 | 0.1022 | 0.000669 | 0.041 | -0.0417 | 0.1276 | 0.74392 | 0.9228 | NaN | 0.1479 | 0.0764 | 0.052826 | 0.3365 | 0.2342 | 0.0952 | 0.013902 | 0.2909 | -0.0335 | 0.1197 | 0.779549 | 0.9535 | NaN | 0.0775 | 0.0587 | 0.186713 | 0.6946 | 0.1961 | 0.0747 | 0.008672 | 0.252 | -0.0766 | 0.0902 | 0.395466 | 0.7606 | NaN | 0.0778 | 0.0436 | 0.074149 | 0.3995 | 0.0482 | 0.0615 | 0.433953 | 0.6955 | 0.1221 | 0.0652 | 0.061168 | 0.8712 | NaN | 0.0773 | 0.0348 | 0.02612 | 0.8627 | 0.115 | 0.0484 | 0.017381 | 0.5917 | 0.0302 | 0.0516 | 0.557577 | 0.9967 | NaN | 0.0604 | 0.0435 | 0.164731 | 0.7516 | 0.0564 | 0.0607 | 0.353045 | 0.6566 | 0.068 | 0.0657 | 0.300614 | 0.8042 |
| valine | 117.0793 | 0.870426 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.2612 | 0.0839 | 0.001862 | 0.0343 | 0.3634 | 0.1229 | 0.003116 | 0.0917 | 0.1829 | 0.1131 | 0.105891 | 0.4395 | NaN | 0.2101 | 0.0786 | 0.007533 | 0.1066 | 0.2164 | 0.1149 | 0.059739 | 0.4283 | 0.1634 | 0.1063 | 0.124417 | 0.6104 | NaN | 0.1438 | 0.0602 | 0.016871 | 0.2387 | 0.2323 | 0.0876 | 0.007991 | 0.2454 | 0.0666 | 0.0816 | 0.414379 | 0.7786 | NaN | 0.0362 | 0.0462 | 0.433112 | 0.718 | 0.0238 | 0.0727 | 0.743686 | 0.873 | 0.05 | 0.0592 | 0.398303 | 0.9735 | NaN | 0.049 | 0.0368 | 0.182515 | 0.9708 | 0.1154 | 0.0575 | 0.044612 | 0.6733 | -0.0026 | 0.0469 | 0.956361 | 0.9967 | NaN | 0.0317 | 0.0459 | 0.490536 | 0.8283 | 0.0117 | 0.0724 | 0.871542 | 0.9452 | 0.0495 | 0.0593 | 0.403838 | 0.8463 |
| phenylalanine | 165.0792 | 2.503736 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.2426 | 0.0854 | 0.004471 | 0.0588 | 0.4285 | 0.1696 | 0.011526 | 0.1645 | 0.1831 | 0.0982 | 0.06233 | 0.3614 | NaN | 0.1842 | 0.0801 | 0.021538 | 0.2162 | 0.3005 | 0.1528 | 0.049295 | 0.4173 | 0.1401 | 0.0934 | 0.133512 | 0.6193 | NaN | 0.1218 | 0.0612 | 0.046799 | 0.4036 | 0.2678 | 0.1204 | 0.026164 | 0.3282 | 0.0673 | 0.0713 | 0.345526 | 0.7211 | NaN | 0.0486 | 0.0464 | 0.294995 | 0.6009 | -0.0602 | 0.0994 | 0.544462 | 0.7679 | 0.086 | 0.0509 | 0.091551 | 0.8712 | NaN | 0.0245 | 0.0374 | 0.512295 | 0.9708 | 0.0614 | 0.0801 | 0.443095 | 0.9977 | 0.0126 | 0.041 | 0.759298 | 0.9967 | NaN | 0.047 | 0.0461 | 0.308044 | 0.7695 | -0.0425 | 0.0983 | 0.665534 | 0.8393 | 0.0773 | 0.0512 | 0.13097 | 0.7232 |
| tyrosine | 181.0741 | 1.297716 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.3852 | 0.0844 | 0.000005 | 0.0004 | 0.4361 | 0.1412 | 0.002017 | 0.0795 | 0.3526 | 0.1044 | 0.00073 | 0.0212 | NaN | 0.2863 | 0.082 | 0.000479 | 0.0204 | 0.1509 | 0.1451 | 0.298478 | 0.6731 | 0.2981 | 0.1002 | 0.002928 | 0.0885 | NaN | 0.207 | 0.0621 | 0.000853 | 0.0336 | 0.1965 | 0.1047 | 0.060629 | 0.4995 | 0.2067 | 0.0767 | 0.007019 | 0.1545 | NaN | 0.0906 | 0.0481 | 0.059785 | 0.3995 | 0.086 | 0.0826 | 0.297787 | 0.6062 | 0.0931 | 0.0579 | 0.10811 | 0.8962 | NaN | 0.032 | 0.0392 | 0.414122 | 0.9708 | 0.03 | 0.0694 | 0.665803 | 0.9977 | 0.0334 | 0.0465 | 0.472428 | 0.9967 | NaN | 0.0559 | 0.0485 | 0.249127 | 0.7516 | 0.0619 | 0.0826 | 0.453814 | 0.7368 | 0.0535 | 0.0592 | 0.366472 | 0.8297 |
| 5-methylthioadenosine | 297.0898 | 4.448414 | Amino Acid | Polyamine Metabolism | 0.3025 | 0.0852 | 0.000382 | 0.0105 | 0.549 | 0.1407 | 0.000096 | 0.0093 | 0.1845 | 0.1054 | 0.079907 | 0.3886 | NaN | 0.2274 | 0.0808 | 0.004893 | 0.0844 | 0.3859 | 0.1323 | 0.003526 | 0.1769 | 0.1332 | 0.1004 | 0.18448 | 0.6656 | NaN | 0.1305 | 0.0623 | 0.036291 | 0.344 | 0.3513 | 0.1019 | 0.000563 | 0.0804 | 0.0143 | 0.0775 | 0.853241 | 0.9569 | NaN | 0.0451 | 0.0475 | 0.34212 | 0.6512 | 0.0607 | 0.0883 | 0.491461 | 0.7353 | 0.0424 | 0.0554 | 0.443683 | 0.9735 | NaN | 0.0146 | 0.0382 | 0.702246 | 0.971 | 0.0691 | 0.0721 | 0.338211 | 0.9977 | -0.01 | 0.044 | 0.82034 | 0.9967 | NaN | 0.0533 | 0.047 | 0.256555 | 0.7516 | 0.047 | 0.088 | 0.593063 | 0.8122 | 0.0594 | 0.0552 | 0.281959 | 0.7999 |
| D-ornithine | 132.0897 | 0.510411 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.2128 | 0.0802 | 0.007941 | 0.0877 | 0.2173 | 0.1143 | 0.057152 | 0.2819 | 0.1896 | 0.1124 | 0.091678 | 0.4217 | NaN | 0.1919 | 0.0743 | 0.009795 | 0.126 | 0.1916 | 0.1004 | 0.056281 | 0.4173 | 0.1715 | 0.1056 | 0.104534 | 0.5745 | NaN | 0.0939 | 0.0576 | 0.103278 | 0.5671 | 0.1586 | 0.0799 | 0.047117 | 0.4603 | 0.035 | 0.082 | 0.66961 | 0.8905 | NaN | 0.0916 | 0.0427 | 0.031963 | 0.3584 | 0.1114 | 0.0618 | 0.071162 | 0.297 | 0.0672 | 0.0586 | 0.251511 | 0.9622 | NaN | 0.0164 | 0.035 | 0.640166 | 0.9708 | 0.0351 | 0.0525 | 0.503701 | 0.9977 | -0.0033 | 0.0467 | 0.943217 | 0.9967 | NaN | 0.1117 | 0.0421 | 0.007881 | 0.7271 | 0.1483 | 0.0602 | 0.013766 | 0.2658 | 0.0738 | 0.0586 | 0.207752 | 0.7294 |
| L-ornithine | 132.0897 | 0.510411 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.2157 | 0.0803 | 0.007254 | 0.0834 | 0.2224 | 0.1155 | 0.054145 | 0.2793 | 0.1943 | 0.1115 | 0.081404 | 0.3905 | NaN | 0.1924 | 0.0745 | 0.009813 | 0.126 | 0.2105 | 0.1011 | 0.037236 | 0.395 | 0.1683 | 0.105 | 0.108922 | 0.577 | NaN | 0.0856 | 0.0579 | 0.139585 | 0.6296 | 0.1601 | 0.0808 | 0.047536 | 0.4603 | 0.0226 | 0.0818 | 0.782828 | 0.9449 | NaN | 0.0932 | 0.0428 | 0.029512 | 0.3584 | 0.112 | 0.0625 | 0.073052 | 0.297 | 0.0674 | 0.0582 | 0.246756 | 0.9622 | NaN | 0.0194 | 0.035 | 0.579744 | 0.9708 | 0.033 | 0.0532 | 0.535391 | 0.9977 | 0.0063 | 0.0464 | 0.892424 | 0.9967 | NaN | 0.1202 | 0.042 | 0.004223 | 0.7271 | 0.1523 | 0.0608 | 0.012226 | 0.265 | 0.0857 | 0.058 | 0.139146 | 0.7232 |
| normethanephrine | 183.0897 | 2.503736 | Benzenoids | phenols | 0.2427 | 0.0853 | 0.004464 | 0.0588 | 0.4286 | 0.1696 | 0.011526 | 0.1645 | 0.1832 | 0.0982 | 0.0622 | 0.3614 | NaN | 0.1843 | 0.0801 | 0.021467 | 0.2162 | 0.3005 | 0.1529 | 0.049295 | 0.4173 | 0.1402 | 0.0934 | 0.133122 | 0.6193 | NaN | 0.1218 | 0.0612 | 0.046679 | 0.4036 | 0.2678 | 0.1204 | 0.026164 | 0.3282 | 0.0674 | 0.0713 | 0.344926 | 0.7211 | NaN | 0.0487 | 0.0464 | 0.294077 | 0.6009 | -0.0603 | 0.0994 | 0.544462 | 0.7679 | 0.0861 | 0.0509 | 0.091048 | 0.8712 | NaN | 0.0246 | 0.0374 | 0.510391 | 0.9708 | 0.0614 | 0.0801 | 0.443095 | 0.9977 | 0.0127 | 0.041 | 0.756547 | 0.9967 | NaN | 0.047 | 0.0461 | 0.307454 | 0.7695 | -0.0425 | 0.0983 | 0.665534 | 0.8393 | 0.0774 | 0.0512 | 0.130561 | 0.7232 |
| D-lyxose | 150.0527 | 0.706673 | Carbohydrate | Pentose Metabolism | -0.3152 | 0.0989 | 0.001435 | 0.0283 | -0.2221 | 0.1386 | 0.108974 | 0.3717 | -0.4107 | 0.1425 | 0.003945 | 0.0947 | NaN | -0.3443 | 0.0907 | 0.000146 | 0.0129 | -0.2741 | 0.1204 | 0.022769 | 0.3387 | -0.4257 | 0.1326 | 0.00132 | 0.0458 | NaN | -0.2506 | 0.0692 | 0.000295 | 0.0161 | -0.17 | 0.0967 | 0.078603 | 0.549 | -0.3222 | 0.1004 | 0.001334 | 0.0818 | NaN | -0.0168 | 0.0549 | 0.760074 | 0.8918 | -0.0285 | 0.0763 | 0.70876 | 0.8608 | -0.0259 | 0.0795 | 0.744157 | 0.9994 | NaN | 0.0176 | 0.0441 | 0.690575 | 0.9708 | -0.0006 | 0.0635 | 0.991842 | 0.9977 | 0.0455 | 0.0629 | 0.469622 | 0.9967 | NaN | -0.0035 | 0.0546 | 0.948491 | 0.9786 | -0.0774 | 0.0748 | 0.30105 | 0.6411 | 0.0712 | 0.0813 | 0.381237 | 0.8318 |
| 5-phospho-alpha-D-ribose-1-diphosphate | 389.977 | 0.999379 | Carbohydrate | Pentose Phosphate Pathway | 0.2397 | 0.0899 | 0.007682 | 0.0865 | 0.1172 | 0.135 | 0.385216 | 0.7018 | 0.3164 | 0.125 | 0.011405 | 0.1749 | NaN | 0.1979 | 0.0838 | 0.018156 | 0.2071 | 0.059 | 0.1193 | 0.620533 | 0.8437 | 0.2749 | 0.1183 | 0.020144 | 0.327 | NaN | 0.0904 | 0.0649 | 0.163654 | 0.6546 | 0.0548 | 0.0947 | 0.562756 | 0.824 | 0.1176 | 0.0927 | 0.204437 | 0.6167 | NaN | 0.0393 | 0.0488 | 0.421317 | 0.7088 | -0.1059 | 0.0733 | 0.1483 | 0.4218 | 0.1763 | 0.0645 | 0.006236 | 0.8712 | NaN | 0.0577 | 0.0388 | 0.137466 | 0.9708 | -0.011 | 0.0606 | 0.856635 | 0.9977 | 0.1166 | 0.0515 | 0.023559 | 0.8496 | NaN | 0.0252 | 0.0486 | 0.604749 | 0.8583 | -0.0924 | 0.0727 | 0.203869 | 0.5437 | 0.1357 | 0.0658 | 0.039288 | 0.6979 |
| Cer t36:0(2OH) | 599.5055 | 24.486198 | Lipid | Ceramide | 0.3344 | 0.0837 | 0.000065 | 0.0024 | 0.2584 | 0.1268 | 0.041615 | 0.2428 | 0.3728 | 0.1141 | 0.001089 | 0.03 | NaN | 0.3219 | 0.0772 | 0.000031 | 0.0056 | 0.2501 | 0.1108 | 0.023993 | 0.3387 | 0.3615 | 0.1067 | 0.000705 | 0.0342 | NaN | 0.2388 | 0.0593 | 0.000056 | 0.0062 | 0.2097 | 0.0881 | 0.017239 | 0.3282 | 0.2789 | 0.0809 | 0.000568 | 0.0522 | NaN | 0.0001 | 0.0482 | 0.998307 | 0.9999 | -0.0213 | 0.0719 | 0.767465 | 0.8754 | 0.0085 | 0.0655 | 0.89661 | 0.9994 | NaN | 0.0361 | 0.038 | 0.34116 | 0.9708 | 0.0187 | 0.0589 | 0.751246 | 0.9977 | 0.0488 | 0.0503 | 0.331193 | 0.9967 | NaN | -0.0177 | 0.0481 | 0.713276 | 0.9155 | -0.0196 | 0.0713 | 0.783774 | 0.9013 | -0.0237 | 0.0662 | 0.720644 | 0.968 |
| PE-Cer d36:1 | 688.5503 | 23.996895 | Lipid | Ceramide phosphoethanolamines | 0.1726 | 0.0828 | 0.037064 | 0.2244 | -0.0551 | 0.1539 | 0.720411 | 0.9045 | 0.2695 | 0.0958 | 0.004926 | 0.0979 | NaN | 0.0971 | 0.0782 | 0.214571 | 0.5835 | 0.0119 | 0.1357 | 0.930304 | 0.9707 | 0.1843 | 0.0953 | 0.05304 | 0.4962 | NaN | 0.129 | 0.0582 | 0.026758 | 0.28 | 0.0974 | 0.1082 | 0.367922 | 0.7724 | 0.1409 | 0.0702 | 0.044796 | 0.3772 | NaN | -0.0664 | 0.045 | 0.139688 | 0.4828 | -0.1614 | 0.0812 | 0.04693 | 0.2515 | -0.019 | 0.0539 | 0.724547 | 0.9994 | NaN | -0.0207 | 0.0358 | 0.562451 | 0.9708 | -0.0846 | 0.068 | 0.213593 | 0.9357 | 0.0085 | 0.0417 | 0.838228 | 0.9967 | NaN | -0.0411 | 0.0445 | 0.355866 | 0.7843 | -0.1917 | 0.08 | 0.016543 | 0.2658 | 0.0301 | 0.053 | 0.570619 | 0.9321 |
| PE-Cer d32:3 | 628.4845 | 25.65966 | Lipid | Ceramide phosphoethanolamines | 0.2347 | 0.0801 | 0.003367 | 0.0526 | 0.0358 | 0.1177 | 0.760595 | 0.9222 | 0.4203 | 0.1053 | 0.000065 | 0.0031 | NaN | 0.1768 | 0.0753 | 0.018895 | 0.2086 | 0.0257 | 0.1033 | 0.80375 | 0.9336 | 0.3479 | 0.1031 | 0.000743 | 0.0342 | NaN | 0.1812 | 0.0562 | 0.001268 | 0.0412 | 0.1538 | 0.0815 | 0.059221 | 0.4995 | 0.2162 | 0.0802 | 0.007014 | 0.1545 | NaN | -0.0254 | 0.0445 | 0.567621 | 0.8059 | -0.1252 | 0.0627 | 0.045701 | 0.2513 | 0.0836 | 0.0612 | 0.172313 | 0.9514 | NaN | 0.0344 | 0.035 | 0.325277 | 0.9708 | -0.008 | 0.0524 | 0.879099 | 0.9977 | 0.0815 | 0.0475 | 0.086457 | 0.9967 | NaN | -0.0085 | 0.044 | 0.847532 | 0.9587 | -0.1092 | 0.0623 | 0.079719 | 0.3895 | 0.0998 | 0.0607 | 0.100516 | 0.7232 |
| PE-Cer d34:3 | 656.5162 | 26.70364 | Lipid | Ceramide phosphoethanolamines | 0.1291 | 0.0837 | 0.12303 | 0.4091 | -0.1025 | 0.1289 | 0.426507 | 0.7255 | 0.3084 | 0.1061 | 0.003646 | 0.0915 | NaN | 0.0884 | 0.0779 | 0.256912 | 0.6275 | -0.0611 | 0.1136 | 0.590655 | 0.8258 | 0.2462 | 0.1023 | 0.016039 | 0.2767 | NaN | 0.1253 | 0.0586 | 0.032473 | 0.3259 | 0.0659 | 0.0916 | 0.472264 | 0.799 | 0.1735 | 0.0775 | 0.025077 | 0.3327 | NaN | -0.0589 | 0.0448 | 0.188983 | 0.5115 | -0.1443 | 0.0678 | 0.033317 | 0.2328 | 0.0105 | 0.0594 | 0.85955 | 0.9994 | NaN | 0.0135 | 0.0357 | 0.704951 | 0.971 | -0.0165 | 0.0577 | 0.775297 | 0.9977 | 0.0418 | 0.0459 | 0.361702 | 0.9967 | NaN | -0.0314 | 0.0444 | 0.479743 | 0.8239 | -0.1108 | 0.0678 | 0.102368 | 0.438 | 0.0339 | 0.059 | 0.565575 | 0.9321 |
| DG 32:0 | 568.5067 | 26.219461 | Lipid | Diacylglycerol | 0.3822 | 0.0787 | 0.000001 | 0.0004 | 0.2981 | 0.1243 | 0.016495 | 0.1821 | 0.4379 | 0.1005 | 0.000013 | 0.001 | NaN | 0.2757 | 0.0778 | 0.000397 | 0.02 | 0.1609 | 0.1147 | 0.160509 | 0.5063 | 0.347 | 0.1027 | 0.000729 | 0.0342 | NaN | 0.2117 | 0.058 | 0.000261 | 0.0161 | 0.183 | 0.0882 | 0.03808 | 0.4042 | 0.2268 | 0.0776 | 0.003461 | 0.1228 | NaN | 0.05 | 0.0462 | 0.279206 | 0.5838 | -0.0201 | 0.0719 | 0.780247 | 0.8826 | 0.1102 | 0.0589 | 0.061275 | 0.8712 | NaN | 0.0485 | 0.0368 | 0.186934 | 0.9708 | -0.0082 | 0.0592 | 0.890209 | 0.9977 | 0.0907 | 0.0461 | 0.049075 | 0.9967 | NaN | 0.0588 | 0.0457 | 0.198033 | 0.7516 | -0.0227 | 0.0713 | 0.750411 | 0.884 | 0.1255 | 0.0583 | 0.031352 | 0.6979 |
| DG 34:0 | 618.5204 | 27.634111 | Lipid | Diacylglycerol | 0.3623 | 0.0804 | 0.000007 | 0.0005 | 0.2236 | 0.1449 | 0.122821 | 0.3746 | 0.4175 | 0.0951 | 0.000011 | 0.001 | NaN | 0.2646 | 0.0784 | 0.000731 | 0.025 | 0.083 | 0.1314 | 0.527598 | 0.7797 | 0.3418 | 0.095 | 0.000322 | 0.0222 | NaN | 0.2122 | 0.0585 | 0.000287 | 0.0161 | 0.1182 | 0.1023 | 0.247966 | 0.6984 | 0.2593 | 0.0708 | 0.00025 | 0.0522 | NaN | 0.0508 | 0.0465 | 0.274505 | 0.5828 | -0.0041 | 0.0801 | 0.959452 | 0.9718 | 0.0834 | 0.0567 | 0.141115 | 0.9514 | NaN | 0.0362 | 0.0372 | 0.330831 | 0.9708 | -0.0367 | 0.0665 | 0.581275 | 0.9977 | 0.0758 | 0.0441 | 0.085186 | 0.9967 | NaN | 0.0599 | 0.0459 | 0.1923 | 0.7516 | -0.0085 | 0.0795 | 0.915069 | 0.9654 | 0.1006 | 0.0561 | 0.072837 | 0.7232 |
| DG 30:1 | 560.4423 | 24.64577 | Lipid | Diacylglycerol | 0.3299 | 0.0816 | 0.000053 | 0.0021 | 0.2259 | 0.1306 | 0.083644 | 0.3252 | 0.4063 | 0.1021 | 0.000069 | 0.0031 | NaN | 0.2388 | 0.0787 | 0.0024 | 0.0497 | 0.1292 | 0.1172 | 0.270048 | 0.637 | 0.3265 | 0.1013 | 0.001271 | 0.0458 | NaN | 0.2023 | 0.0587 | 0.000566 | 0.024 | 0.1696 | 0.0912 | 0.062853 | 0.5028 | 0.2319 | 0.0764 | 0.002413 | 0.111 | NaN | 0.0627 | 0.046 | 0.173137 | 0.5115 | -0.0071 | 0.0728 | 0.922667 | 0.9554 | 0.1089 | 0.0583 | 0.061856 | 0.8712 | NaN | 0.0901 | 0.0361 | 0.012569 | 0.7645 | 0.0371 | 0.0597 | 0.534053 | 0.9977 | 0.1322 | 0.0441 | 0.002727 | 0.4891 | NaN | 0.0671 | 0.0456 | 0.1409 | 0.7516 | -0.0131 | 0.0722 | 0.855699 | 0.9335 | 0.1229 | 0.0578 | 0.033635 | 0.6979 |
| DG 32:1 | 588.4736 | 25.42276 | Lipid | Diacylglycerol | 0.368 | 0.0804 | 0.000005 | 0.0004 | 0.2309 | 0.1223 | 0.059067 | 0.2819 | 0.4828 | 0.1039 | 0.000003 | 0.0005 | NaN | 0.275 | 0.078 | 0.000424 | 0.02 | 0.1542 | 0.1092 | 0.157853 | 0.5063 | 0.3945 | 0.1054 | 0.000183 | 0.0202 | NaN | 0.2349 | 0.0579 | 0.00005 | 0.0062 | 0.197 | 0.0847 | 0.020054 | 0.3282 | 0.2696 | 0.0799 | 0.000739 | 0.0583 | NaN | 0.0419 | 0.0468 | 0.371018 | 0.6693 | -0.0552 | 0.0692 | 0.425062 | 0.6926 | 0.1325 | 0.0615 | 0.031102 | 0.8712 | NaN | 0.0747 | 0.0366 | 0.041441 | 0.9656 | 0.0274 | 0.0563 | 0.626395 | 0.9977 | 0.1206 | 0.0477 | 0.011379 | 0.6141 | NaN | 0.049 | 0.0463 | 0.289787 | 0.7695 | -0.0506 | 0.0686 | 0.460962 | 0.744 | 0.1415 | 0.0612 | 0.020676 | 0.6979 |
| DG 33:1 | 602.4901 | 25.90679 | Lipid | Diacylglycerol | 0.3317 | 0.0812 | 0.000044 | 0.002 | 0.2219 | 0.1211 | 0.066963 | 0.2957 | 0.4256 | 0.1072 | 0.000072 | 0.0031 | NaN | 0.2585 | 0.0773 | 0.000825 | 0.025 | 0.1859 | 0.1067 | 0.081496 | 0.441 | 0.3444 | 0.106 | 0.001161 | 0.0458 | NaN | 0.2361 | 0.0575 | 0.00004 | 0.0062 | 0.1928 | 0.0838 | 0.021503 | 0.3282 | 0.2747 | 0.0785 | 0.000466 | 0.0522 | NaN | 0.0068 | 0.0468 | 0.884837 | 0.9579 | -0.0794 | 0.0685 | 0.246802 | 0.5603 | 0.084 | 0.0623 | 0.177708 | 0.9514 | NaN | 0.0754 | 0.0363 | 0.037748 | 0.9471 | 0.0588 | 0.0551 | 0.286324 | 0.9834 | 0.0939 | 0.048 | 0.050413 | 0.9967 | NaN | 0.0043 | 0.0465 | 0.926879 | 0.9724 | -0.0673 | 0.0679 | 0.321565 | 0.6453 | 0.0707 | 0.0629 | 0.260663 | 0.7654 |
| DG 34:1 | 616.5049 | 26.494192 | Lipid | Diacylglycerol | 0.3759 | 0.0799 | 0.000003 | 0.0004 | 0.2891 | 0.1269 | 0.022771 | 0.2091 | 0.4441 | 0.1012 | 0.000011 | 0.001 | NaN | 0.2887 | 0.0772 | 0.000185 | 0.0129 | 0.2156 | 0.1132 | 0.056758 | 0.4173 | 0.3603 | 0.1017 | 0.000398 | 0.0244 | NaN | 0.211 | 0.0586 | 0.00032 | 0.0161 | 0.1867 | 0.0896 | 0.037272 | 0.4042 | 0.2226 | 0.0787 | 0.004671 | 0.1228 | NaN | 0.0458 | 0.0467 | 0.326525 | 0.6369 | -0.0555 | 0.0734 | 0.449683 | 0.7032 | 0.13 | 0.0586 | 0.026618 | 0.8712 | NaN | 0.0784 | 0.0365 | 0.031888 | 0.8777 | 0.0658 | 0.0588 | 0.262862 | 0.9821 | 0.0913 | 0.0465 | 0.049558 | 0.9967 | NaN | 0.0571 | 0.0461 | 0.215724 | 0.7516 | -0.0405 | 0.0726 | 0.577234 | 0.8075 | 0.1367 | 0.0584 | 0.019239 | 0.6979 |
| DG 35:1 | 630.5215 | 27.154875 | Lipid | Diacylglycerol | 0.3059 | 0.0812 | 0.000165 | 0.0051 | 0.2624 | 0.1406 | 0.062077 | 0.2856 | 0.3381 | 0.0977 | 0.000541 | 0.0166 | NaN | 0.2358 | 0.077 | 0.002199 | 0.0486 | 0.2045 | 0.1244 | 0.100155 | 0.4459 | 0.2727 | 0.0952 | 0.004176 | 0.1048 | NaN | 0.1743 | 0.0586 | 0.00293 | 0.0735 | 0.2194 | 0.0976 | 0.024508 | 0.3282 | 0.1509 | 0.0742 | 0.041953 | 0.3772 | NaN | 0.0498 | 0.0455 | 0.273473 | 0.5828 | -0.0327 | 0.0792 | 0.679793 | 0.8471 | 0.0964 | 0.0542 | 0.075275 | 0.8712 | NaN | 0.0557 | 0.0362 | 0.123553 | 0.9708 | 0.0624 | 0.0642 | 0.331194 | 0.9977 | 0.0562 | 0.0432 | 0.193418 | 0.9967 | NaN | 0.0537 | 0.0451 | 0.233585 | 0.7516 | -0.0156 | 0.0783 | 0.841993 | 0.924 | 0.094 | 0.0544 | 0.084034 | 0.7232 |
| DG 36:1 | 644.5369 | 28.001514 | Lipid | Diacylglycerol | 0.3543 | 0.0814 | 0.000014 | 0.0008 | 0.2892 | 0.1389 | 0.037289 | 0.2428 | 0.3867 | 0.099 | 0.000094 | 0.0037 | NaN | 0.2635 | 0.0787 | 0.000809 | 0.025 | 0.1886 | 0.1247 | 0.130571 | 0.4744 | 0.3077 | 0.0985 | 0.001787 | 0.058 | NaN | 0.1546 | 0.0608 | 0.010941 | 0.1776 | 0.1246 | 0.0998 | 0.211954 | 0.6538 | 0.1653 | 0.0771 | 0.031956 | 0.3392 | NaN | 0.0618 | 0.0465 | 0.184279 | 0.5115 | -0.0144 | 0.0788 | 0.854998 | 0.9253 | 0.1103 | 0.0561 | 0.04914 | 0.8712 | NaN | 0.0525 | 0.0372 | 0.158207 | 0.9708 | 0.0413 | 0.0643 | 0.521075 | 0.9977 | 0.0605 | 0.0449 | 0.178167 | 0.9967 | NaN | 0.0729 | 0.0459 | 0.112295 | 0.7516 | -0.0062 | 0.078 | 0.936714 | 0.9719 | 0.1225 | 0.0557 | 0.027834 | 0.6979 |
| DG 32:2 | 586.4577 | 24.862595 | Lipid | Diacylglycerol | 0.3805 | 0.0799 | 0.000002 | 0.0004 | 0.1761 | 0.1302 | 0.176027 | 0.4519 | 0.5131 | 0.0969 | 0.0 | <.0001 | NaN | 0.3004 | 0.0767 | 0.000089 | 0.0098 | 0.0895 | 0.1162 | 0.440844 | 0.7563 | 0.4455 | 0.0958 | 0.000003 | 0.0014 | NaN | 0.2359 | 0.0579 | 0.000046 | 0.0062 | 0.1405 | 0.0907 | 0.121374 | 0.577 | 0.3114 | 0.0745 | 0.00003 | 0.0163 | NaN | 0.0358 | 0.047 | 0.446231 | 0.7294 | -0.1067 | 0.072 | 0.138377 | 0.4085 | 0.1435 | 0.0596 | 0.016018 | 0.8712 | NaN | 0.0944 | 0.0363 | 0.009193 | 0.7645 | 0.0196 | 0.059 | 0.739024 | 0.9977 | 0.1569 | 0.0447 | 0.000447 | 0.1235 | NaN | 0.0494 | 0.0464 | 0.286355 | 0.7695 | -0.0981 | 0.0714 | 0.169617 | 0.5381 | 0.1617 | 0.0587 | 0.005876 | 0.6979 |
| DG 34:2 | 614.4888 | 25.732864 | Lipid | Diacylglycerol | 0.3365 | 0.08 | 0.000026 | 0.0013 | 0.1939 | 0.1249 | 0.120548 | 0.3728 | 0.4495 | 0.104 | 0.000016 | 0.0011 | NaN | 0.2673 | 0.076 | 0.000435 | 0.02 | 0.159 | 0.11 | 0.148264 | 0.4937 | 0.3712 | 0.1031 | 0.00032 | 0.0222 | NaN | 0.2055 | 0.0577 | 0.000369 | 0.017 | 0.1596 | 0.0869 | 0.066259 | 0.5225 | 0.2381 | 0.0799 | 0.002874 | 0.122 | NaN | 0.0087 | 0.0464 | 0.850627 | 0.9461 | -0.1099 | 0.0698 | 0.115121 | 0.3784 | 0.1249 | 0.0603 | 0.038388 | 0.8712 | NaN | 0.0814 | 0.0358 | 0.022871 | 0.8627 | 0.0513 | 0.0565 | 0.363817 | 0.9977 | 0.1102 | 0.047 | 0.019075 | 0.8099 | NaN | 0.0203 | 0.0458 | 0.656949 | 0.8716 | -0.088 | 0.0691 | 0.203158 | 0.5437 | 0.1247 | 0.0604 | 0.039102 | 0.6979 |
| DG 35:2 | 628.5046 | 26.1662 | Lipid | Diacylglycerol | 0.3893 | 0.0836 | 0.000003 | 0.0004 | 0.2933 | 0.129 | 0.02296 | 0.2091 | 0.4552 | 0.1081 | 0.000025 | 0.0016 | NaN | 0.3195 | 0.0793 | 0.000056 | 0.0077 | 0.2516 | 0.1136 | 0.026794 | 0.3521 | 0.3812 | 0.1059 | 0.00032 | 0.0222 | NaN | 0.24 | 0.0605 | 0.000073 | 0.0068 | 0.2617 | 0.0886 | 0.003134 | 0.173 | 0.2255 | 0.0836 | 0.006958 | 0.1545 | NaN | 0.0469 | 0.0488 | 0.335597 | 0.6432 | -0.0425 | 0.0744 | 0.567347 | 0.7754 | 0.1189 | 0.0626 | 0.057659 | 0.8712 | NaN | 0.0929 | 0.0379 | 0.01417 | 0.7645 | 0.0774 | 0.0595 | 0.19313 | 0.9357 | 0.1072 | 0.0487 | 0.02773 | 0.8504 | NaN | 0.0547 | 0.0482 | 0.256364 | 0.7516 | -0.0349 | 0.0736 | 0.635452 | 0.8215 | 0.1274 | 0.0624 | 0.041077 | 0.6979 |
| DG 34:3 | 612.4738 | 25.196987 | Lipid | Diacylglycerol | 0.3405 | 0.0799 | 0.00002 | 0.0011 | 0.1729 | 0.1208 | 0.152481 | 0.4298 | 0.4785 | 0.1034 | 0.000004 | 0.0005 | NaN | 0.2641 | 0.0763 | 0.000541 | 0.0213 | 0.1276 | 0.1067 | 0.231853 | 0.5936 | 0.3997 | 0.1029 | 0.000103 | 0.0187 | NaN | 0.2143 | 0.0575 | 0.000192 | 0.0151 | 0.1634 | 0.0837 | 0.050779 | 0.4751 | 0.2647 | 0.0796 | 0.000886 | 0.0611 | NaN | -0.0146 | 0.0468 | 0.755716 | 0.8904 | -0.1205 | 0.0671 | 0.072556 | 0.297 | 0.0868 | 0.063 | 0.168199 | 0.9514 | NaN | 0.0787 | 0.0359 | 0.028313 | 0.8683 | 0.0263 | 0.0548 | 0.631229 | 0.9977 | 0.131 | 0.0469 | 0.005226 | 0.4891 | NaN | 0.0107 | 0.046 | 0.816303 | 0.9499 | -0.0845 | 0.0665 | 0.203781 | 0.5437 | 0.1035 | 0.0624 | 0.097277 | 0.7232 |
| DG 35:3 | 626.49 | 25.472881 | Lipid | Diacylglycerol | 0.3738 | 0.0809 | 0.000004 | 0.0004 | 0.1945 | 0.1216 | 0.109781 | 0.3717 | 0.518 | 0.1059 | 0.000001 | 0.0003 | NaN | 0.3275 | 0.0757 | 0.000015 | 0.0042 | 0.1783 | 0.1067 | 0.094606 | 0.4459 | 0.4639 | 0.1017 | 0.000005 | 0.0014 | NaN | 0.2543 | 0.0578 | 0.000011 | 0.006 | 0.2407 | 0.0826 | 0.003589 | 0.1766 | 0.2877 | 0.0823 | 0.000472 | 0.0522 | NaN | 0.0327 | 0.0474 | 0.489785 | 0.7552 | -0.106 | 0.0681 | 0.119794 | 0.3845 | 0.1595 | 0.0627 | 0.011013 | 0.8712 | NaN | 0.072 | 0.037 | 0.051568 | 0.9656 | 0.0097 | 0.0557 | 0.862226 | 0.9977 | 0.1358 | 0.0489 | 0.005539 | 0.4891 | NaN | 0.0358 | 0.0469 | 0.446339 | 0.8178 | -0.1046 | 0.0675 | 0.121512 | 0.4626 | 0.1662 | 0.0625 | 0.00783 | 0.6979 |
| DG 36:3 | 640.5052 | 25.970724 | Lipid | Diacylglycerol | 0.2625 | 0.0859 | 0.002245 | 0.0387 | 0.0779 | 0.1219 | 0.522969 | 0.8001 | 0.4491 | 0.1192 | 0.000165 | 0.0061 | NaN | 0.221 | 0.0801 | 0.005783 | 0.0887 | 0.1182 | 0.1068 | 0.268563 | 0.637 | 0.3723 | 0.116 | 0.001328 | 0.0458 | NaN | 0.1599 | 0.0612 | 0.00902 | 0.166 | 0.1124 | 0.0846 | 0.183997 | 0.652 | 0.2105 | 0.0911 | 0.020911 | 0.3181 | NaN | 0.0006 | 0.0476 | 0.990785 | 0.9999 | -0.0908 | 0.0658 | 0.167256 | 0.4504 | 0.1185 | 0.0674 | 0.078728 | 0.8712 | NaN | 0.079 | 0.0371 | 0.03339 | 0.8777 | 0.0301 | 0.0543 | 0.579353 | 0.9977 | 0.1368 | 0.0515 | 0.007875 | 0.4891 | NaN | 0.0374 | 0.0468 | 0.424756 | 0.8178 | -0.0711 | 0.0653 | 0.276256 | 0.6201 | 0.1699 | 0.0655 | 0.009524 | 0.6979 |
| DG 36:4 | 638.4888 | 25.322704 | Lipid | Diacylglycerol | 0.2937 | 0.084 | 0.000471 | 0.0118 | 0.044 | 0.1527 | 0.773388 | 0.9222 | 0.4041 | 0.0973 | 0.000033 | 0.0018 | NaN | 0.2532 | 0.0783 | 0.001223 | 0.0338 | 0.0717 | 0.134 | 0.592433 | 0.8258 | 0.356 | 0.0933 | 0.000135 | 0.0187 | NaN | 0.1874 | 0.0599 | 0.001753 | 0.0484 | 0.1446 | 0.1062 | 0.173193 | 0.6495 | 0.2135 | 0.0742 | 0.004032 | 0.1228 | NaN | 0.0549 | 0.0466 | 0.238234 | 0.5457 | -0.1226 | 0.0817 | 0.133416 | 0.4016 | 0.1515 | 0.0542 | 0.00522 | 0.8712 | NaN | 0.0944 | 0.0365 | 0.00961 | 0.7645 | -0.0065 | 0.068 | 0.923427 | 0.9977 | 0.1487 | 0.0415 | 0.000342 | 0.1235 | NaN | 0.0801 | 0.0458 | 0.080119 | 0.7496 | -0.1064 | 0.0811 | 0.189704 | 0.5437 | 0.1791 | 0.053 | 0.000731 | 0.4034 |
| DG 38:4 | 666.5223 | 26.351738 | Lipid | Diacylglycerol | 0.2034 | 0.0851 | 0.016887 | 0.1377 | 0.0651 | 0.1186 | 0.583111 | 0.8296 | 0.3416 | 0.1209 | 0.004729 | 0.0979 | NaN | 0.1836 | 0.0788 | 0.01987 | 0.2151 | 0.0983 | 0.104 | 0.344451 | 0.702 | 0.2944 | 0.1148 | 0.01037 | 0.2054 | NaN | 0.1183 | 0.0604 | 0.050378 | 0.4089 | 0.0999 | 0.0824 | 0.225644 | 0.6655 | 0.1348 | 0.0903 | 0.13567 | 0.5306 | NaN | 0.0069 | 0.0462 | 0.881636 | 0.9579 | -0.0703 | 0.0639 | 0.271323 | 0.5824 | 0.1036 | 0.0652 | 0.112199 | 0.8976 | NaN | 0.0391 | 0.0367 | 0.287083 | 0.9708 | -0.0156 | 0.053 | 0.76838 | 0.9977 | 0.0999 | 0.0508 | 0.049455 | 0.9967 | NaN | 0.0321 | 0.0456 | 0.48187 | 0.8239 | -0.0744 | 0.0634 | 0.240371 | 0.5769 | 0.1577 | 0.0637 | 0.013219 | 0.6979 |
| DG 36:5 | 636.472 | 24.87105 | Lipid | Diacylglycerol | 0.175 | 0.0834 | 0.035848 | 0.2223 | -0.0094 | 0.1177 | 0.936371 | 0.9682 | 0.3551 | 0.1143 | 0.001891 | 0.0497 | NaN | 0.1414 | 0.0775 | 0.068166 | 0.3516 | -0.0193 | 0.1033 | 0.851995 | 0.9418 | 0.3112 | 0.1085 | 0.004136 | 0.1048 | NaN | 0.1088 | 0.059 | 0.065139 | 0.4439 | 0.0393 | 0.0823 | 0.633124 | 0.8442 | 0.1885 | 0.0843 | 0.025317 | 0.3327 | NaN | -0.0738 | 0.0453 | 0.103418 | 0.4581 | -0.1612 | 0.0617 | 0.009023 | 0.1672 | 0.0179 | 0.0647 | 0.781528 | 0.9994 | NaN | 0.0577 | 0.0355 | 0.104071 | 0.9708 | -0.0042 | 0.0524 | 0.936079 | 0.9977 | 0.1266 | 0.0477 | 0.007975 | 0.4891 | NaN | -0.0365 | 0.0448 | 0.415239 | 0.8132 | -0.1441 | 0.0615 | 0.019062 | 0.2716 | 0.0777 | 0.0633 | 0.219661 | 0.7294 |
| DG 38:5 | 664.5056 | 25.86453 | Lipid | Diacylglycerol | 0.2569 | 0.0865 | 0.002975 | 0.0483 | 0.1965 | 0.1237 | 0.112115 | 0.3717 | 0.3117 | 0.1199 | 0.009342 | 0.1563 | NaN | 0.1853 | 0.0817 | 0.02335 | 0.2243 | 0.2072 | 0.1079 | 0.054908 | 0.4173 | 0.2054 | 0.1189 | 0.083985 | 0.5586 | NaN | 0.1393 | 0.062 | 0.024617 | 0.28 | 0.1481 | 0.0863 | 0.086242 | 0.549 | 0.1216 | 0.0889 | 0.171474 | 0.5737 | NaN | -0.0042 | 0.0479 | 0.930875 | 0.9723 | -0.0553 | 0.069 | 0.422312 | 0.6917 | 0.0527 | 0.0652 | 0.419179 | 0.9735 | NaN | 0.0558 | 0.0376 | 0.13803 | 0.9708 | 0.0496 | 0.056 | 0.376303 | 0.9977 | 0.0616 | 0.0508 | 0.225577 | 0.9967 | NaN | 0.0045 | 0.0474 | 0.924569 | 0.9724 | -0.0474 | 0.0683 | 0.487612 | 0.7613 | 0.0604 | 0.0651 | 0.353718 | 0.8297 |
| FA 17:0 | 270.256 | 22.96632 | Lipid | Fatty Acid | 0.2131 | 0.0814 | 0.008824 | 0.0937 | 0.2106 | 0.1216 | 0.083364 | 0.3252 | 0.2018 | 0.1093 | 0.064812 | 0.3614 | NaN | 0.1952 | 0.0753 | 0.009563 | 0.126 | 0.1568 | 0.1077 | 0.145478 | 0.4927 | 0.1947 | 0.1024 | 0.057395 | 0.4962 | NaN | 0.1449 | 0.0575 | 0.011781 | 0.1806 | 0.1926 | 0.084 | 0.021885 | 0.3282 | 0.1015 | 0.0786 | 0.196903 | 0.614 | NaN | 0.0316 | 0.0442 | 0.474543 | 0.7484 | 0.0059 | 0.0676 | 0.929939 | 0.9554 | 0.0559 | 0.0575 | 0.330685 | 0.9622 | NaN | 0.0379 | 0.0353 | 0.282279 | 0.9708 | 0.029 | 0.0557 | 0.601736 | 0.9977 | 0.0424 | 0.0452 | 0.348292 | 0.9967 | NaN | 0.0276 | 0.0439 | 0.52968 | 0.8373 | 0.0035 | 0.0671 | 0.958133 | 0.9831 | 0.0495 | 0.0576 | 0.390277 | 0.8329 |
| FA 18:3 | 278.2229 | 22.803661 | Lipid | Fatty Acid | 0.2339 | 0.081 | 0.003857 | 0.0532 | 0.1565 | 0.1211 | 0.196393 | 0.4734 | 0.2916 | 0.1079 | 0.006872 | 0.1185 | NaN | 0.2231 | 0.0748 | 0.002848 | 0.0531 | 0.1812 | 0.1057 | 0.086469 | 0.4459 | 0.2664 | 0.1016 | 0.008747 | 0.1857 | NaN | 0.1636 | 0.0572 | 0.00422 | 0.0935 | 0.2076 | 0.0828 | 0.012194 | 0.2845 | 0.1249 | 0.0799 | 0.117915 | 0.5085 | NaN | -0.005 | 0.0447 | 0.910626 | 0.963 | -0.0756 | 0.0668 | 0.257529 | 0.5687 | 0.0604 | 0.0587 | 0.303706 | 0.9622 | NaN | 0.0336 | 0.0354 | 0.34267 | 0.9708 | 0.0256 | 0.0547 | 0.640424 | 0.9977 | 0.04 | 0.0462 | 0.387105 | 0.9967 | NaN | 0.0145 | 0.0442 | 0.741789 | 0.9202 | -0.0448 | 0.0661 | 0.497537 | 0.7736 | 0.0696 | 0.0585 | 0.234381 | 0.7365 |
| AC 3:0 | 217.1321 | 1.629795 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.2506 | 0.0859 | 0.003528 | 0.0526 | 0.6012 | 0.1396 | 0.000017 | 0.0092 | 0.0937 | 0.1061 | 0.377567 | 0.7082 | NaN | 0.1874 | 0.0808 | 0.020394 | 0.2162 | 0.4757 | 0.1277 | 0.000196 | 0.0464 | 0.048 | 0.1005 | 0.6334 | 0.8939 | NaN | 0.1709 | 0.0608 | 0.004911 | 0.1027 | 0.3931 | 0.1013 | 0.000104 | 0.0576 | 0.0664 | 0.0752 | 0.377766 | 0.7398 | NaN | 0.0699 | 0.0465 | 0.132809 | 0.4825 | 0.1886 | 0.085 | 0.026429 | 0.2227 | 0.0222 | 0.0549 | 0.685546 | 0.9994 | NaN | 0.0168 | 0.0378 | 0.655429 | 0.9708 | 0.119 | 0.0721 | 0.09889 | 0.7937 | -0.0257 | 0.0433 | 0.552105 | 0.9967 | NaN | 0.088 | 0.0459 | 0.055181 | 0.7271 | 0.1561 | 0.0858 | 0.068799 | 0.3895 | 0.0638 | 0.0545 | 0.242205 | 0.7389 |
| AC 4:0 | 231.1476 | 2.899889 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.2597 | 0.0867 | 0.002731 | 0.0457 | 0.417 | 0.1322 | 0.001608 | 0.0683 | 0.1474 | 0.1135 | 0.194119 | 0.5449 | NaN | 0.2489 | 0.08 | 0.00187 | 0.0458 | 0.3348 | 0.1182 | 0.004611 | 0.1934 | 0.1567 | 0.1062 | 0.140173 | 0.6249 | NaN | 0.0723 | 0.0635 | 0.254899 | 0.7568 | 0.1544 | 0.0999 | 0.122081 | 0.577 | 0.0063 | 0.0822 | 0.938725 | 0.9766 | NaN | 0.0653 | 0.0471 | 0.166161 | 0.5067 | 0.0842 | 0.0775 | 0.277494 | 0.5869 | 0.0619 | 0.0587 | 0.291629 | 0.9622 | NaN | 0.045 | 0.0379 | 0.234792 | 0.9708 | 0.104 | 0.0632 | 0.099542 | 0.7937 | 0.0047 | 0.0466 | 0.919745 | 0.9967 | NaN | 0.0653 | 0.0468 | 0.162907 | 0.7516 | 0.0883 | 0.0767 | 0.249632 | 0.5864 | 0.0568 | 0.0589 | 0.334463 | 0.8205 |
| AC 8:1 | 285.1943 | 9.563584 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.345 | 0.0854 | 0.000053 | 0.0021 | 0.4749 | 0.1221 | 0.000101 | 0.0093 | 0.2674 | 0.1175 | 0.022928 | 0.2583 | NaN | 0.3466 | 0.0784 | 0.00001 | 0.0042 | 0.4526 | 0.1058 | 0.000019 | 0.0103 | 0.2723 | 0.1098 | 0.013116 | 0.2413 | NaN | 0.2003 | 0.0617 | 0.001178 | 0.0407 | 0.3039 | 0.0884 | 0.000583 | 0.0804 | 0.1044 | 0.0862 | 0.225845 | 0.6205 | NaN | -0.0096 | 0.0494 | 0.845937 | 0.9461 | 0.0303 | 0.0773 | 0.695326 | 0.8567 | -0.0271 | 0.0642 | 0.6734 | 0.9994 | NaN | 0.0207 | 0.039 | 0.594698 | 0.9708 | 0.1123 | 0.0607 | 0.064442 | 0.6841 | -0.0508 | 0.0503 | 0.312374 | 0.9967 | NaN | -0.0055 | 0.0489 | 0.910427 | 0.9724 | 0.0477 | 0.076 | 0.530198 | 0.7867 | -0.0366 | 0.0644 | 0.570599 | 0.9321 |
| AC 5:0 (OH) | 261.1578 | 1.981441 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.2855 | 0.087 | 0.001028 | 0.021 | 0.4027 | 0.1326 | 0.002391 | 0.088 | 0.1988 | 0.1143 | 0.082052 | 0.3905 | NaN | 0.2448 | 0.081 | 0.002521 | 0.0497 | 0.303 | 0.1196 | 0.011327 | 0.2842 | 0.1739 | 0.1076 | 0.106149 | 0.5745 | NaN | 0.1742 | 0.0621 | 0.005022 | 0.1027 | 0.2956 | 0.0928 | 0.001455 | 0.1338 | 0.0794 | 0.0826 | 0.336542 | 0.7118 | NaN | 0.1145 | 0.0468 | 0.014541 | 0.3584 | 0.0981 | 0.0767 | 0.200903 | 0.4973 | 0.1356 | 0.0582 | 0.019901 | 0.8712 | NaN | 0.058 | 0.0382 | 0.12876 | 0.9708 | 0.0679 | 0.064 | 0.288607 | 0.9834 | 0.049 | 0.047 | 0.297945 | 0.9967 | NaN | 0.1076 | 0.0466 | 0.020925 | 0.7271 | 0.0823 | 0.0765 | 0.282224 | 0.6236 | 0.1316 | 0.0584 | 0.024309 | 0.6979 |
| FA 8:1 (DiC) | 172.074 | 4.380399 | Lipid | Fatty Acid, Dicarboxylate | 0.1873 | 0.0861 | 0.02968 | 0.21 | 0.4792 | 0.1483 | 0.001234 | 0.0568 | 0.0546 | 0.1041 | 0.600177 | 0.8451 | NaN | 0.1487 | 0.0802 | 0.063579 | 0.3472 | 0.388 | 0.1325 | 0.003417 | 0.1769 | 0.0316 | 0.0979 | 0.746776 | 0.9421 | NaN | 0.0233 | 0.0624 | 0.708724 | 0.9414 | 0.2619 | 0.1083 | 0.015615 | 0.3192 | -0.079 | 0.0746 | 0.289574 | 0.6745 | NaN | 0.05 | 0.0461 | 0.277526 | 0.5838 | 0.0723 | 0.0881 | 0.41168 | 0.6798 | 0.0382 | 0.0535 | 0.475366 | 0.9735 | NaN | 0.0556 | 0.0368 | 0.130883 | 0.9708 | 0.1532 | 0.0699 | 0.028551 | 0.6225 | 0.0146 | 0.0421 | 0.72941 | 0.9967 | NaN | 0.0562 | 0.0456 | 0.218176 | 0.7516 | 0.0316 | 0.0886 | 0.720878 | 0.8612 | 0.0645 | 0.0533 | 0.226439 | 0.7294 |
| FA 9:1 (DiC) | 186.0894 | 6.299434 | Lipid | Fatty Acid, Dicarboxylate | 0.2294 | 0.0828 | 0.00561 | 0.0704 | 0.484 | 0.1233 | 0.000087 | 0.0093 | 0.0592 | 0.1087 | 0.586039 | 0.8382 | NaN | 0.1825 | 0.0774 | 0.018381 | 0.2071 | 0.3768 | 0.1125 | 0.000809 | 0.0744 | 0.0361 | 0.1022 | 0.723978 | 0.9342 | NaN | 0.049 | 0.0606 | 0.419494 | 0.8456 | 0.2216 | 0.0947 | 0.019317 | 0.3282 | -0.0488 | 0.0777 | 0.530092 | 0.826 | NaN | 0.1001 | 0.0442 | 0.023353 | 0.3584 | 0.1568 | 0.0732 | 0.032331 | 0.2309 | 0.0594 | 0.0557 | 0.285974 | 0.9622 | NaN | 0.0858 | 0.0354 | 0.015234 | 0.7645 | 0.179 | 0.0587 | 0.002281 | 0.2518 | 0.031 | 0.0439 | 0.479984 | 0.9967 | NaN | 0.0943 | 0.0439 | 0.031829 | 0.7271 | 0.1244 | 0.074 | 0.092849 | 0.4133 | 0.0737 | 0.0556 | 0.184949 | 0.7294 |
| FA 12:1 (DiC) | 228.1364 | 15.499843 | Lipid | Fatty Acid, Dicarboxylate | -0.2344 | 0.0808 | 0.003734 | 0.0529 | -0.2281 | 0.1283 | 0.075368 | 0.313 | -0.2365 | 0.1038 | 0.022679 | 0.2583 | NaN | -0.1672 | 0.0764 | 0.028517 | 0.2422 | -0.1029 | 0.1166 | 0.377825 | 0.7136 | -0.1831 | 0.0992 | 0.065018 | 0.4962 | NaN | -0.1331 | 0.0577 | 0.021082 | 0.2569 | -0.0888 | 0.0917 | 0.332901 | 0.7705 | -0.1492 | 0.0744 | 0.044838 | 0.3772 | NaN | -0.0044 | 0.0446 | 0.920597 | 0.9698 | -0.073 | 0.0703 | 0.298686 | 0.6062 | 0.0343 | 0.0568 | 0.546645 | 0.9885 | NaN | 0.0238 | 0.0358 | 0.506679 | 0.9708 | -0.0328 | 0.0588 | 0.576375 | 0.9977 | 0.0648 | 0.0445 | 0.145177 | 0.9967 | NaN | -0.0003 | 0.0443 | 0.995426 | 0.9972 | -0.1114 | 0.0688 | 0.105476 | 0.4479 | 0.0728 | 0.0573 | 0.203581 | 0.7294 |
| FA 28:2 (DiC) | 450.3724 | 22.945812 | Lipid | Fatty Acid, Dicarboxylate | -0.1725 | 0.0864 | 0.045849 | 0.2457 | -0.35 | 0.1185 | 0.003151 | 0.0917 | 0.0256 | 0.1227 | 0.834648 | 0.9565 | NaN | -0.1779 | 0.0797 | 0.025597 | 0.2243 | -0.2814 | 0.1057 | 0.007762 | 0.238 | -0.0149 | 0.1156 | 0.897489 | 0.9798 | NaN | -0.0808 | 0.0614 | 0.188393 | 0.6946 | -0.088 | 0.0906 | 0.331092 | 0.7705 | -0.0746 | 0.0872 | 0.39254 | 0.7576 | NaN | -0.1118 | 0.0453 | 0.013478 | 0.3584 | -0.172 | 0.0652 | 0.008284 | 0.1672 | -0.0595 | 0.063 | 0.345395 | 0.9622 | NaN | -0.0309 | 0.037 | 0.404231 | 0.9708 | -0.0596 | 0.0569 | 0.294765 | 0.9835 | 0.0003 | 0.0496 | 0.99499 | 0.9967 | NaN | -0.0727 | 0.0454 | 0.109696 | 0.7516 | -0.1383 | 0.0659 | 0.035751 | 0.3022 | -0.013 | 0.0632 | 0.836827 | 0.9809 |
| SN-glycero-3-phosphocholine | 257.1031 | 0.614226 | Lipid | Phosphatidylcholine | 0.2019 | 0.084 | 0.016241 | 0.1377 | 0.024 | 0.1332 | 0.857275 | 0.9521 | 0.3025 | 0.1077 | 0.004964 | 0.0979 | NaN | 0.199 | 0.0775 | 0.010257 | 0.1287 | 0.0706 | 0.117 | 0.546143 | 0.7852 | 0.2859 | 0.101 | 0.004662 | 0.1119 | NaN | 0.0581 | 0.0607 | 0.338594 | 0.792 | -0.0773 | 0.0933 | 0.406996 | 0.784 | 0.1502 | 0.0792 | 0.057887 | 0.4204 | NaN | 0.0605 | 0.045 | 0.179304 | 0.5115 | 0.0616 | 0.0712 | 0.386886 | 0.6687 | 0.0629 | 0.0588 | 0.285004 | 0.9622 | NaN | 0.0404 | 0.0362 | 0.264309 | 0.9708 | 0.0282 | 0.0592 | 0.633728 | 0.9977 | 0.0498 | 0.0462 | 0.28082 | 0.9967 | NaN | 0.0961 | 0.0442 | 0.029671 | 0.7271 | 0.1315 | 0.0699 | 0.059934 | 0.387 | 0.0782 | 0.0585 | 0.181549 | 0.7294 |
| PC 34:0/PE 37:0 | 761.5923 | 25.413399 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2026 | 0.0831 | 0.014833 | 0.1321 | -0.343 | 0.0998 | 0.000587 | 0.0405 | 0.0256 | 0.1376 | 0.852543 | 0.9565 | NaN | -0.1622 | 0.0775 | 0.03642 | 0.2832 | -0.2548 | 0.091 | 0.005131 | 0.1934 | 0.0384 | 0.1291 | 0.766181 | 0.9436 | NaN | -0.0952 | 0.0595 | 0.109247 | 0.5674 | -0.1616 | 0.0747 | 0.030475 | 0.3505 | 0.0057 | 0.0975 | 0.953223 | 0.9766 | NaN | -0.0939 | 0.0441 | 0.033322 | 0.3584 | -0.1065 | 0.058 | 0.066522 | 0.2844 | -0.0814 | 0.0706 | 0.249002 | 0.9622 | NaN | -0.0671 | 0.0355 | 0.058845 | 0.9656 | -0.1335 | 0.0464 | 0.00404 | 0.307 | 0.0365 | 0.0555 | 0.5105 | 0.9967 | NaN | -0.0694 | 0.0441 | 0.116015 | 0.7516 | -0.1146 | 0.0572 | 0.04524 | 0.3202 | -0.0008 | 0.0709 | 0.991003 | 0.996 |
| PC 40:4/PE 43:4 | 837.6238 | 25.627386 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2333 | 0.084 | 0.005514 | 0.0704 | 0.2676 | 0.1194 | 0.025038 | 0.2194 | 0.2437 | 0.1205 | 0.043164 | 0.3531 | NaN | 0.2222 | 0.0777 | 0.004218 | 0.0751 | 0.2415 | 0.1048 | 0.02119 | 0.3387 | 0.2257 | 0.1132 | 0.046111 | 0.4545 | NaN | 0.1808 | 0.059 | 0.002179 | 0.0573 | 0.1886 | 0.0838 | 0.024413 | 0.3282 | 0.1532 | 0.0862 | 0.075323 | 0.455 | NaN | 0.0027 | 0.0462 | 0.953368 | 0.9818 | 0.0445 | 0.0672 | 0.508174 | 0.75 | -0.007 | 0.0648 | 0.914517 | 0.9994 | NaN | -0.006 | 0.037 | 0.871068 | 0.9722 | 0.0021 | 0.0563 | 0.969691 | 0.9977 | -0.0161 | 0.0508 | 0.75081 | 0.9967 | NaN | -0.0211 | 0.046 | 0.646407 | 0.8687 | 0.0319 | 0.0669 | 0.633264 | 0.8206 | -0.0536 | 0.0654 | 0.41266 | 0.8487 |
| PC 31:5/PE 34:5 | 707.509 | 25.409264 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2675 | 0.0798 | 0.000807 | 0.0186 | 0.1287 | 0.1284 | 0.316193 | 0.6383 | 0.3597 | 0.1001 | 0.000327 | 0.0113 | NaN | 0.2083 | 0.0752 | 0.005611 | 0.0887 | 0.1402 | 0.1124 | 0.212153 | 0.5647 | 0.287 | 0.0983 | 0.003493 | 0.0964 | NaN | 0.1148 | 0.0582 | 0.04857 | 0.4089 | 0.0774 | 0.0899 | 0.38923 | 0.7775 | 0.1344 | 0.0777 | 0.083749 | 0.4613 | NaN | 0.024 | 0.0445 | 0.589083 | 0.8139 | -0.0464 | 0.07 | 0.506953 | 0.75 | 0.0842 | 0.0565 | 0.136153 | 0.9514 | NaN | 0.0752 | 0.0348 | 0.030616 | 0.8777 | 0.032 | 0.0575 | 0.577871 | 0.9977 | 0.1078 | 0.043 | 0.012238 | 0.6141 | NaN | 0.0524 | 0.0437 | 0.230354 | 0.7516 | -0.0449 | 0.0694 | 0.517357 | 0.7783 | 0.1283 | 0.055 | 0.019644 | 0.6979 |
| PC 35:5/PE 38:5 | 765.5672 | 25.150826 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.3013 | 0.0832 | 0.000295 | 0.0086 | -0.4873 | 0.1246 | 0.000091 | 0.0093 | -0.1497 | 0.1123 | 0.182606 | 0.5263 | NaN | -0.2589 | 0.0777 | 0.00086 | 0.025 | -0.3443 | 0.1169 | 0.003238 | 0.1769 | -0.1478 | 0.1053 | 0.160185 | 0.6552 | NaN | -0.1348 | 0.0609 | 0.026884 | 0.28 | -0.2215 | 0.0957 | 0.020656 | 0.3282 | -0.0945 | 0.0799 | 0.236529 | 0.6205 | NaN | -0.1009 | 0.0455 | 0.026561 | 0.3584 | -0.128 | 0.0753 | 0.088852 | 0.3206 | -0.0738 | 0.0579 | 0.202686 | 0.9514 | NaN | -0.0573 | 0.0369 | 0.12052 | 0.9708 | -0.0805 | 0.0633 | 0.203562 | 0.9357 | -0.0422 | 0.0458 | 0.356637 | 0.9967 | NaN | -0.0931 | 0.0453 | 0.039895 | 0.7271 | -0.094 | 0.076 | 0.216324 | 0.5528 | -0.0874 | 0.0578 | 0.13061 | 0.7232 |
| PE 36:2 | 620.5388 | 26.788805 | Lipid | Phosphatidylethanolamine | 0.2786 | 0.0845 | 0.000983 | 0.0209 | 0.1502 | 0.1283 | 0.241723 | 0.5446 | 0.3827 | 0.1101 | 0.000511 | 0.0166 | NaN | 0.2198 | 0.0795 | 0.005694 | 0.0887 | 0.1731 | 0.1121 | 0.122538 | 0.4674 | 0.3023 | 0.1081 | 0.005158 | 0.1186 | NaN | 0.1431 | 0.061 | 0.019024 | 0.2387 | 0.1246 | 0.0894 | 0.163479 | 0.6267 | 0.1559 | 0.0844 | 0.064698 | 0.4338 | NaN | 0.0205 | 0.047 | 0.663512 | 0.846 | -0.0615 | 0.0704 | 0.382213 | 0.6674 | 0.0953 | 0.0616 | 0.121843 | 0.9473 | NaN | 0.0691 | 0.0369 | 0.061457 | 0.9656 | 0.0521 | 0.0575 | 0.364591 | 0.9977 | 0.0866 | 0.0481 | 0.071632 | 0.9967 | NaN | 0.0412 | 0.0464 | 0.3745 | 0.8007 | -0.0415 | 0.0697 | 0.551947 | 0.7972 | 0.1157 | 0.061 | 0.057839 | 0.702 |
| PS 35:4 | 769.496 | 24.213146 | Lipid | Phosphatidylserine | 0.2429 | 0.0832 | 0.003498 | 0.0526 | 0.3788 | 0.1136 | 0.00085 | 0.0427 | 0.1133 | 0.1188 | 0.340045 | 0.7068 | NaN | 0.1717 | 0.0787 | 0.029111 | 0.2435 | 0.2983 | 0.1021 | 0.003494 | 0.1769 | 0.0406 | 0.1135 | 0.720596 | 0.9342 | NaN | 0.1682 | 0.0588 | 0.004237 | 0.0935 | 0.2917 | 0.0789 | 0.000216 | 0.0596 | 0.0589 | 0.0845 | 0.485641 | 0.8173 | NaN | 0.0201 | 0.0457 | 0.659318 | 0.846 | 0.045 | 0.0683 | 0.509796 | 0.7504 | -0.0121 | 0.0617 | 0.844871 | 0.9994 | NaN | 0.0191 | 0.0365 | 0.602032 | 0.9708 | 0.0463 | 0.0561 | 0.409752 | 0.9977 | -0.0045 | 0.0485 | 0.92634 | 0.9967 | NaN | 0.0043 | 0.0455 | 0.925288 | 0.9724 | 0.039 | 0.0679 | 0.565429 | 0.8024 | -0.034 | 0.0619 | 0.583385 | 0.9367 |
| PS 40:4 | 839.5813 | 25.223974 | Lipid | Phosphatidylserine | -0.2421 | 0.0897 | 0.006951 | 0.0816 | -0.3207 | 0.1177 | 0.006437 | 0.1275 | -0.114 | 0.1372 | 0.405968 | 0.7347 | NaN | -0.1936 | 0.0837 | 0.020807 | 0.2162 | -0.1948 | 0.1086 | 0.072958 | 0.4408 | -0.1067 | 0.1287 | 0.406958 | 0.8023 | NaN | -0.0814 | 0.065 | 0.210584 | 0.7091 | -0.0436 | 0.0903 | 0.629229 | 0.8438 | -0.1346 | 0.0967 | 0.163808 | 0.5601 | NaN | -0.0309 | 0.0488 | 0.527165 | 0.7799 | -0.0902 | 0.0667 | 0.176646 | 0.4578 | 0.0562 | 0.0712 | 0.430077 | 0.9735 | NaN | -0.0634 | 0.0387 | 0.101093 | 0.9708 | -0.127 | 0.0538 | 0.018222 | 0.5917 | 0.0166 | 0.0559 | 0.766756 | 0.9967 | NaN | -0.0458 | 0.0483 | 0.342917 | 0.7759 | -0.1032 | 0.0658 | 0.116537 | 0.4593 | 0.0337 | 0.0713 | 0.636829 | 0.9483 |
| PS 42:6 | 863.5603 | 25.18495 | Lipid | Phosphatidylserine | -0.2779 | 0.0839 | 0.000927 | 0.0205 | -0.2823 | 0.1339 | 0.035063 | 0.2428 | -0.26 | 0.1075 | 0.015602 | 0.2153 | NaN | -0.2335 | 0.0784 | 0.002885 | 0.0531 | -0.1918 | 0.12 | 0.109947 | 0.4669 | -0.2301 | 0.1015 | 0.02331 | 0.3478 | NaN | -0.1004 | 0.0616 | 0.102741 | 0.5671 | -0.0587 | 0.0983 | 0.550193 | 0.8202 | -0.1235 | 0.0785 | 0.115604 | 0.5065 | NaN | -0.0753 | 0.0459 | 0.100839 | 0.4561 | -0.0662 | 0.0746 | 0.374255 | 0.6609 | -0.0782 | 0.0573 | 0.171903 | 0.9514 | NaN | -0.0372 | 0.0371 | 0.316786 | 0.9708 | -0.0125 | 0.0625 | 0.841561 | 0.9977 | -0.0512 | 0.0452 | 0.257609 | 0.9967 | NaN | -0.093 | 0.0452 | 0.03969 | 0.7271 | -0.037 | 0.0745 | 0.619597 | 0.8191 | -0.1269 | 0.0561 | 0.023578 | 0.6979 |
| PS 39:7 | 819.5096 | 24.150833 | Lipid | Phosphatidylserine | -0.1555 | 0.0862 | 0.071346 | 0.3144 | -0.4356 | 0.1304 | 0.000838 | 0.0427 | 0.0292 | 0.1131 | 0.796276 | 0.948 | NaN | -0.155 | 0.0796 | 0.051535 | 0.3365 | -0.3915 | 0.1145 | 0.000627 | 0.0744 | 0.0087 | 0.1063 | 0.934957 | 0.9876 | NaN | -0.1432 | 0.0603 | 0.017611 | 0.2387 | -0.1769 | 0.0987 | 0.073108 | 0.549 | -0.1621 | 0.0807 | 0.04456 | 0.3772 | NaN | -0.0712 | 0.0456 | 0.11808 | 0.4618 | -0.1515 | 0.0749 | 0.043142 | 0.2513 | -0.0051 | 0.0582 | 0.92981 | 0.9994 | NaN | -0.0454 | 0.0367 | 0.215939 | 0.9708 | -0.1395 | 0.0617 | 0.023811 | 0.6225 | 0.0096 | 0.0457 | 0.83327 | 0.9967 | NaN | -0.0247 | 0.0457 | 0.588575 | 0.8527 | -0.1769 | 0.0732 | 0.01568 | 0.2658 | 0.0857 | 0.0578 | 0.137933 | 0.7232 |
| LysoPC 14:0 | 467.3013 | 21.544027 | Lipid | Lysolipid, PC | 0.2105 | 0.0843 | 0.01251 | 0.117 | 0.0877 | 0.1379 | 0.524733 | 0.8001 | 0.2963 | 0.1045 | 0.004558 | 0.0979 | NaN | 0.1276 | 0.0801 | 0.111068 | 0.4199 | 0.0751 | 0.1211 | 0.535348 | 0.7797 | 0.205 | 0.1037 | 0.04809 | 0.4577 | NaN | 0.116 | 0.06 | 0.053167 | 0.4157 | 0.1507 | 0.0955 | 0.11462 | 0.577 | 0.0948 | 0.0789 | 0.229793 | 0.6205 | NaN | 0.0085 | 0.0459 | 0.853545 | 0.9461 | -0.0735 | 0.0745 | 0.323829 | 0.6384 | 0.0662 | 0.057 | 0.245392 | 0.9622 | NaN | 0.0717 | 0.036 | 0.046537 | 0.9656 | 0.0417 | 0.0614 | 0.496975 | 0.9977 | 0.0946 | 0.0437 | 0.030507 | 0.8863 | NaN | 0.0385 | 0.0452 | 0.394208 | 0.8117 | -0.0687 | 0.0739 | 0.352293 | 0.6566 | 0.1105 | 0.0558 | 0.047805 | 0.6979 |
| norhyodeoxycholic acid | 378.2799 | 22.721872 | Lipid | Secondary Bile Acid Metabolism | 0.1515 | 0.0833 | 0.069065 | 0.3125 | 0.3564 | 0.1201 | 0.002996 | 0.0917 | -0.0294 | 0.1126 | 0.793866 | 0.948 | NaN | 0.1057 | 0.0778 | 0.174181 | 0.5312 | 0.1795 | 0.1154 | 0.11982 | 0.4674 | -0.026 | 0.1056 | 0.805427 | 0.9546 | NaN | 0.1129 | 0.0586 | 0.054223 | 0.4157 | 0.1516 | 0.089 | 0.088511 | 0.549 | 0.084 | 0.0801 | 0.294702 | 0.6783 | NaN | 0.046 | 0.0443 | 0.298776 | 0.6019 | 0.0579 | 0.0701 | 0.408462 | 0.6798 | 0.0418 | 0.0579 | 0.470666 | 0.9735 | NaN | 0.0483 | 0.0354 | 0.172501 | 0.9708 | 0.0425 | 0.0581 | 0.46434 | 0.9977 | 0.0495 | 0.0454 | 0.275005 | 0.9967 | NaN | -0.0073 | 0.0444 | 0.868539 | 0.9644 | 0.0163 | 0.0706 | 0.817053 | 0.9093 | -0.0248 | 0.0579 | 0.668134 | 0.9564 |
| SM d36:2 | 728.5813 | 24.159441 | Lipid | Sphingomyelin | 0.2288 | 0.0843 | 0.006664 | 0.08 | 0.23 | 0.1334 | 0.084627 | 0.3267 | 0.2231 | 0.1089 | 0.04054 | 0.3497 | NaN | 0.2121 | 0.078 | 0.006565 | 0.0979 | 0.2765 | 0.1157 | 0.016887 | 0.3007 | 0.1863 | 0.103 | 0.070684 | 0.5067 | NaN | 0.1854 | 0.0591 | 0.001691 | 0.0484 | 0.2567 | 0.0909 | 0.004743 | 0.2014 | 0.1293 | 0.0782 | 0.098257 | 0.4716 | NaN | -0.0516 | 0.0467 | 0.26907 | 0.5828 | -0.028 | 0.0745 | 0.707346 | 0.8608 | -0.0579 | 0.0592 | 0.32751 | 0.9622 | NaN | 0.0436 | 0.0366 | 0.232932 | 0.9708 | 0.0924 | 0.0599 | 0.123027 | 0.8645 | 0.0091 | 0.0458 | 0.843208 | 0.9967 | NaN | -0.0373 | 0.0462 | 0.419238 | 0.8132 | 0.0044 | 0.0735 | 0.951865 | 0.9788 | -0.059 | 0.0593 | 0.31967 | 0.8169 |
| DHEA sulfate | 368.1666 | 15.235868 | Lipid | Steroid | 0.3102 | 0.1066 | 0.003624 | 0.0526 | 0.4019 | 0.1493 | 0.007109 | 0.1308 | 0.2516 | 0.1502 | 0.093844 | 0.4281 | NaN | 0.1984 | 0.1018 | 0.051355 | 0.3365 | 0.2734 | 0.1356 | 0.043825 | 0.4171 | 0.1358 | 0.1458 | 0.351705 | 0.767 | NaN | 0.1064 | 0.0776 | 0.17014 | 0.6546 | 0.2603 | 0.1059 | 0.013974 | 0.2967 | -0.045 | 0.1116 | 0.687054 | 0.903 | NaN | 0.0354 | 0.0584 | 0.544303 | 0.7928 | 0.0604 | 0.086 | 0.482844 | 0.7322 | 0.0103 | 0.0794 | 0.896902 | 0.9994 | NaN | 0.0577 | 0.0465 | 0.214204 | 0.9708 | 0.0733 | 0.0707 | 0.299656 | 0.9835 | 0.048 | 0.0619 | 0.437784 | 0.9967 | NaN | 0.0512 | 0.0578 | 0.375693 | 0.8007 | 0.0412 | 0.0858 | 0.630682 | 0.8191 | 0.0605 | 0.0789 | 0.442751 | 0.8627 |
| cortisone | 360.1939 | 13.359143 | Lipid | Steroid | -0.2898 | 0.0819 | 0.000399 | 0.0105 | -0.2488 | 0.1269 | 0.049886 | 0.2757 | -0.2959 | 0.1093 | 0.006766 | 0.1185 | NaN | -0.2819 | 0.0755 | 0.000187 | 0.0129 | -0.306 | 0.1096 | 0.005256 | 0.1934 | -0.2729 | 0.1028 | 0.007935 | 0.1752 | NaN | -0.1509 | 0.0592 | 0.010886 | 0.1776 | -0.1999 | 0.0882 | 0.023384 | 0.3282 | -0.1269 | 0.0809 | 0.116743 | 0.5074 | NaN | -0.0333 | 0.0458 | 0.466484 | 0.7407 | 0.0818 | 0.0723 | 0.257564 | 0.5687 | -0.1054 | 0.0583 | 0.070415 | 0.8712 | NaN | 0.0143 | 0.037 | 0.698639 | 0.971 | 0.0597 | 0.0594 | 0.315203 | 0.9977 | -0.0157 | 0.0472 | 0.740366 | 0.9967 | NaN | -0.0349 | 0.0454 | 0.441413 | 0.8178 | 0.0419 | 0.0713 | 0.557025 | 0.8007 | -0.0848 | 0.0589 | 0.150465 | 0.7294 |
| urate | 168.0287 | 0.995372 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.2769 | 0.0898 | 0.002055 | 0.0366 | 0.275 | 0.1283 | 0.032058 | 0.2396 | 0.2483 | 0.1302 | 0.056551 | 0.3614 | NaN | 0.2057 | 0.0848 | 0.015283 | 0.1834 | 0.1759 | 0.1155 | 0.127771 | 0.4744 | 0.1764 | 0.1246 | 0.157085 | 0.652 | NaN | 0.1038 | 0.0655 | 0.112831 | 0.5674 | 0.1831 | 0.0903 | 0.042608 | 0.4355 | 0.0123 | 0.0967 | 0.899008 | 0.9707 | NaN | 0.0442 | 0.0493 | 0.370421 | 0.6693 | -0.0703 | 0.0737 | 0.340458 | 0.6506 | 0.1601 | 0.0665 | 0.016047 | 0.8712 | NaN | 0.0353 | 0.0395 | 0.370998 | 0.9708 | 0.0014 | 0.0601 | 0.98195 | 0.9977 | 0.0611 | 0.0538 | 0.255845 | 0.9967 | NaN | 0.0326 | 0.0491 | 0.5068 | 0.8283 | -0.0713 | 0.0731 | 0.32926 | 0.6453 | 0.1348 | 0.0672 | 0.045016 | 0.6979 |
| dipeptide (glutamate-phenylalanine) | 294.1236 | 2.800813 | Peptide | Dipeptide | 0.2669 | 0.0848 | 0.001658 | 0.0316 | 0.2456 | 0.1179 | 0.037301 | 0.2428 | 0.3112 | 0.1215 | 0.010413 | 0.1691 | NaN | 0.2382 | 0.0787 | 0.002493 | 0.0497 | 0.1739 | 0.1053 | 0.098492 | 0.4459 | 0.2922 | 0.1141 | 0.010419 | 0.2054 | NaN | 0.1599 | 0.0606 | 0.008283 | 0.1577 | 0.1297 | 0.084 | 0.122743 | 0.577 | 0.1754 | 0.0881 | 0.046414 | 0.3772 | NaN | 0.0729 | 0.0462 | 0.114466 | 0.4618 | 0.074 | 0.0652 | 0.256384 | 0.5687 | 0.0905 | 0.0651 | 0.164137 | 0.9514 | NaN | -0.0608 | 0.038 | 0.109444 | 0.9708 | -0.0717 | 0.0556 | 0.197568 | 0.9357 | -0.0517 | 0.0528 | 0.326857 | 0.9967 | NaN | 0.048 | 0.0462 | 0.298928 | 0.7695 | 0.0356 | 0.0655 | 0.586967 | 0.8122 | 0.0751 | 0.0656 | 0.251675 | 0.7533 |
| dipeptide (histidine-tyrosine) | 341.1487 | 2.509147 | Peptide | Dipeptide | 0.2307 | 0.0873 | 0.008202 | 0.0888 | 0.3489 | 0.1363 | 0.010471 | 0.1606 | 0.1619 | 0.1128 | 0.151124 | 0.5142 | NaN | 0.1836 | 0.0815 | 0.024193 | 0.2243 | 0.2634 | 0.1219 | 0.030667 | 0.3624 | 0.1222 | 0.1066 | 0.251754 | 0.6818 | NaN | 0.044 | 0.0638 | 0.490594 | 0.8908 | 0.0799 | 0.1021 | 0.433928 | 0.7964 | 0.004 | 0.0821 | 0.96083 | 0.9768 | NaN | 0.1062 | 0.0464 | 0.022077 | 0.3584 | 0.1414 | 0.0755 | 0.061024 | 0.2766 | 0.0973 | 0.0579 | 0.092857 | 0.8712 | NaN | 0.0315 | 0.0379 | 0.40614 | 0.9708 | 0.0613 | 0.0642 | 0.339669 | 0.9977 | 0.0118 | 0.0464 | 0.79917 | 0.9967 | NaN | 0.1016 | 0.0461 | 0.027537 | 0.7271 | 0.1204 | 0.0755 | 0.110707 | 0.4558 | 0.0996 | 0.0579 | 0.085435 | 0.7232 |
| L-gamma-glutamyl-L-isoleucine | 260.1368 | 4.586305 | Peptide | Gamma-glutamyl Amino Acid | 0.2867 | 0.0841 | 0.000649 | 0.0156 | 0.4662 | 0.1297 | 0.000323 | 0.0255 | 0.1645 | 0.1088 | 0.130707 | 0.4747 | NaN | 0.2436 | 0.0785 | 0.001909 | 0.0458 | 0.3297 | 0.1202 | 0.006104 | 0.2106 | 0.1509 | 0.1022 | 0.139544 | 0.6249 | NaN | 0.1431 | 0.0609 | 0.018731 | 0.2387 | 0.3111 | 0.0926 | 0.000782 | 0.0863 | 0.0347 | 0.0789 | 0.659702 | 0.8899 | NaN | 0.0736 | 0.0461 | 0.110661 | 0.4618 | 0.0766 | 0.0786 | 0.330306 | 0.6466 | 0.0724 | 0.0563 | 0.198662 | 0.9514 | NaN | 0.0592 | 0.037 | 0.109359 | 0.9708 | 0.1608 | 0.0615 | 0.00895 | 0.494 | -0.0033 | 0.045 | 0.941328 | 0.9967 | NaN | 0.0877 | 0.0455 | 0.054046 | 0.7271 | 0.0834 | 0.0777 | 0.283121 | 0.6236 | 0.0913 | 0.0561 | 0.103673 | 0.7232 |
| NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN | NaN |
| N-acetyl-L-alanine | 131.0588 | 1.468751 | Amino Acid | Acetyl Amino Acid | 0.1446 | 0.0803 | 0.071594 | 0.3144 | 0.3244 | 0.1178 | 0.005885 | 0.1275 | 0.0174 | 0.107 | 0.871053 | 0.9655 | NaN | 0.139 | 0.0742 | 0.06104 | 0.3472 | 0.27 | 0.1044 | 0.009658 | 0.2539 | 0.0297 | 0.1004 | 0.767561 | 0.9436 | NaN | 0.0574 | 0.0571 | 0.314993 | 0.782 | 0.1394 | 0.0865 | 0.107358 | 0.577 | 0.0008 | 0.0758 | 0.991382 | 0.9973 | NaN | 0.0763 | 0.0423 | 0.071099 | 0.3995 | 0.1436 | 0.0651 | 0.027429 | 0.2227 | 0.0247 | 0.055 | 0.653688 | 0.9994 | NaN | 0.1077 | 0.0333 | 0.001218 | 0.5305 | 0.1937 | 0.0512 | 0.000154 | 0.085 | 0.0457 | 0.043 | 0.28845 | 0.9967 | NaN | 0.086 | 0.0419 | 0.039871 | 0.7271 | 0.113 | 0.0656 | 0.084976 | 0.3942 | 0.0666 | 0.0548 | 0.223961 | 0.7294 |
| N-acetyl-L-aspartic acid | 175.0479 | 0.965545 | Amino Acid | Acetyl Amino Acid | -0.1886 | 0.0928 | 0.042179 | 0.2354 | -0.1936 | 0.147 | 0.187938 | 0.4652 | -0.162 | 0.12 | 0.176978 | 0.5263 | NaN | -0.1462 | 0.0864 | 0.09057 | 0.3948 | -0.1354 | 0.13 | 0.29748 | 0.6731 | -0.127 | 0.1132 | 0.261884 | 0.6818 | NaN | -0.0838 | 0.0661 | 0.205057 | 0.7091 | -0.0321 | 0.1049 | 0.759411 | 0.8919 | -0.119 | 0.085 | 0.161776 | 0.5601 | NaN | -0.0069 | 0.0499 | 0.890015 | 0.9579 | 0.0046 | 0.0806 | 0.954163 | 0.9682 | -0.0081 | 0.0628 | 0.897453 | 0.9994 | NaN | -0.0351 | 0.0398 | 0.377819 | 0.9708 | 0.0849 | 0.067 | 0.205154 | 0.9357 | -0.1075 | 0.0478 | 0.024627 | 0.8496 | NaN | 0.0038 | 0.0496 | 0.938631 | 0.9776 | -0.0168 | 0.0797 | 0.833161 | 0.9191 | 0.022 | 0.0632 | 0.727665 | 0.968 |
| N-acetyl-DL-serine | 147.0529 | 0.853391 | Amino Acid | Acetyl Amino Acid | 0.0912 | 0.0908 | 0.315489 | 0.6791 | 0.1939 | 0.1143 | 0.089945 | 0.3424 | -0.0771 | 0.1454 | 0.595945 | 0.8415 | NaN | 0.0927 | 0.084 | 0.269353 | 0.6436 | 0.0656 | 0.1048 | 0.531094 | 0.7797 | 0.0099 | 0.1384 | 0.94309 | 0.9876 | NaN | 0.0257 | 0.0642 | 0.688552 | 0.9341 | 0.0874 | 0.0813 | 0.282392 | 0.7284 | -0.0904 | 0.1028 | 0.378929 | 0.7398 | NaN | 0.0606 | 0.0477 | 0.203728 | 0.5151 | 0.0895 | 0.0619 | 0.148412 | 0.4218 | 0.0339 | 0.075 | 0.651106 | 0.9994 | NaN | 0.0858 | 0.0379 | 0.023648 | 0.8627 | 0.129 | 0.05 | 0.009914 | 0.4975 | 0.0145 | 0.0589 | 0.805329 | 0.9967 | NaN | 0.0455 | 0.0474 | 0.33742 | 0.7759 | 0.048 | 0.0623 | 0.440752 | 0.7284 | 0.0541 | 0.0751 | 0.471522 | 0.8648 |
| N-acetyl-L-leucine | 173.1045 | 7.169957 | Amino Acid | Acetyl Amino Acid | 0.1109 | 0.087 | 0.202088 | 0.554 | 0.2597 | 0.1111 | 0.019458 | 0.1918 | -0.065 | 0.1343 | 0.628526 | 0.859 | NaN | 0.0591 | 0.0811 | 0.466081 | 0.7817 | 0.0917 | 0.1059 | 0.386248 | 0.7136 | -0.0572 | 0.126 | 0.649966 | 0.8939 | NaN | 0.0884 | 0.0611 | 0.148136 | 0.6542 | 0.1618 | 0.0787 | 0.039833 | 0.4149 | -0.0129 | 0.0954 | 0.89278 | 0.9707 | NaN | 0.1025 | 0.0453 | 0.023753 | 0.3584 | 0.1128 | 0.061 | 0.064315 | 0.2844 | 0.1004 | 0.0691 | 0.146309 | 0.9514 | NaN | 0.004 | 0.037 | 0.91369 | 0.9722 | 0.0101 | 0.0525 | 0.847006 | 0.9977 | -0.0043 | 0.0544 | 0.936707 | 0.9967 | NaN | 0.0972 | 0.0451 | 0.030991 | 0.7271 | 0.0742 | 0.0615 | 0.227689 | 0.5642 | 0.1406 | 0.0689 | 0.041248 | 0.6979 |
| N-alpha-acetyl-L-lysine | 188.1158 | 0.893928 | Amino Acid | Acetyl Amino Acid | -0.0812 | 0.0798 | 0.309356 | 0.675 | -0.1599 | 0.1126 | 0.155719 | 0.4298 | 0.0106 | 0.1118 | 0.924336 | 0.9888 | NaN | -0.029 | 0.0745 | 0.697237 | 0.9341 | -0.0662 | 0.1013 | 0.513383 | 0.7797 | 0.0486 | 0.1052 | 0.644149 | 0.8939 | NaN | -0.0106 | 0.0565 | 0.851406 | 0.9805 | -0.1351 | 0.0783 | 0.084565 | 0.549 | 0.1089 | 0.079 | 0.168269 | 0.5664 | NaN | 0.0495 | 0.0423 | 0.242161 | 0.5478 | 0.0301 | 0.0622 | 0.628581 | 0.8088 | 0.0714 | 0.0572 | 0.211475 | 0.9514 | NaN | 0.0144 | 0.0339 | 0.671151 | 0.9708 | -0.0403 | 0.0508 | 0.428466 | 0.9977 | 0.0688 | 0.0447 | 0.12398 | 0.9967 | NaN | 0.0342 | 0.042 | 0.415118 | 0.8132 | 0.0306 | 0.0617 | 0.620279 | 0.8191 | 0.0408 | 0.0574 | 0.478016 | 0.8651 |
| trans-4-hydroxyproline | 131.0586 | 0.616758 | Amino Acid | Arginine and Proline Metabolism | -0.0875 | 0.0844 | 0.30013 | 0.6636 | -0.0802 | 0.1145 | 0.483558 | 0.7831 | -0.1075 | 0.1235 | 0.383931 | 0.7088 | NaN | -0.1214 | 0.078 | 0.119609 | 0.4431 | -0.1161 | 0.1002 | 0.246778 | 0.6081 | -0.1458 | 0.1158 | 0.207978 | 0.6714 | NaN | -0.0988 | 0.0592 | 0.09472 | 0.5647 | -0.0523 | 0.08 | 0.513249 | 0.8105 | -0.1552 | 0.0866 | 0.073205 | 0.454 | NaN | -0.0369 | 0.0445 | 0.406384 | 0.701 | -0.0383 | 0.0615 | 0.533045 | 0.7623 | -0.0335 | 0.0638 | 0.59894 | 0.9994 | NaN | -0.0044 | 0.0358 | 0.902975 | 0.9722 | 0.0232 | 0.0513 | 0.651636 | 0.9977 | -0.0375 | 0.05 | 0.453482 | 0.9967 | NaN | -0.0243 | 0.0442 | 0.582319 | 0.8527 | -0.026 | 0.0611 | 0.670541 | 0.8407 | -0.0216 | 0.0639 | 0.73612 | 0.968 |
| m-hydroxymandelic acid | 168.0402 | 2.245258 | Amino Acid | catecholamine | 0.0172 | 0.085 | 0.839757 | 0.9457 | 0.0648 | 0.1401 | 0.643598 | 0.8665 | -0.0239 | 0.1071 | 0.823548 | 0.9565 | NaN | 0.0212 | 0.0786 | 0.787722 | 0.9749 | 0.0563 | 0.1229 | 0.647085 | 0.8459 | -0.0198 | 0.1005 | 0.843483 | 0.9708 | NaN | -0.0054 | 0.0599 | 0.927881 | 0.9968 | 0.0072 | 0.0981 | 0.941833 | 0.9762 | -0.0256 | 0.0758 | 0.735823 | 0.9305 | NaN | -0.0296 | 0.0447 | 0.508002 | 0.7704 | -0.1102 | 0.0752 | 0.142884 | 0.4129 | 0.0252 | 0.0551 | 0.647552 | 0.9994 | NaN | -0.0147 | 0.0359 | 0.680853 | 0.9708 | 0.04 | 0.0623 | 0.520402 | 0.9977 | -0.0503 | 0.043 | 0.241995 | 0.9967 | NaN | -0.0381 | 0.0444 | 0.389949 | 0.8116 | -0.0905 | 0.0747 | 0.225683 | 0.5642 | -0.0032 | 0.0552 | 0.953558 | 0.996 |
| phosphocreatine | 211.0126 | 13.180015 | Amino Acid | Creatine Metabolism | 0.0565 | 0.0835 | 0.498158 | 0.8017 | -0.0115 | 0.1101 | 0.916699 | 0.967 | 0.1363 | 0.1264 | 0.280723 | 0.6622 | NaN | 0.0664 | 0.0772 | 0.389193 | 0.7434 | 0.0325 | 0.097 | 0.737504 | 0.89 | 0.1264 | 0.1185 | 0.286211 | 0.6902 | NaN | 0.0565 | 0.0587 | 0.335076 | 0.7904 | 0.0386 | 0.077 | 0.616185 | 0.8437 | 0.0733 | 0.0899 | 0.414665 | 0.7786 | NaN | -0.0933 | 0.0439 | 0.033665 | 0.3584 | -0.1593 | 0.0576 | 0.005658 | 0.1623 | -0.0003 | 0.0658 | 0.996199 | 0.9994 | NaN | -0.0237 | 0.0353 | 0.501338 | 0.9708 | -0.0307 | 0.0489 | 0.530843 | 0.9977 | -0.0164 | 0.0517 | 0.75142 | 0.9967 | NaN | -0.0887 | 0.0436 | 0.041907 | 0.7271 | -0.1396 | 0.0574 | 0.014974 | 0.2658 | -0.0168 | 0.066 | 0.798658 | 0.9748 |
| 5-oxoproline | 129.0429 | 1.13778 | Amino Acid | Creatine Metabolism | -0.0855 | 0.0904 | 0.344126 | 0.6908 | 0.1259 | 0.1489 | 0.39771 | 0.7124 | -0.2198 | 0.1112 | 0.048148 | 0.3542 | NaN | -0.0904 | 0.0835 | 0.278989 | 0.6471 | 0.1149 | 0.1306 | 0.378995 | 0.7136 | -0.2205 | 0.104 | 0.034027 | 0.4269 | NaN | -0.0406 | 0.0637 | 0.523978 | 0.8998 | -0.0896 | 0.1062 | 0.398555 | 0.7775 | -0.0147 | 0.0828 | 0.859378 | 0.9576 | NaN | 0.0432 | 0.0478 | 0.366151 | 0.6693 | 0.1564 | 0.0785 | 0.04644 | 0.2513 | -0.027 | 0.0592 | 0.648606 | 0.9994 | NaN | -0.0231 | 0.0382 | 0.545295 | 0.9708 | -0.024 | 0.0669 | 0.72022 | 0.9977 | -0.0277 | 0.0464 | 0.550608 | 0.9967 | NaN | 0.0171 | 0.0474 | 0.719153 | 0.9166 | 0.1427 | 0.0781 | 0.067779 | 0.3895 | -0.0601 | 0.0588 | 0.306409 | 0.8042 |
| creatine | 131.0694 | 0.679577 | Amino Acid | Creatine Metabolism | -0.045 | 0.0934 | 0.630115 | 0.8777 | 0.0625 | 0.1616 | 0.699106 | 0.8949 | -0.0911 | 0.1161 | 0.432814 | 0.7481 | NaN | -0.1503 | 0.0875 | 0.085859 | 0.3825 | 0.0191 | 0.1422 | 0.89329 | 0.9575 | -0.2044 | 0.1108 | 0.06515 | 0.4962 | NaN | -0.036 | 0.0657 | 0.584015 | 0.9166 | 0.0267 | 0.113 | 0.813508 | 0.9217 | -0.0456 | 0.0825 | 0.580711 | 0.8571 | NaN | -0.0132 | 0.0492 | 0.787553 | 0.9001 | -0.0746 | 0.0869 | 0.39037 | 0.6692 | -0.0035 | 0.0601 | 0.953692 | 0.9994 | NaN | -0.006 | 0.0394 | 0.879218 | 0.9722 | -0.0092 | 0.0721 | 0.898294 | 0.9977 | -0.0006 | 0.0472 | 0.990533 | 0.9967 | NaN | -0.014 | 0.0488 | 0.773367 | 0.9362 | -0.1094 | 0.086 | 0.203173 | 0.5437 | 0.0192 | 0.0603 | 0.750049 | 0.9732 |
| glutamate | 147.0536 | 0.611569 | Amino Acid | Creatine Metabolism | 0.031 | 0.0891 | 0.728096 | 0.9158 | -0.043 | 0.1282 | 0.737393 | 0.9126 | 0.095 | 0.1222 | 0.437028 | 0.7481 | NaN | 0.066 | 0.0825 | 0.423828 | 0.7661 | 0.0371 | 0.1135 | 0.743706 | 0.89 | 0.1154 | 0.1145 | 0.313345 | 0.7142 | NaN | 0.0251 | 0.0627 | 0.688755 | 0.9341 | 0.0008 | 0.0897 | 0.992953 | 0.9998 | 0.051 | 0.0868 | 0.556736 | 0.8398 | NaN | -0.0187 | 0.0469 | 0.689539 | 0.8515 | -0.0577 | 0.0685 | 0.399903 | 0.6771 | 0.0137 | 0.0631 | 0.828497 | 0.9994 | NaN | -0.0187 | 0.0376 | 0.619472 | 0.9708 | 0.0081 | 0.0571 | 0.887215 | 0.9977 | -0.0415 | 0.0497 | 0.403794 | 0.9967 | NaN | -0.0031 | 0.0465 | 0.947639 | 0.9786 | 0.0163 | 0.0683 | 0.810822 | 0.9093 | -0.0226 | 0.0634 | 0.721612 | 0.968 |
| betaine | 117.0793 | 0.650488 | Amino Acid | Glycine, Serine and Threonine Metabolism | -0.0375 | 0.0853 | 0.6605 | 0.8782 | -0.0333 | 0.1178 | 0.777216 | 0.9222 | -0.0527 | 0.1225 | 0.667224 | 0.8854 | NaN | -0.005 | 0.0791 | 0.949557 | 0.9933 | -0.0357 | 0.1033 | 0.729649 | 0.8852 | -0.0013 | 0.1157 | 0.991194 | 0.9993 | NaN | 0.0226 | 0.0602 | 0.706845 | 0.9414 | 0.0273 | 0.0825 | 0.740944 | 0.8816 | 0.0146 | 0.0871 | 0.867005 | 0.9625 | NaN | -0.0355 | 0.0448 | 0.428626 | 0.7148 | -0.0612 | 0.0629 | 0.330213 | 0.6466 | -0.0039 | 0.0631 | 0.950755 | 0.9994 | NaN | -0.0015 | 0.036 | 0.966351 | 0.9912 | -0.0088 | 0.0524 | 0.866676 | 0.9977 | 0.0038 | 0.0496 | 0.939466 | 0.9967 | NaN | -0.0383 | 0.0445 | 0.389001 | 0.8116 | -0.0252 | 0.0626 | 0.687158 | 0.8461 | -0.0502 | 0.0629 | 0.424893 | 0.8529 |
| homoserine | 119.0581 | 0.684298 | Amino Acid | Glycine, Serine and Threonine Metabolism | -0.0878 | 0.0838 | 0.294557 | 0.6636 | -0.0962 | 0.1211 | 0.427132 | 0.7255 | -0.077 | 0.1151 | 0.503936 | 0.8016 | NaN | -0.1149 | 0.0774 | 0.137467 | 0.4502 | 0.0194 | 0.1088 | 0.858492 | 0.9418 | -0.1627 | 0.1091 | 0.136047 | 0.6206 | NaN | -0.0104 | 0.0593 | 0.860959 | 0.9805 | 0.0052 | 0.0855 | 0.951656 | 0.9764 | -0.0116 | 0.082 | 0.887661 | 0.9707 | NaN | -0.0652 | 0.0439 | 0.137777 | 0.4828 | -0.0437 | 0.0651 | 0.502263 | 0.7453 | -0.0939 | 0.0586 | 0.109186 | 0.8962 | NaN | 0.0106 | 0.0355 | 0.765958 | 0.9722 | 0.0128 | 0.0543 | 0.813381 | 0.9977 | 0.0108 | 0.0468 | 0.817017 | 0.9967 | NaN | -0.0635 | 0.0436 | 0.145233 | 0.7516 | -0.0582 | 0.0644 | 0.365902 | 0.6653 | -0.0746 | 0.059 | 0.206082 | 0.7294 |
| sarcosine | 89.0478 | 0.671801 | Amino Acid | Glycine, Serine and Threonine Metabolism | -0.0221 | 0.0777 | 0.775984 | 0.9192 | 0.0165 | 0.1183 | 0.889124 | 0.9558 | -0.0513 | 0.103 | 0.618657 | 0.8559 | NaN | -0.0932 | 0.0725 | 0.198772 | 0.557 | -0.0348 | 0.1043 | 0.738506 | 0.89 | -0.1269 | 0.0978 | 0.194516 | 0.6714 | NaN | 0.0041 | 0.0547 | 0.940829 | 0.9968 | 0.0374 | 0.0826 | 0.651053 | 0.8476 | -0.0044 | 0.0732 | 0.951697 | 0.9766 | NaN | -0.0016 | 0.0409 | 0.969279 | 0.9898 | -0.074 | 0.0633 | 0.242007 | 0.5571 | 0.0395 | 0.0531 | 0.457658 | 0.9735 | NaN | -0.0463 | 0.0326 | 0.155833 | 0.9708 | -0.0418 | 0.0526 | 0.426915 | 0.9977 | -0.0487 | 0.0414 | 0.239447 | 0.9967 | NaN | 0.0003 | 0.0406 | 0.994061 | 0.9972 | -0.0769 | 0.0627 | 0.220535 | 0.5569 | 0.0489 | 0.0532 | 0.358452 | 0.8297 |
| serine | 105.0421 | 0.978105 | Amino Acid | Glycine, Serine and Threonine Metabolism | 0.0636 | 0.0896 | 0.477712 | 0.7919 | -0.056 | 0.1595 | 0.725403 | 0.9045 | 0.1244 | 0.1073 | 0.246206 | 0.615 | NaN | -0.0022 | 0.0837 | 0.979453 | 0.9933 | -0.1808 | 0.1407 | 0.198779 | 0.5489 | 0.0781 | 0.1017 | 0.442589 | 0.8338 | NaN | 0.0111 | 0.0632 | 0.860794 | 0.9805 | -0.0277 | 0.1115 | 0.803727 | 0.9217 | 0.0371 | 0.0768 | 0.629053 | 0.8703 | NaN | 0.0628 | 0.047 | 0.180915 | 0.5115 | -0.0342 | 0.0855 | 0.689356 | 0.8532 | 0.101 | 0.0546 | 0.064416 | 0.8712 | NaN | 0.0157 | 0.0378 | 0.678351 | 0.9708 | 0.0254 | 0.0711 | 0.720526 | 0.9977 | 0.0151 | 0.0438 | 0.730847 | 0.9967 | NaN | 0.0365 | 0.0467 | 0.434904 | 0.8178 | -0.0012 | 0.0849 | 0.988578 | 0.9976 | 0.05 | 0.0555 | 0.367618 | 0.8297 |
| 3-hydroxypyruvic acid | 104.0115 | 0.910453 | Amino Acid | Glycine, serine, and threonine metabolism | -0.1743 | 0.0849 | 0.040204 | 0.2336 | -0.2041 | 0.1277 | 0.10992 | 0.3717 | -0.1222 | 0.1167 | 0.295143 | 0.6793 | NaN | -0.1188 | 0.0795 | 0.135178 | 0.4468 | -0.1846 | 0.112 | 0.099376 | 0.4459 | -0.0579 | 0.1112 | 0.602686 | 0.8877 | NaN | -0.0651 | 0.0607 | 0.283222 | 0.7662 | -0.119 | 0.0899 | 0.185796 | 0.652 | -0.0446 | 0.0833 | 0.592231 | 0.8601 | NaN | 0.0203 | 0.0459 | 0.658935 | 0.846 | -0.0193 | 0.0704 | 0.783657 | 0.8828 | 0.0789 | 0.0609 | 0.195035 | 0.9514 | NaN | -0.028 | 0.0364 | 0.442167 | 0.9708 | -0.0229 | 0.0583 | 0.693733 | 0.9977 | -0.0314 | 0.0474 | 0.508006 | 0.9967 | NaN | -0.023 | 0.0452 | 0.611386 | 0.8587 | -0.075 | 0.0689 | 0.276368 | 0.6201 | 0.0349 | 0.061 | 0.567547 | 0.9321 |
| L-histidine | 155.0693 | 0.637818 | Amino Acid | Histidine Metabolism | 0.0521 | 0.0909 | 0.566777 | 0.8447 | -0.0256 | 0.1304 | 0.844212 | 0.9472 | 0.1143 | 0.1251 | 0.361101 | 0.7082 | NaN | -0.011 | 0.0848 | 0.896941 | 0.9933 | -0.1586 | 0.1159 | 0.171091 | 0.5189 | 0.0734 | 0.1181 | 0.53435 | 0.8742 | NaN | 0.0105 | 0.0641 | 0.869989 | 0.9805 | 0.0056 | 0.0912 | 0.951168 | 0.9764 | 0.0157 | 0.0895 | 0.860458 | 0.9576 | NaN | -0.0095 | 0.0479 | 0.842629 | 0.9461 | 0.0298 | 0.07 | 0.669875 | 0.8442 | -0.0483 | 0.0651 | 0.4576 | 0.9735 | NaN | -0.0482 | 0.0383 | 0.208628 | 0.9708 | -0.0532 | 0.0578 | 0.357008 | 0.9977 | -0.0437 | 0.051 | 0.391877 | 0.9967 | NaN | -0.0103 | 0.0475 | 0.8286 | 0.9529 | -0.0055 | 0.0694 | 0.936463 | 0.9719 | -0.0153 | 0.0651 | 0.814215 | 0.9748 |
| 5-aminopentanoate | 117.079 | 0.650918 | Amino Acid | Lysine Metabolism | -0.0453 | 0.1035 | 0.661539 | 0.8782 | -0.0419 | 0.1426 | 0.768684 | 0.9222 | -0.0622 | 0.1487 | 0.675845 | 0.8876 | NaN | -0.0073 | 0.0959 | 0.939626 | 0.9933 | -0.0472 | 0.1251 | 0.706103 | 0.8798 | -0.0006 | 0.1405 | 0.996464 | 0.9993 | NaN | 0.0248 | 0.073 | 0.733404 | 0.9415 | 0.0298 | 0.0999 | 0.7652 | 0.8968 | 0.016 | 0.1057 | 0.87978 | 0.9674 | NaN | -0.0414 | 0.0543 | 0.446607 | 0.7294 | -0.0733 | 0.0762 | 0.336115 | 0.6487 | -0.0024 | 0.0766 | 0.974589 | 0.9994 | NaN | -0.0058 | 0.0437 | 0.893835 | 0.9722 | -0.0128 | 0.0635 | 0.839635 | 0.9977 | -0.0013 | 0.0602 | 0.983195 | 0.9967 | NaN | -0.0455 | 0.0539 | 0.399054 | 0.8117 | -0.0304 | 0.0758 | 0.688826 | 0.8461 | -0.0593 | 0.0764 | 0.437256 | 0.8627 |
| glutarylcarnitine | 275.1374 | 1.605139 | Amino Acid | Lysine Metabolism | -0.0223 | 0.0876 | 0.798805 | 0.9303 | 0.2512 | 0.1343 | 0.061446 | 0.285 | -0.2096 | 0.1119 | 0.061062 | 0.3614 | NaN | -0.045 | 0.081 | 0.578377 | 0.8743 | 0.1944 | 0.1189 | 0.102064 | 0.449 | -0.2264 | 0.1045 | 0.030279 | 0.3979 | NaN | -0.0248 | 0.0616 | 0.686747 | 0.9341 | 0.1165 | 0.0958 | 0.223894 | 0.6655 | -0.1385 | 0.0797 | 0.082334 | 0.4613 | NaN | 0.0042 | 0.0461 | 0.927163 | 0.9722 | 0.046 | 0.0744 | 0.536255 | 0.7649 | -0.0095 | 0.0596 | 0.873964 | 0.9994 | NaN | 0.0644 | 0.0368 | 0.079595 | 0.9708 | 0.1318 | 0.0597 | 0.027195 | 0.6225 | 0.0146 | 0.0469 | 0.75534 | 0.9967 | NaN | -0.0045 | 0.0457 | 0.921137 | 0.9724 | 0.048 | 0.0738 | 0.51553 | 0.7783 | -0.032 | 0.0594 | 0.589644 | 0.9367 |
| lysine | 146.1055 | 0.511165 | Amino Acid | Lysine Metabolism | 0.2151 | 0.0847 | 0.011119 | 0.1096 | 0.2601 | 0.1386 | 0.060628 | 0.2836 | 0.1934 | 0.1064 | 0.069132 | 0.3664 | NaN | 0.1153 | 0.0813 | 0.156022 | 0.4921 | 0.1467 | 0.125 | 0.240396 | 0.6051 | 0.1046 | 0.104 | 0.314416 | 0.7142 | NaN | 0.0719 | 0.0612 | 0.239832 | 0.7437 | 0.0416 | 0.101 | 0.680556 | 0.8696 | 0.096 | 0.0766 | 0.209893 | 0.6205 | NaN | 0.0208 | 0.046 | 0.651463 | 0.846 | 0.0462 | 0.0769 | 0.54746 | 0.769 | -0.0044 | 0.0567 | 0.938399 | 0.9994 | NaN | 0.009 | 0.0369 | 0.806973 | 0.9722 | 0.0586 | 0.0634 | 0.355222 | 0.9977 | -0.017 | 0.0445 | 0.702639 | 0.9967 | NaN | 0.0398 | 0.0455 | 0.38092 | 0.8087 | 0.1004 | 0.0751 | 0.181376 | 0.5427 | -0.002 | 0.0568 | 0.972404 | 0.996 |
| N6,N6,N6-trimethyl-L-lysine | 188.1515 | 0.598599 | Amino Acid | Lysine Metabolism | -0.154 | 0.0846 | 0.068666 | 0.3125 | -0.2345 | 0.1202 | 0.050987 | 0.2759 | -0.1036 | 0.1182 | 0.380695 | 0.7082 | NaN | -0.0876 | 0.0795 | 0.270516 | 0.6436 | -0.176 | 0.1066 | 0.098943 | 0.4459 | -0.0218 | 0.1134 | 0.847529 | 0.9708 | NaN | -0.0456 | 0.0604 | 0.450111 | 0.8568 | -0.07 | 0.087 | 0.420696 | 0.7926 | -0.0067 | 0.0846 | 0.93654 | 0.9766 | NaN | 0.0051 | 0.0454 | 0.910354 | 0.963 | -0.0506 | 0.0666 | 0.447479 | 0.7017 | 0.0431 | 0.0614 | 0.483129 | 0.9759 | NaN | -0.0282 | 0.0361 | 0.435702 | 0.9708 | -0.0455 | 0.0552 | 0.409515 | 0.9977 | -0.0132 | 0.0481 | 0.783676 | 0.9967 | NaN | -0.0156 | 0.0449 | 0.72859 | 0.918 | -0.0609 | 0.0659 | 0.355459 | 0.6566 | 0.0158 | 0.0614 | 0.797151 | 0.9748 |
| pipecolate | 129.079 | 0.940523 | Amino Acid | Lysine Metabolism | -0.0247 | 0.0853 | 0.772025 | 0.9192 | 0.0076 | 0.131 | 0.953674 | 0.974 | -0.042 | 0.1113 | 0.705978 | 0.8959 | NaN | 0.0103 | 0.0791 | 0.896572 | 0.9933 | -0.009 | 0.115 | 0.93739 | 0.9726 | 0.0073 | 0.1053 | 0.944619 | 0.9876 | NaN | -0.0513 | 0.0599 | 0.392257 | 0.8313 | -0.0837 | 0.0916 | 0.360516 | 0.7705 | -0.0342 | 0.0788 | 0.664178 | 0.8899 | NaN | -0.0068 | 0.0449 | 0.879964 | 0.9579 | -0.0611 | 0.0701 | 0.383255 | 0.6674 | 0.0367 | 0.0573 | 0.521636 | 0.9885 | NaN | -0.0166 | 0.036 | 0.643795 | 0.9708 | -0.0167 | 0.0583 | 0.775003 | 0.9977 | -0.0169 | 0.045 | 0.707693 | 0.9967 | NaN | 0.0073 | 0.0445 | 0.870051 | 0.9644 | -0.0427 | 0.0696 | 0.539703 | 0.7906 | 0.0461 | 0.0574 | 0.421603 | 0.8525 |
| N-(tert-Butoxycarbonyl)-L-methionine | 249.1031 | 13.127769 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | -0.0507 | 0.0814 | 0.533523 | 0.8257 | -0.1149 | 0.1194 | 0.335718 | 0.6612 | 0.0031 | 0.1098 | 0.977741 | 0.994 | NaN | -0.0566 | 0.0752 | 0.452112 | 0.7771 | -0.1297 | 0.1045 | 0.214521 | 0.5647 | -0.0009 | 0.103 | 0.992834 | 0.9993 | NaN | -0.0486 | 0.0572 | 0.396066 | 0.8313 | -0.0622 | 0.0837 | 0.457492 | 0.7964 | -0.0393 | 0.0778 | 0.613092 | 0.8637 | NaN | 0.0278 | 0.0429 | 0.517958 | 0.7769 | 0.0115 | 0.0648 | 0.859424 | 0.9253 | 0.0443 | 0.0563 | 0.432025 | 0.9735 | NaN | 0.0249 | 0.0344 | 0.468519 | 0.9708 | 0.022 | 0.0538 | 0.682396 | 0.9977 | 0.0279 | 0.0443 | 0.528698 | 0.9967 | NaN | 0.0227 | 0.0426 | 0.594755 | 0.8527 | -0.0335 | 0.0639 | 0.600291 | 0.8122 | 0.0714 | 0.0563 | 0.204131 | 0.7294 |
| hypotaurine | 109.0016 | 0.502127 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.0404 | 0.0824 | 0.624448 | 0.8777 | 0.0232 | 0.1135 | 0.837649 | 0.9436 | 0.0946 | 0.1204 | 0.432056 | 0.7481 | NaN | 0.0178 | 0.0764 | 0.81571 | 0.9803 | 0.0252 | 0.0996 | 0.799918 | 0.9315 | 0.051 | 0.1137 | 0.653829 | 0.8956 | NaN | 0.0476 | 0.0579 | 0.411571 | 0.8406 | -0.0161 | 0.0794 | 0.839296 | 0.9257 | 0.1065 | 0.0849 | 0.209727 | 0.6205 | NaN | 0.0243 | 0.0433 | 0.575016 | 0.8059 | 0.0529 | 0.0606 | 0.382955 | 0.6674 | 0.0066 | 0.0622 | 0.915163 | 0.9994 | NaN | 0.0566 | 0.0345 | 0.10162 | 0.9708 | 0.0805 | 0.0499 | 0.106533 | 0.7937 | 0.0358 | 0.0487 | 0.461784 | 0.9967 | NaN | 0.0422 | 0.0429 | 0.325141 | 0.7727 | 0.1042 | 0.0596 | 0.080496 | 0.3895 | -0.015 | 0.0624 | 0.810127 | 0.9748 |
| methionine | 149.0516 | 0.977423 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.0653 | 0.087 | 0.45282 | 0.7691 | 0.0688 | 0.16 | 0.666971 | 0.8808 | 0.0721 | 0.103 | 0.483898 | 0.7845 | NaN | 0.0065 | 0.0812 | 0.936032 | 0.9933 | -0.0916 | 0.1434 | 0.522702 | 0.7797 | 0.0379 | 0.0972 | 0.696428 | 0.9182 | NaN | -0.0135 | 0.0615 | 0.825738 | 0.9805 | -0.0159 | 0.1122 | 0.887108 | 0.9527 | -0.0085 | 0.0735 | 0.907763 | 0.9711 | NaN | 0.0958 | 0.0453 | 0.034484 | 0.3592 | 0.0036 | 0.086 | 0.966584 | 0.9772 | 0.1315 | 0.0516 | 0.010905 | 0.8712 | NaN | 0.0262 | 0.0367 | 0.475077 | 0.9708 | 0.0567 | 0.071 | 0.424806 | 0.9977 | 0.0162 | 0.0417 | 0.698346 | 0.9967 | NaN | 0.0793 | 0.0451 | 0.078537 | 0.7496 | 0.0551 | 0.085 | 0.517085 | 0.7783 | 0.0873 | 0.0525 | 0.096235 | 0.7232 |
| S-adenosyl-L-homocysteine | 384.121 | 1.490665 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.1423 | 0.0791 | 0.071897 | 0.3144 | 0.1668 | 0.1242 | 0.179051 | 0.4576 | 0.1205 | 0.1033 | 0.243467 | 0.6109 | NaN | 0.1334 | 0.0731 | 0.067994 | 0.3516 | 0.1012 | 0.1102 | 0.358676 | 0.7021 | 0.1234 | 0.0968 | 0.202328 | 0.6714 | NaN | 0.0815 | 0.0559 | 0.145206 | 0.6464 | 0.1212 | 0.0868 | 0.162534 | 0.6267 | 0.0381 | 0.074 | 0.606367 | 0.8637 | NaN | -0.0309 | 0.0425 | 0.466811 | 0.7407 | -0.0546 | 0.0685 | 0.425774 | 0.6926 | -0.0013 | 0.0539 | 0.980793 | 0.9994 | NaN | 0.0528 | 0.0335 | 0.115315 | 0.9708 | 0.1181 | 0.0545 | 0.030163 | 0.6225 | 0.0063 | 0.0423 | 0.882312 | 0.9967 | NaN | 0.0055 | 0.042 | 0.895697 | 0.9724 | -0.0127 | 0.0676 | 0.850603 | 0.9298 | 0.0281 | 0.0537 | 0.601345 | 0.9367 |
| S-Allyl-L-cysteine | 161.0512 | 1.868486 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.1059 | 0.0892 | 0.234986 | 0.588 | 0.4487 | 0.1815 | 0.013431 | 0.1655 | 0.0074 | 0.1013 | 0.941971 | 0.9916 | NaN | 0.0703 | 0.0828 | 0.396281 | 0.7491 | 0.3517 | 0.1615 | 0.029374 | 0.3624 | -0.0166 | 0.0952 | 0.861878 | 0.9708 | NaN | 0.0169 | 0.0633 | 0.789066 | 0.9615 | 0.2682 | 0.1292 | 0.037959 | 0.4042 | -0.0605 | 0.0718 | 0.399834 | 0.7663 | NaN | 0.0236 | 0.0472 | 0.616784 | 0.8244 | 0.0667 | 0.1034 | 0.519142 | 0.7556 | 0.0157 | 0.052 | 0.762186 | 0.9994 | NaN | -0.0471 | 0.0379 | 0.21448 | 0.9708 | 0.0554 | 0.0856 | 0.517904 | 0.9977 | -0.0762 | 0.0404 | 0.059338 | 0.9967 | NaN | 0.0015 | 0.0469 | 0.974853 | 0.9951 | 0.0132 | 0.1037 | 0.898718 | 0.9614 | 0.0005 | 0.0521 | 0.991664 | 0.996 |
| 3,4-hydroxyphenyl-lactate | 182.0573 | 3.796673 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.1302 | 0.0907 | 0.151328 | 0.4641 | 0.1634 | 0.1237 | 0.186326 | 0.4633 | 0.0731 | 0.1329 | 0.582574 | 0.8382 | NaN | 0.0901 | 0.0844 | 0.285851 | 0.6553 | -0.0544 | 0.1173 | 0.64263 | 0.8459 | 0.1071 | 0.1247 | 0.390386 | 0.8005 | NaN | 0.0168 | 0.0646 | 0.795457 | 0.965 | -0.0273 | 0.0892 | 0.759399 | 0.8919 | 0.0476 | 0.0942 | 0.613548 | 0.8637 | NaN | 0.0638 | 0.0478 | 0.182039 | 0.5115 | 0.1251 | 0.0657 | 0.057129 | 0.2719 | 0.003 | 0.0686 | 0.965185 | 0.9994 | NaN | 0.0614 | 0.0383 | 0.108351 | 0.9708 | 0.1046 | 0.0546 | 0.05521 | 0.6733 | 0.0092 | 0.0538 | 0.864717 | 0.9967 | NaN | 0.0675 | 0.0474 | 0.154905 | 0.7516 | 0.0992 | 0.0657 | 0.131331 | 0.4865 | 0.0379 | 0.0685 | 0.579633 | 0.9367 |
| 3-methoxytyrosine | 211.0857 | 1.982335 | Amino Acid | Phenylalanine and Tyrosine Metabolism | -0.1709 | 0.0812 | 0.035383 | 0.2219 | -0.1199 | 0.136 | 0.377966 | 0.6978 | -0.2191 | 0.1007 | 0.029668 | 0.2924 | NaN | -0.0927 | 0.077 | 0.228428 | 0.5924 | -0.0397 | 0.1207 | 0.742497 | 0.89 | -0.1492 | 0.0976 | 0.126184 | 0.6104 | NaN | -0.0815 | 0.0578 | 0.158712 | 0.6546 | -0.141 | 0.0943 | 0.135065 | 0.5905 | -0.0611 | 0.0744 | 0.411012 | 0.7786 | NaN | -0.0168 | 0.0437 | 0.701386 | 0.8602 | 0.0068 | 0.0737 | 0.925989 | 0.9554 | -0.022 | 0.0541 | 0.684045 | 0.9994 | NaN | -0.0369 | 0.0348 | 0.289041 | 0.9708 | -0.0596 | 0.0605 | 0.324952 | 0.9977 | -0.0305 | 0.0423 | 0.470709 | 0.9967 | NaN | -0.0461 | 0.0431 | 0.284616 | 0.7695 | -0.0226 | 0.0729 | 0.756401 | 0.8842 | -0.0561 | 0.0536 | 0.294839 | 0.8042 |
| phenylacetic acid | 136.0526 | 4.193451 | Amino Acid | Phenylalanine and Tyrosine Metabolism | -0.0746 | 0.0775 | 0.336184 | 0.6908 | 0.2059 | 0.1355 | 0.128673 | 0.3869 | -0.1944 | 0.0934 | 0.03739 | 0.3329 | NaN | -0.1004 | 0.0716 | 0.161284 | 0.5058 | 0.1368 | 0.1203 | 0.255417 | 0.6149 | -0.2061 | 0.0871 | 0.018031 | 0.3016 | NaN | -0.0406 | 0.0546 | 0.457655 | 0.863 | 0.14 | 0.0949 | 0.140255 | 0.5905 | -0.1173 | 0.0669 | 0.079638 | 0.4613 | NaN | 0.0079 | 0.041 | 0.846877 | 0.9461 | 0.031 | 0.0744 | 0.676745 | 0.8471 | -0.0121 | 0.0501 | 0.809518 | 0.9994 | NaN | 0.01 | 0.0329 | 0.761934 | 0.9722 | 0.0438 | 0.0614 | 0.476127 | 0.9977 | -0.0043 | 0.0394 | 0.912985 | 0.9967 | NaN | 0.0049 | 0.0407 | 0.904343 | 0.9724 | -0.0264 | 0.0744 | 0.722667 | 0.8612 | 0.0135 | 0.0505 | 0.790045 | 0.9748 |
| hypaphorine | 246.137 | 4.095109 | Amino Acid | Tryptophan Metabolism | 0.0199 | 0.0842 | 0.812793 | 0.9386 | -0.0949 | 0.1208 | 0.432427 | 0.73 | 0.1186 | 0.1155 | 0.30443 | 0.6859 | NaN | 0.0406 | 0.0779 | 0.602475 | 0.8868 | -0.042 | 0.1068 | 0.693909 | 0.8728 | 0.1262 | 0.1082 | 0.243332 | 0.6818 | NaN | 0.0088 | 0.0593 | 0.881802 | 0.9865 | -0.052 | 0.0846 | 0.539046 | 0.8173 | 0.0597 | 0.0822 | 0.467604 | 0.8005 | NaN | -0.0785 | 0.0442 | 0.075481 | 0.3995 | -0.13 | 0.0637 | 0.041141 | 0.2513 | -0.0275 | 0.0602 | 0.647632 | 0.9994 | NaN | -0.0168 | 0.0355 | 0.636456 | 0.9708 | -0.0679 | 0.0535 | 0.204298 | 0.9357 | 0.0294 | 0.047 | 0.531184 | 0.9967 | NaN | -0.0703 | 0.0439 | 0.108738 | 0.7516 | -0.1138 | 0.0634 | 0.072784 | 0.3895 | -0.0276 | 0.0603 | 0.647667 | 0.9483 |
| 5-hydroxytryptophan | 220.0946 | 2.440203 | Amino acid | Tryptophan Metabolism | 0.0405 | 0.0879 | 0.64533 | 0.8782 | 0.0615 | 0.1339 | 0.646129 | 0.8671 | 0.0184 | 0.1154 | 0.873337 | 0.9661 | NaN | 0.0119 | 0.0815 | 0.884215 | 0.9933 | -0.0077 | 0.1184 | 0.947893 | 0.9799 | 0.0043 | 0.1083 | 0.968575 | 0.9948 | NaN | -0.0613 | 0.0621 | 0.324074 | 0.782 | -0.0195 | 0.094 | 0.835232 | 0.9257 | -0.0894 | 0.082 | 0.275228 | 0.6721 | NaN | 0.0505 | 0.0461 | 0.272992 | 0.5828 | 0.065 | 0.0716 | 0.364275 | 0.659 | 0.0357 | 0.0592 | 0.547092 | 0.9885 | NaN | 0.0339 | 0.037 | 0.359514 | 0.9708 | 0.0256 | 0.0596 | 0.667078 | 0.9977 | 0.0394 | 0.0465 | 0.396874 | 0.9967 | NaN | 0.0512 | 0.0457 | 0.262779 | 0.7516 | 0.0043 | 0.0714 | 0.952176 | 0.9788 | 0.0831 | 0.059 | 0.159019 | 0.7294 |
| indole-3-acetate | 175.064 | 8.37482 | Amino Acid | Tryptophan Metabolism | -0.1058 | 0.083 | 0.202735 | 0.554 | -0.0887 | 0.11 | 0.419917 | 0.7244 | -0.1092 | 0.126 | 0.386066 | 0.7104 | NaN | -0.0689 | 0.0772 | 0.372157 | 0.7361 | 0.0406 | 0.0998 | 0.684457 | 0.8726 | -0.1192 | 0.118 | 0.312657 | 0.7142 | NaN | -0.055 | 0.0586 | 0.34802 | 0.793 | -0.005 | 0.0775 | 0.948208 | 0.9764 | -0.1285 | 0.0887 | 0.147388 | 0.5464 | NaN | -0.02 | 0.044 | 0.648752 | 0.846 | -0.0186 | 0.0593 | 0.754111 | 0.8746 | -0.0099 | 0.0652 | 0.879751 | 0.9994 | NaN | -0.0261 | 0.0352 | 0.457981 | 0.9708 | 0.0349 | 0.0494 | 0.479731 | 0.9977 | -0.1024 | 0.0501 | 0.040931 | 0.9967 | NaN | -0.0487 | 0.0434 | 0.262525 | 0.7516 | -0.06 | 0.0584 | 0.304129 | 0.6419 | -0.0262 | 0.0652 | 0.687451 | 0.9564 |
| indolelactic acid | 205.1461 | 5.755592 | Amino Acid | Tryptophan Metabolism | 0.2068 | 0.0819 | 0.011603 | 0.1124 | 0.1321 | 0.1403 | 0.346207 | 0.675 | 0.2358 | 0.1009 | 0.019476 | 0.251 | NaN | 0.1468 | 0.077 | 0.056597 | 0.3415 | 0.0817 | 0.1238 | 0.50895 | 0.7797 | 0.1758 | 0.0971 | 0.070127 | 0.5067 | NaN | 0.0686 | 0.0592 | 0.246146 | 0.7548 | 0.0726 | 0.0983 | 0.460248 | 0.7964 | 0.0564 | 0.0753 | 0.454234 | 0.791 | NaN | 0.0055 | 0.0446 | 0.901205 | 0.9579 | -0.1215 | 0.0763 | 0.111384 | 0.3743 | 0.0808 | 0.0534 | 0.130477 | 0.9514 | NaN | 0.0413 | 0.0354 | 0.243137 | 0.9708 | 0.0305 | 0.0628 | 0.627896 | 0.9977 | 0.0461 | 0.0424 | 0.277195 | 0.9967 | NaN | 0.0292 | 0.0441 | 0.507548 | 0.8283 | -0.0938 | 0.0757 | 0.21533 | 0.5528 | 0.1005 | 0.053 | 0.057883 | 0.702 |
| kynurenine | 208.0858 | 2.196904 | Amino Acid | Tryptophan Metabolism | 0.0996 | 0.0868 | 0.250872 | 0.6074 | 0.0118 | 0.1356 | 0.930445 | 0.9682 | 0.1633 | 0.1115 | 0.143095 | 0.4991 | NaN | 0.084 | 0.0803 | 0.295628 | 0.6634 | 0.0326 | 0.119 | 0.784437 | 0.9193 | 0.1396 | 0.105 | 0.183668 | 0.6656 | NaN | 0.0024 | 0.0616 | 0.968347 | 0.9971 | -0.0223 | 0.0948 | 0.814056 | 0.9217 | 0.0263 | 0.0809 | 0.744596 | 0.9363 | NaN | 0.0258 | 0.0458 | 0.573432 | 0.8059 | -0.0525 | 0.0726 | 0.470197 | 0.719 | 0.0734 | 0.0577 | 0.203505 | 0.9514 | NaN | 0.0571 | 0.0365 | 0.117847 | 0.9708 | 0.0175 | 0.0603 | 0.771157 | 0.9977 | 0.0871 | 0.0448 | 0.052159 | 0.9967 | NaN | 0.0511 | 0.0453 | 0.259168 | 0.7516 | -0.0376 | 0.0721 | 0.602268 | 0.8128 | 0.1083 | 0.0571 | 0.058072 | 0.702 |
| tryptophan | 204.0898 | 3.571538 | Amino Acid | Tryptophan Metabolism | 0.0982 | 0.0796 | 0.21745 | 0.5715 | 0.0438 | 0.1099 | 0.690387 | 0.892 | 0.1607 | 0.1142 | 0.159277 | 0.5202 | NaN | 0.0717 | 0.0738 | 0.331469 | 0.701 | 0.0351 | 0.0965 | 0.716137 | 0.8811 | 0.1265 | 0.1078 | 0.240491 | 0.6818 | NaN | 0.055 | 0.0561 | 0.327208 | 0.7853 | 0.0556 | 0.0766 | 0.468271 | 0.799 | 0.0671 | 0.0819 | 0.412845 | 0.7786 | NaN | 0.0062 | 0.0422 | 0.882601 | 0.9579 | -0.0189 | 0.0591 | 0.74925 | 0.8744 | 0.0232 | 0.0597 | 0.697606 | 0.9994 | NaN | -0.0036 | 0.0338 | 0.914503 | 0.9722 | -0.0149 | 0.049 | 0.761067 | 0.9977 | 0.0119 | 0.047 | 0.800348 | 0.9967 | NaN | -0.0117 | 0.0419 | 0.780905 | 0.9432 | -0.0474 | 0.0586 | 0.418005 | 0.7078 | 0.0207 | 0.0599 | 0.729532 | 0.968 |
| 4-hydroxyphenylethanol | 138.0682 | 6.78909 | Amino Acid | Tyrosine Metabolism | 0.0945 | 0.0845 | 0.263073 | 0.6259 | 0.1031 | 0.1313 | 0.43197 | 0.73 | 0.0858 | 0.1102 | 0.435897 | 0.7481 | NaN | 0.0701 | 0.0783 | 0.370466 | 0.7361 | 0.1116 | 0.115 | 0.331743 | 0.6989 | 0.0566 | 0.1038 | 0.585568 | 0.8877 | NaN | 0.0258 | 0.0598 | 0.665796 | 0.9288 | 0.1425 | 0.0909 | 0.117041 | 0.577 | -0.0404 | 0.0791 | 0.609562 | 0.8637 | NaN | 0.0179 | 0.0446 | 0.688196 | 0.8515 | -0.0396 | 0.0711 | 0.577091 | 0.7754 | 0.0441 | 0.0567 | 0.43659 | 0.9735 | NaN | 0.0161 | 0.0358 | 0.651876 | 0.9708 | -0.0179 | 0.0589 | 0.761665 | 0.9977 | 0.0414 | 0.0445 | 0.352564 | 0.9967 | NaN | 0.0233 | 0.0443 | 0.598126 | 0.8554 | -0.0633 | 0.0705 | 0.369512 | 0.6653 | 0.0737 | 0.0564 | 0.191662 | 0.7294 |
| proline | 115.0634 | 0.68809 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.1396 | 0.0886 | 0.114893 | 0.3958 | 0.1154 | 0.1247 | 0.354932 | 0.685 | 0.1615 | 0.1245 | 0.194741 | 0.5449 | NaN | 0.0229 | 0.085 | 0.787811 | 0.9749 | -0.0535 | 0.1144 | 0.640083 | 0.8459 | 0.0534 | 0.1213 | 0.660127 | 0.9005 | NaN | 0.0214 | 0.0632 | 0.734803 | 0.9415 | 0.0322 | 0.0878 | 0.713571 | 0.8816 | -0.0001 | 0.0903 | 0.999397 | 0.9994 | NaN | 0.002 | 0.0472 | 0.966823 | 0.9898 | -0.0251 | 0.0677 | 0.711375 | 0.8608 | 0.035 | 0.0648 | 0.589123 | 0.9975 | NaN | -0.0061 | 0.0379 | 0.87168 | 0.9722 | 0.0082 | 0.056 | 0.883952 | 0.9977 | -0.0214 | 0.0513 | 0.677032 | 0.9967 | NaN | -0.0047 | 0.0469 | 0.919832 | 0.9724 | -0.0159 | 0.0671 | 0.813141 | 0.9093 | 0.0109 | 0.0652 | 0.866762 | 0.9885 |
| N-acetyl-DL-methionine | 191.0621 | 1.239334 | Amino Acid | Acetyl Amino Acid | -0.0824 | 0.0845 | 0.329582 | 0.6891 | -0.0666 | 0.1147 | 0.561661 | 0.8159 | -0.1329 | 0.1248 | 0.286925 | 0.6683 | NaN | -0.0246 | 0.0789 | 0.755017 | 0.9649 | -0.054 | 0.1007 | 0.591705 | 0.8258 | -0.0443 | 0.12 | 0.71231 | 0.9317 | NaN | -0.0843 | 0.0593 | 0.155336 | 0.6546 | -0.118 | 0.0795 | 0.137603 | 0.5905 | -0.0579 | 0.089 | 0.515665 | 0.826 | NaN | -0.0806 | 0.0442 | 0.067994 | 0.3995 | -0.1059 | 0.0607 | 0.080995 | 0.3118 | -0.0478 | 0.0645 | 0.458936 | 0.9735 | NaN | 0.0378 | 0.0358 | 0.291856 | 0.9708 | 0.0424 | 0.0512 | 0.408104 | 0.9977 | 0.0278 | 0.0511 | 0.58561 | 0.9967 | NaN | -0.0739 | 0.0439 | 0.092326 | 0.7516 | -0.0706 | 0.0607 | 0.244687 | 0.5776 | -0.0771 | 0.0642 | 0.229905 | 0.7294 |
| 4-acetamidobutanoate | 145.0737 | 1.814703 | Amino Acid | Arginine and proline metabolism | -0.0136 | 0.0879 | 0.877211 | 0.9457 | -0.0518 | 0.141 | 0.713174 | 0.9029 | -0.0008 | 0.1133 | 0.994295 | 0.997 | NaN | -0.0363 | 0.0814 | 0.655133 | 0.9303 | -0.1631 | 0.1243 | 0.189618 | 0.5395 | -0.0058 | 0.1063 | 0.956801 | 0.9893 | NaN | -0.0007 | 0.0619 | 0.990969 | 0.9992 | 0.0009 | 0.0987 | 0.992417 | 0.9998 | -0.0203 | 0.0802 | 0.800602 | 0.9477 | NaN | -0.0276 | 0.0462 | 0.55075 | 0.7979 | -0.0919 | 0.0751 | 0.220866 | 0.5278 | 0.0295 | 0.0582 | 0.61216 | 0.9994 | NaN | 0.0365 | 0.037 | 0.324253 | 0.9708 | 0.0407 | 0.0628 | 0.517192 | 0.9977 | 0.0308 | 0.0457 | 0.49974 | 0.9967 | NaN | -0.021 | 0.0458 | 0.646823 | 0.8687 | -0.0921 | 0.0745 | 0.216322 | 0.5528 | 0.0349 | 0.0583 | 0.549679 | 0.9167 |
| 4-hydroxy-L-proline | 131.0579 | 0.616786 | Amino Acid | Arginine and proline metabolism | -0.0788 | 0.0832 | 0.34336 | 0.6908 | -0.0541 | 0.1157 | 0.639929 | 0.8658 | -0.1191 | 0.1184 | 0.314226 | 0.6905 | NaN | -0.098 | 0.0768 | 0.202181 | 0.5637 | -0.1024 | 0.1015 | 0.312984 | 0.6823 | -0.1253 | 0.1109 | 0.258484 | 0.6818 | NaN | -0.1069 | 0.0582 | 0.066121 | 0.4451 | -0.085 | 0.0805 | 0.290717 | 0.7395 | -0.1272 | 0.0833 | 0.126812 | 0.5265 | NaN | 0.0008 | 0.044 | 0.984844 | 0.9995 | 0.0377 | 0.0623 | 0.545334 | 0.7679 | -0.042 | 0.0612 | 0.492557 | 0.9851 | NaN | 0.0246 | 0.0353 | 0.485148 | 0.9708 | 0.0761 | 0.0514 | 0.138255 | 0.8645 | -0.0294 | 0.0481 | 0.541533 | 0.9967 | NaN | 0.0086 | 0.0436 | 0.843686 | 0.9563 | 0.0442 | 0.0617 | 0.47428 | 0.7523 | -0.0318 | 0.0613 | 0.604369 | 0.9367 |
| S-3-methyl-2-oxopentanoate | 130.0634 | 4.355281 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.0704 | 0.0891 | 0.429303 | 0.7595 | 0.1914 | 0.1202 | 0.111269 | 0.3717 | -0.063 | 0.1294 | 0.626251 | 0.859 | NaN | 0.0614 | 0.0825 | 0.456286 | 0.7771 | 0.0897 | 0.1083 | 0.407574 | 0.7328 | -0.0281 | 0.1218 | 0.817552 | 0.9616 | NaN | -0.0001 | 0.063 | 0.999209 | 0.9992 | 0.1285 | 0.0843 | 0.127378 | 0.5811 | -0.149 | 0.091 | 0.101619 | 0.4836 | NaN | 0.0629 | 0.0467 | 0.178262 | 0.5115 | 0.0108 | 0.0664 | 0.870443 | 0.9311 | 0.1292 | 0.0663 | 0.051515 | 0.8712 | NaN | 0.0386 | 0.0376 | 0.304036 | 0.9708 | 0.0824 | 0.0538 | 0.125934 | 0.8645 | -0.0115 | 0.0524 | 0.82625 | 0.9967 | NaN | 0.049 | 0.0465 | 0.291492 | 0.7695 | -0.0172 | 0.0662 | 0.794774 | 0.9064 | 0.1273 | 0.0665 | 0.055406 | 0.702 |
| 4-methyl-2-oxopentanoate | 130.0634 | 4.760282 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.0382 | 0.0859 | 0.656797 | 0.8782 | 0.1721 | 0.1175 | 0.14309 | 0.415 | -0.1051 | 0.1224 | 0.39065 | 0.714 | NaN | 0.0274 | 0.0794 | 0.730285 | 0.9573 | 0.0663 | 0.1061 | 0.531815 | 0.7797 | -0.0719 | 0.1153 | 0.532683 | 0.8742 | NaN | -0.0264 | 0.0606 | 0.66254 | 0.9288 | 0.1276 | 0.0821 | 0.120068 | 0.577 | -0.1886 | 0.0854 | 0.027261 | 0.3354 | NaN | 0.0408 | 0.0451 | 0.365004 | 0.6693 | -0.0192 | 0.0649 | 0.767921 | 0.8754 | 0.1065 | 0.0635 | 0.093526 | 0.8712 | NaN | 0.0276 | 0.0362 | 0.445446 | 0.9708 | 0.0747 | 0.0525 | 0.155024 | 0.8645 | -0.0234 | 0.0497 | 0.637696 | 0.9967 | NaN | 0.0277 | 0.0448 | 0.536359 | 0.8373 | -0.0402 | 0.0645 | 0.533849 | 0.79 | 0.0989 | 0.0636 | 0.119826 | 0.7232 |
| methyl-acetoacetate | 116.0478 | 2.239242 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.1271 | 0.0857 | 0.138132 | 0.4388 | 0.2393 | 0.1115 | 0.031928 | 0.2396 | -0.0245 | 0.1298 | 0.850035 | 0.9565 | NaN | 0.0939 | 0.0796 | 0.238509 | 0.6038 | 0.1424 | 0.101 | 0.15883 | 0.5063 | -0.0235 | 0.1217 | 0.847176 | 0.9708 | NaN | 0.0127 | 0.0611 | 0.83551 | 0.9805 | 0.1496 | 0.0788 | 0.057651 | 0.499 | -0.1579 | 0.0916 | 0.08468 | 0.4613 | NaN | 0.0323 | 0.0454 | 0.476651 | 0.7496 | -0.0074 | 0.0634 | 0.907404 | 0.9488 | 0.0751 | 0.0666 | 0.259434 | 0.9622 | NaN | 0.0446 | 0.0363 | 0.21885 | 0.9708 | 0.0918 | 0.0505 | 0.069291 | 0.6957 | -0.0153 | 0.0524 | 0.770663 | 0.9967 | NaN | 0.0221 | 0.0452 | 0.624544 | 0.8641 | -0.0305 | 0.0632 | 0.629246 | 0.8191 | 0.0804 | 0.0666 | 0.227933 | 0.7294 |
| methyl-malonate | 118.027 | 1.412051 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.0529 | 0.086 | 0.538195 | 0.8275 | 0.2123 | 0.122 | 0.081897 | 0.3252 | -0.0743 | 0.119 | 0.532133 | 0.8099 | NaN | 0.022 | 0.0798 | 0.782266 | 0.9727 | 0.1892 | 0.1071 | 0.077362 | 0.4408 | -0.1162 | 0.1117 | 0.298197 | 0.7079 | NaN | 0.1513 | 0.06 | 0.011715 | 0.1806 | 0.2322 | 0.0833 | 0.005296 | 0.2088 | 0.0666 | 0.0853 | 0.434567 | 0.7865 | NaN | -0.0804 | 0.0453 | 0.075917 | 0.3995 | -0.0073 | 0.068 | 0.914775 | 0.9527 | -0.1357 | 0.06 | 0.023568 | 0.8712 | NaN | 0.0126 | 0.0363 | 0.728456 | 0.971 | 0.001 | 0.0562 | 0.986096 | 0.9977 | 0.0213 | 0.0483 | 0.659235 | 0.9967 | NaN | -0.0672 | 0.045 | 0.135208 | 0.7516 | -0.0012 | 0.0674 | 0.98542 | 0.9974 | -0.1195 | 0.0603 | 0.047508 | 0.6979 |
| 3-amino-5-hydroxybenzoic acid | 153.0414 | 1.468679 | Benzenoids | Benzoic acid and derivatives | -0.0688 | 0.0822 | 0.402551 | 0.7358 | -0.0972 | 0.1067 | 0.362502 | 0.6924 | -0.0507 | 0.1296 | 0.695847 | 0.8959 | NaN | -0.0203 | 0.0766 | 0.791433 | 0.9752 | 0.0039 | 0.096 | 0.967863 | 0.9835 | -0.0276 | 0.1218 | 0.820786 | 0.9616 | NaN | 0.0029 | 0.0581 | 0.960889 | 0.9971 | 0.0644 | 0.0763 | 0.398607 | 0.7775 | -0.1 | 0.0915 | 0.27407 | 0.6721 | NaN | -0.0789 | 0.0429 | 0.066288 | 0.3995 | -0.1288 | 0.056 | 0.021368 | 0.2134 | 0.0107 | 0.0667 | 0.872786 | 0.9994 | NaN | -0.0219 | 0.0347 | 0.52864 | 0.9708 | -0.0497 | 0.0475 | 0.295198 | 0.9835 | 0.0111 | 0.0524 | 0.833037 | 0.9967 | NaN | -0.0541 | 0.0428 | 0.206201 | 0.7516 | -0.1188 | 0.0557 | 0.032937 | 0.2981 | 0.0513 | 0.0668 | 0.442704 | 0.8627 |
| bis(2-ethylhexyl)phthalate | 390.2777 | 23.077421 | Benzenoids | Benzoic acids and derivatives | 0.0194 | 0.0826 | 0.814731 | 0.9389 | -0.015 | 0.1053 | 0.886701 | 0.9558 | 0.11 | 0.1329 | 0.407721 | 0.7355 | NaN | 0.0543 | 0.0765 | 0.477837 | 0.7897 | -0.0381 | 0.0924 | 0.680172 | 0.8726 | 0.1935 | 0.1254 | 0.122723 | 0.6104 | NaN | 0.0097 | 0.0581 | 0.867343 | 0.9805 | -0.0456 | 0.0735 | 0.535079 | 0.8173 | 0.0829 | 0.0941 | 0.378378 | 0.7398 | NaN | -0.0156 | 0.0435 | 0.719711 | 0.8731 | -0.0157 | 0.0564 | 0.780197 | 0.8826 | -0.0017 | 0.0688 | 0.979788 | 0.9994 | NaN | -0.0074 | 0.0348 | 0.832259 | 0.9722 | -0.0492 | 0.0466 | 0.2911 | 0.9835 | 0.0615 | 0.0536 | 0.250712 | 0.9967 | NaN | -0.0252 | 0.0431 | 0.559573 | 0.8527 | -0.032 | 0.0559 | 0.567144 | 0.8027 | -0.0045 | 0.069 | 0.948058 | 0.996 |
| monoethylhexyl phthalic acid | 278.1524 | 20.82011 | Benzenoids | Benzoic acids and derivatives | -0.1761 | 0.0817 | 0.031084 | 0.2145 | -0.1211 | 0.1459 | 0.406541 | 0.7124 | -0.1856 | 0.0984 | 0.059182 | 0.3614 | NaN | -0.1592 | 0.0756 | 0.0353 | 0.2784 | -0.1183 | 0.1279 | 0.354962 | 0.7021 | -0.1688 | 0.0925 | 0.067966 | 0.5067 | NaN | -0.1134 | 0.0578 | 0.049675 | 0.4089 | 0.0237 | 0.1033 | 0.81821 | 0.9217 | -0.1763 | 0.0688 | 0.010344 | 0.1877 | NaN | -0.0716 | 0.0434 | 0.098746 | 0.4561 | -0.0941 | 0.0779 | 0.227222 | 0.5371 | -0.0589 | 0.0516 | 0.2542 | 0.9622 | NaN | -0.0601 | 0.0348 | 0.084144 | 0.9708 | -0.1042 | 0.0643 | 0.104916 | 0.7937 | -0.0396 | 0.0407 | 0.330328 | 0.9967 | NaN | -0.0491 | 0.0433 | 0.256699 | 0.7516 | -0.1188 | 0.0769 | 0.122416 | 0.4628 | -0.0149 | 0.0524 | 0.776667 | 0.9748 |
| 3-hydroxybenzyl alcohol | 124.0521 | 5.697804 | Benzenoids | benzyl alcohols | 0.1762 | 0.0762 | 0.020801 | 0.164 | 0.3293 | 0.1241 | 0.007978 | 0.1421 | 0.0869 | 0.0954 | 0.36257 | 0.7082 | NaN | 0.1333 | 0.0712 | 0.061212 | 0.3472 | 0.2318 | 0.1121 | 0.038645 | 0.395 | 0.0599 | 0.0899 | 0.505384 | 0.8742 | NaN | -0.0048 | 0.0558 | 0.930877 | 0.9968 | 0.1271 | 0.0914 | 0.164563 | 0.6267 | -0.0811 | 0.0693 | 0.242161 | 0.6246 | NaN | 0.0176 | 0.0412 | 0.66955 | 0.846 | 0.019 | 0.0721 | 0.791957 | 0.8867 | 0.0164 | 0.0494 | 0.739703 | 0.9994 | NaN | 0.0036 | 0.033 | 0.914083 | 0.9722 | 0.0522 | 0.0588 | 0.374964 | 0.9977 | -0.023 | 0.0389 | 0.553986 | 0.9967 | NaN | 0.0349 | 0.0407 | 0.391119 | 0.8116 | 0.0515 | 0.0707 | 0.466302 | 0.7446 | 0.0262 | 0.0494 | 0.596144 | 0.9367 |
| phenylethanolamine | 137.0845 | 2.631094 | Benzenoids | Halobenzenes | 0.1507 | 0.0834 | 0.070923 | 0.3144 | 0.1362 | 0.1508 | 0.366406 | 0.695 | 0.1509 | 0.0996 | 0.129808 | 0.4747 | NaN | 0.1238 | 0.0774 | 0.110015 | 0.4199 | 0.1307 | 0.1323 | 0.323221 | 0.6906 | 0.1212 | 0.094 | 0.197474 | 0.6714 | NaN | 0.0302 | 0.0597 | 0.613741 | 0.9231 | -0.0385 | 0.1072 | 0.719296 | 0.8816 | 0.0516 | 0.0718 | 0.472755 | 0.8005 | NaN | 0.0994 | 0.0437 | 0.023078 | 0.3584 | 0.1159 | 0.0804 | 0.149093 | 0.4218 | 0.0974 | 0.051 | 0.056034 | 0.8712 | NaN | 0.0779 | 0.0351 | 0.026569 | 0.8627 | 0.0864 | 0.0669 | 0.196186 | 0.9357 | 0.0734 | 0.0402 | 0.06787 | 0.9967 | NaN | 0.1062 | 0.0433 | 0.014133 | 0.7271 | 0.1257 | 0.0795 | 0.114042 | 0.4593 | 0.1018 | 0.051 | 0.045905 | 0.6979 |
| epinephrine | 183.0886 | 0.92338 | Benzenoids | phenols | 0.2115 | 0.083 | 0.010804 | 0.1096 | 0.2134 | 0.1108 | 0.054097 | 0.2793 | 0.2226 | 0.1243 | 0.073383 | 0.3735 | NaN | 0.1363 | 0.0786 | 0.082719 | 0.3825 | 0.1245 | 0.0998 | 0.212214 | 0.5647 | 0.1453 | 0.1195 | 0.223795 | 0.6714 | NaN | 0.1005 | 0.0594 | 0.090654 | 0.556 | 0.1036 | 0.079 | 0.189587 | 0.652 | 0.1114 | 0.0894 | 0.212394 | 0.6205 | NaN | 0.0525 | 0.0447 | 0.24011 | 0.546 | 0.0361 | 0.0616 | 0.557245 | 0.7737 | 0.059 | 0.0653 | 0.366641 | 0.9622 | NaN | 0.0243 | 0.036 | 0.499996 | 0.9708 | 0.0217 | 0.0512 | 0.670848 | 0.9977 | 0.0316 | 0.0515 | 0.539511 | 0.9967 | NaN | 0.0519 | 0.0444 | 0.242211 | 0.7516 | 0.058 | 0.0606 | 0.338282 | 0.6496 | 0.0357 | 0.0658 | 0.586764 | 0.9367 |
| fluvoxamino acid | 304.1505 | 6.009206 | Benzenoids | Trifluoromethylbenzenes | 0.0437 | 0.0862 | 0.611809 | 0.8736 | 0.14 | 0.1675 | 0.403417 | 0.7124 | 0.0054 | 0.0998 | 0.957179 | 0.9916 | NaN | 0.0395 | 0.0797 | 0.620448 | 0.9037 | 0.1244 | 0.147 | 0.397477 | 0.7241 | 0.0034 | 0.0936 | 0.971394 | 0.9948 | NaN | 0.0087 | 0.0607 | 0.8863 | 0.9865 | -0.1148 | 0.1196 | 0.337256 | 0.7705 | 0.0467 | 0.0707 | 0.508882 | 0.8238 | NaN | 0.0388 | 0.0453 | 0.39074 | 0.6828 | 0.1146 | 0.0894 | 0.199881 | 0.4973 | 0.0128 | 0.0513 | 0.803183 | 0.9994 | NaN | 0.0599 | 0.0361 | 0.097327 | 0.9708 | 0.1073 | 0.074 | 0.147208 | 0.8645 | 0.0422 | 0.0401 | 0.293772 | 0.9967 | NaN | 0.0065 | 0.045 | 0.884967 | 0.9712 | 0.0272 | 0.0897 | 0.761695 | 0.8852 | -0.0005 | 0.0514 | 0.991487 | 0.996 |
| allose | 180.0642 | 1.594537 | Carbohydrate | Aldohexose sugar | -0.0157 | 0.0995 | 0.874481 | 0.9457 | 0.0516 | 0.1309 | 0.693686 | 0.8926 | -0.0848 | 0.1513 | 0.574964 | 0.8352 | NaN | 0.0034 | 0.0921 | 0.970287 | 0.9933 | -0.0109 | 0.1156 | 0.925021 | 0.9689 | -0.0205 | 0.1431 | 0.886006 | 0.9776 | NaN | -0.0558 | 0.0699 | 0.424819 | 0.8487 | 0.0335 | 0.0915 | 0.714014 | 0.8816 | -0.1883 | 0.1062 | 0.076188 | 0.455 | NaN | -0.0004 | 0.0523 | 0.993749 | 0.9999 | 0.0087 | 0.0703 | 0.901212 | 0.9458 | 0.0001 | 0.078 | 0.999414 | 0.9994 | NaN | 0.0426 | 0.0419 | 0.308819 | 0.9708 | 0.0936 | 0.0575 | 0.103704 | 0.7937 | -0.0239 | 0.0612 | 0.696619 | 0.9967 | NaN | 0.019 | 0.0519 | 0.71484 | 0.9155 | 0.01 | 0.0697 | 0.886286 | 0.9587 | 0.0398 | 0.0782 | 0.610736 | 0.9391 |
| glucaric acid | 210.0387 | 0.884294 | Carbohydrate | Aminosugar Metabolism | 0.0264 | 0.0843 | 0.754463 | 0.9192 | -0.0755 | 0.1259 | 0.54843 | 0.8065 | 0.1042 | 0.1127 | 0.3551 | 0.7082 | NaN | 0.0417 | 0.0779 | 0.592724 | 0.8776 | -0.0266 | 0.111 | 0.810907 | 0.9349 | 0.1037 | 0.1056 | 0.326205 | 0.732 | NaN | 0.0708 | 0.0592 | 0.231134 | 0.7309 | 0.0115 | 0.0885 | 0.896196 | 0.9599 | 0.1057 | 0.0795 | 0.183471 | 0.5977 | NaN | -0.0033 | 0.0443 | 0.940797 | 0.9731 | -0.0165 | 0.0677 | 0.807237 | 0.8909 | 0.0202 | 0.0583 | 0.728654 | 0.9994 | NaN | 0.033 | 0.0355 | 0.35188 | 0.9708 | 0.0203 | 0.0563 | 0.717749 | 0.9977 | 0.0425 | 0.0456 | 0.351349 | 0.9967 | NaN | 0.0207 | 0.0439 | 0.636838 | 0.8685 | 0.0059 | 0.0673 | 0.92959 | 0.9718 | 0.0424 | 0.0582 | 0.46637 | 0.8639 |
| glucuronic acid | 194.042 | 0.662189 | Carbohydrate | Aminosugar Metabolism | 0.1096 | 0.0872 | 0.20872 | 0.5594 | 0.0796 | 0.1236 | 0.519392 | 0.8001 | 0.1291 | 0.1225 | 0.292014 | 0.6773 | NaN | 0.0609 | 0.0813 | 0.453757 | 0.7771 | 0.0175 | 0.1093 | 0.872727 | 0.9428 | 0.0864 | 0.1157 | 0.455534 | 0.8391 | NaN | 0.0013 | 0.0621 | 0.983775 | 0.9992 | 0.0819 | 0.0861 | 0.341563 | 0.7705 | -0.0669 | 0.089 | 0.45213 | 0.7898 | NaN | -0.0189 | 0.0464 | 0.684214 | 0.8515 | -0.0188 | 0.0667 | 0.777865 | 0.8826 | -0.0337 | 0.0639 | 0.598246 | 0.9994 | NaN | -0.0207 | 0.0371 | 0.577742 | 0.9708 | -0.0364 | 0.0553 | 0.509987 | 0.9977 | -0.0045 | 0.0501 | 0.928298 | 0.9967 | NaN | 0.0118 | 0.0459 | 0.797639 | 0.9482 | -0.0253 | 0.0662 | 0.702676 | 0.8504 | 0.0389 | 0.0635 | 0.540319 | 0.9121 |
| lactose | 342.1173 | 0.670231 | Carbohydrate | Aminosugar Metabolism | 0.1451 | 0.0813 | 0.074406 | 0.3184 | 0.0312 | 0.1141 | 0.784548 | 0.9222 | 0.253 | 0.1139 | 0.026338 | 0.2796 | NaN | 0.0827 | 0.0763 | 0.27872 | 0.6471 | 0.0168 | 0.1002 | 0.866751 | 0.942 | 0.1681 | 0.1108 | 0.129386 | 0.6104 | NaN | 0.0388 | 0.0581 | 0.504301 | 0.8921 | -0.0902 | 0.0801 | 0.260388 | 0.7102 | 0.1636 | 0.0815 | 0.044552 | 0.3772 | NaN | 0.067 | 0.043 | 0.118565 | 0.4618 | 0.1255 | 0.0602 | 0.037037 | 0.243 | 0.0079 | 0.0616 | 0.898084 | 0.9994 | NaN | 0.059 | 0.0344 | 0.086317 | 0.9708 | 0.0434 | 0.0506 | 0.391256 | 0.9977 | 0.0768 | 0.0471 | 0.102836 | 0.9967 | NaN | 0.0849 | 0.0424 | 0.045232 | 0.7271 | 0.1124 | 0.0598 | 0.060294 | 0.387 | 0.0605 | 0.0608 | 0.319418 | 0.8169 |
| N-acetyl-D-glucosamine | 221.0905 | 0.68895 | Carbohydrate | Aminosugar Metabolism | 0.1929 | 0.0916 | 0.035175 | 0.2219 | 0.0419 | 0.1201 | 0.7275 | 0.9045 | 0.3856 | 0.1399 | 0.005859 | 0.1115 | NaN | 0.1475 | 0.0854 | 0.08407 | 0.3825 | -0.0952 | 0.1081 | 0.378479 | 0.7136 | 0.3869 | 0.1306 | 0.003047 | 0.0885 | NaN | 0.0206 | 0.0663 | 0.755593 | 0.9454 | -0.0008 | 0.0841 | 0.992108 | 0.9998 | 0.0731 | 0.1073 | 0.49569 | 0.8203 | NaN | 0.047 | 0.049 | 0.336918 | 0.6435 | 0.0189 | 0.0645 | 0.769151 | 0.8754 | 0.0707 | 0.0765 | 0.3557 | 0.9622 | NaN | 0.0312 | 0.0393 | 0.427188 | 0.9708 | 0.0355 | 0.0534 | 0.50605 | 0.9977 | 0.0291 | 0.0605 | 0.63099 | 0.9967 | NaN | 0.0565 | 0.0485 | 0.244247 | 0.7516 | 0.0171 | 0.0639 | 0.789131 | 0.9029 | 0.1049 | 0.0758 | 0.166184 | 0.7294 |
| N-acetylneuraminate | 309.1045 | 0.672557 | Carbohydrate | Aminosugar Metabolism | -0.0332 | 0.0833 | 0.690133 | 0.8901 | -0.1179 | 0.1166 | 0.311984 | 0.6377 | 0.0237 | 0.1186 | 0.841362 | 0.9565 | NaN | 0.0038 | 0.0773 | 0.960881 | 0.9933 | -0.0683 | 0.1031 | 0.507746 | 0.7797 | 0.0598 | 0.1115 | 0.591773 | 0.8877 | NaN | 0.0381 | 0.0588 | 0.51658 | 0.8967 | 0.0577 | 0.0836 | 0.489548 | 0.8029 | 0.0219 | 0.084 | 0.794246 | 0.9477 | NaN | 0.0079 | 0.0439 | 0.857687 | 0.9469 | -0.0452 | 0.0629 | 0.472119 | 0.7199 | 0.064 | 0.0607 | 0.291817 | 0.9622 | NaN | 0.0163 | 0.0352 | 0.643314 | 0.9708 | -0.0581 | 0.0519 | 0.263167 | 0.9821 | 0.0878 | 0.0473 | 0.063265 | 0.9967 | NaN | 0.011 | 0.0435 | 0.801157 | 0.9482 | -0.0623 | 0.0621 | 0.316037 | 0.6453 | 0.0868 | 0.0606 | 0.151893 | 0.7294 |
| 2-deoxy-D-glucose | 164.0684 | 0.704827 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | 0.0714 | 0.0835 | 0.392636 | 0.7224 | 0.1473 | 0.1147 | 0.198981 | 0.4761 | 0.0008 | 0.1199 | 0.994677 | 0.997 | NaN | 0.1105 | 0.0773 | 0.152912 | 0.4907 | 0.0207 | 0.1044 | 0.843177 | 0.9389 | 0.1271 | 0.1162 | 0.273817 | 0.6833 | NaN | -0.0404 | 0.0593 | 0.495536 | 0.8921 | -0.0455 | 0.083 | 0.583805 | 0.8371 | -0.0457 | 0.0849 | 0.590758 | 0.8601 | NaN | 0.0612 | 0.0438 | 0.162213 | 0.5058 | 0.1195 | 0.0608 | 0.049496 | 0.2517 | 0.0028 | 0.0616 | 0.963428 | 0.9994 | NaN | 0.0561 | 0.0351 | 0.109857 | 0.9708 | 0.1026 | 0.0504 | 0.041991 | 0.6733 | 0.0071 | 0.0484 | 0.882765 | 0.9967 | NaN | 0.0573 | 0.0435 | 0.187633 | 0.7516 | 0.0862 | 0.061 | 0.157777 | 0.5311 | 0.0295 | 0.0617 | 0.632351 | 0.9483 |
| glucose | 180.0636 | 0.649866 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | -0.0046 | 0.1013 | 0.963665 | 0.9784 | 0.1251 | 0.1423 | 0.379244 | 0.6978 | -0.0997 | 0.1433 | 0.486658 | 0.7855 | NaN | -0.1263 | 0.0954 | 0.1857 | 0.5452 | -0.0721 | 0.1306 | 0.581081 | 0.8209 | -0.2063 | 0.1358 | 0.128739 | 0.6104 | NaN | -0.0437 | 0.0712 | 0.539762 | 0.9005 | -0.0327 | 0.101 | 0.745842 | 0.8816 | -0.0636 | 0.1016 | 0.531197 | 0.826 | NaN | 0.063 | 0.0531 | 0.236174 | 0.5455 | 0.1409 | 0.0752 | 0.061142 | 0.2766 | -0.0086 | 0.074 | 0.907453 | 0.9994 | NaN | -0.0043 | 0.0427 | 0.920069 | 0.9722 | 0.0078 | 0.0638 | 0.90224 | 0.9977 | -0.0143 | 0.0581 | 0.805042 | 0.9967 | NaN | 0.0363 | 0.0528 | 0.492069 | 0.8283 | 0.1081 | 0.0752 | 0.150359 | 0.5225 | -0.0313 | 0.074 | 0.672472 | 0.9564 |
| glyceraldehyde | 90.0314 | 1.593113 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | -0.0388 | 0.0997 | 0.697453 | 0.8953 | -0.0031 | 0.1233 | 0.979845 | 0.987 | -0.0811 | 0.1672 | 0.627688 | 0.859 | NaN | -0.0124 | 0.0924 | 0.893564 | 0.9933 | -0.0299 | 0.1083 | 0.782365 | 0.9189 | -0.0063 | 0.1582 | 0.968003 | 0.9948 | NaN | -0.0637 | 0.0701 | 0.363452 | 0.8068 | 0.0068 | 0.0861 | 0.937417 | 0.9762 | -0.1994 | 0.1175 | 0.08976 | 0.4613 | NaN | 0.0049 | 0.0525 | 0.926123 | 0.9722 | 0.01 | 0.0661 | 0.879493 | 0.9354 | 0.0027 | 0.0862 | 0.974645 | 0.9994 | NaN | 0.042 | 0.042 | 0.317787 | 0.9708 | 0.0829 | 0.0544 | 0.12712 | 0.8645 | -0.0288 | 0.0676 | 0.669773 | 0.9967 | NaN | 0.012 | 0.0521 | 0.817615 | 0.9499 | -0.0003 | 0.0656 | 0.995959 | 0.9991 | 0.0399 | 0.0864 | 0.644367 | 0.9483 |
| ascorbate | 176.0311 | 1.087867 | Cofactors and Vitamins | Ascorbate and Aldarate Metabolism | 0.1166 | 0.0843 | 0.166622 | 0.4815 | 0.1526 | 0.1375 | 0.267048 | 0.5804 | 0.0949 | 0.1063 | 0.37218 | 0.7082 | NaN | 0.1463 | 0.0778 | 0.060202 | 0.3472 | 0.1896 | 0.1201 | 0.114342 | 0.4674 | 0.1181 | 0.0996 | 0.235599 | 0.6818 | NaN | 0.113 | 0.0591 | 0.055881 | 0.4216 | 0.0694 | 0.0968 | 0.473328 | 0.799 | 0.1283 | 0.0746 | 0.085602 | 0.4613 | NaN | 0.0705 | 0.0443 | 0.111857 | 0.4618 | 0.044 | 0.0744 | 0.55385 | 0.772 | 0.096 | 0.0541 | 0.07588 | 0.8712 | NaN | 0.0681 | 0.0354 | 0.05469 | 0.9656 | 0.1859 | 0.0586 | 0.001513 | 0.2446 | -0.0015 | 0.0433 | 0.97154 | 0.9967 | NaN | 0.0696 | 0.044 | 0.11382 | 0.7516 | 0.087 | 0.0732 | 0.234305 | 0.5698 | 0.066 | 0.0546 | 0.226602 | 0.7294 |
| dethiobiotin | 214.1178 | 7.308711 | Cofactors and Vitamins | biotin metabolism | 0.0379 | 0.0892 | 0.67058 | 0.8782 | -0.0209 | 0.1344 | 0.876169 | 0.9558 | 0.1031 | 0.1183 | 0.383571 | 0.7088 | NaN | 0.0486 | 0.0824 | 0.555573 | 0.8543 | 0.02 | 0.1182 | 0.865685 | 0.942 | 0.1004 | 0.111 | 0.365485 | 0.782 | NaN | 0.0329 | 0.0627 | 0.600209 | 0.9166 | 0.123 | 0.0941 | 0.191131 | 0.652 | -0.0396 | 0.0852 | 0.642096 | 0.8795 | NaN | -0.0146 | 0.0469 | 0.756255 | 0.8904 | -0.1148 | 0.0714 | 0.107553 | 0.3711 | 0.0707 | 0.0607 | 0.243871 | 0.9622 | NaN | -0.0235 | 0.0376 | 0.531948 | 0.9708 | -0.0416 | 0.0597 | 0.485191 | 0.9977 | -0.0073 | 0.0482 | 0.8793 | 0.9967 | NaN | 0.0146 | 0.0465 | 0.754345 | 0.9221 | -0.0889 | 0.071 | 0.210571 | 0.5528 | 0.1006 | 0.0604 | 0.095455 | 0.7232 |
| biliverdin | 582.2489 | 18.410517 | Cofactors and Vitamins | Hemoglobin and Porphyrin Metabolism | -0.1496 | 0.096 | 0.119263 | 0.4014 | -0.2092 | 0.1581 | 0.185656 | 0.4633 | -0.1253 | 0.1201 | 0.296967 | 0.6793 | NaN | -0.1687 | 0.0886 | 0.056918 | 0.3415 | -0.2567 | 0.1378 | 0.062429 | 0.4362 | -0.1387 | 0.1125 | 0.217773 | 0.6714 | NaN | -0.0419 | 0.0683 | 0.539334 | 0.9005 | -0.1271 | 0.111 | 0.252148 | 0.703 | -0.0001 | 0.0864 | 0.998862 | 0.9994 | NaN | -0.0566 | 0.0508 | 0.265604 | 0.5828 | -0.0625 | 0.0858 | 0.466322 | 0.7154 | -0.0468 | 0.0621 | 0.451161 | 0.9735 | NaN | 0.0314 | 0.0411 | 0.444564 | 0.9708 | 0.062 | 0.072 | 0.389275 | 0.9977 | 0.0123 | 0.0491 | 0.801488 | 0.9967 | NaN | -0.0222 | 0.0507 | 0.662003 | 0.8742 | -0.0319 | 0.0855 | 0.709219 | 0.8511 | -0.0124 | 0.0625 | 0.842769 | 0.9809 |
| bilirubin | 584.265 | 12.192934 | Cofactors and Vitamins | Hemoglobin and Porphyrin Metabolism | 0.1254 | 0.0897 | 0.16194 | 0.4783 | 0.298 | 0.1324 | 0.024359 | 0.2169 | -0.0048 | 0.1193 | 0.96776 | 0.9929 | NaN | 0.0818 | 0.0835 | 0.327062 | 0.6998 | 0.1551 | 0.1217 | 0.202445 | 0.5505 | -0.0163 | 0.1119 | 0.884108 | 0.9776 | NaN | 0.0076 | 0.0639 | 0.905294 | 0.9918 | 0.1395 | 0.0952 | 0.142985 | 0.5917 | -0.101 | 0.0844 | 0.231683 | 0.6205 | NaN | 0.1013 | 0.0468 | 0.030563 | 0.3584 | 0.1848 | 0.0707 | 0.008994 | 0.1672 | 0.0448 | 0.0612 | 0.464386 | 0.9735 | NaN | 0.0376 | 0.038 | 0.322768 | 0.9708 | 0.1068 | 0.0603 | 0.076277 | 0.6995 | -0.0157 | 0.0482 | 0.745002 | 0.9967 | NaN | 0.0983 | 0.0465 | 0.034575 | 0.7271 | 0.1519 | 0.0712 | 0.032934 | 0.2981 | 0.0632 | 0.0612 | 0.302194 | 0.8042 |
| nicotinamide | 122.0481 | 1.119239 | Cofactors and Vitamins | Nicotinate and Nicotinamide Metabolism | 0.1365 | 0.0839 | 0.103616 | 0.3755 | 0.0952 | 0.1538 | 0.536041 | 0.8052 | 0.1563 | 0.0991 | 0.114894 | 0.4498 | NaN | 0.1338 | 0.0775 | 0.084192 | 0.3825 | 0.0623 | 0.1352 | 0.645014 | 0.8459 | 0.1575 | 0.0928 | 0.089845 | 0.5595 | NaN | 0.0962 | 0.0591 | 0.103355 | 0.5671 | 0.0994 | 0.1072 | 0.353622 | 0.7705 | 0.0901 | 0.0708 | 0.203088 | 0.6167 | NaN | 0.0497 | 0.0444 | 0.262869 | 0.5828 | 0.0855 | 0.0822 | 0.298048 | 0.6062 | 0.0393 | 0.0519 | 0.449107 | 0.9735 | NaN | 0.0319 | 0.0357 | 0.370971 | 0.9708 | 0.1258 | 0.0674 | 0.061811 | 0.6733 | -0.0067 | 0.0411 | 0.869791 | 0.9967 | NaN | 0.0461 | 0.0441 | 0.29557 | 0.7695 | 0.0767 | 0.0816 | 0.346874 | 0.6513 | 0.037 | 0.052 | 0.476439 | 0.8651 |
| pantothenate | 219.1106 | 3.27496 | Cofactors and Vitamins | Pantothenate and CoA Metabolism | 0.0722 | 0.0829 | 0.38378 | 0.7181 | 0.046 | 0.1333 | 0.730124 | 0.9057 | 0.0486 | 0.1089 | 0.655769 | 0.885 | NaN | 0.0357 | 0.077 | 0.642967 | 0.9286 | 0.0582 | 0.117 | 0.618936 | 0.8436 | 0.0017 | 0.103 | 0.986691 | 0.9993 | NaN | -0.0356 | 0.0589 | 0.545448 | 0.9015 | 0.0206 | 0.0932 | 0.824925 | 0.9229 | -0.0691 | 0.0778 | 0.373901 | 0.7398 | NaN | 0.0373 | 0.0436 | 0.392097 | 0.6828 | 0.0519 | 0.0713 | 0.466573 | 0.7154 | 0.02 | 0.056 | 0.720653 | 0.9994 | NaN | 0.0072 | 0.0351 | 0.836359 | 0.9722 | 0.0593 | 0.0591 | 0.314947 | 0.9977 | -0.0311 | 0.0441 | 0.480387 | 0.9967 | NaN | 0.0329 | 0.0433 | 0.448056 | 0.8178 | 0.0202 | 0.0709 | 0.775684 | 0.8958 | 0.0361 | 0.056 | 0.519414 | 0.8961 |
| pterin | 163.067 | 1.601121 | Cofactors and Vitamins | Pterin Metabolism | -0.1086 | 0.0835 | 0.193573 | 0.5397 | -0.0163 | 0.1216 | 0.893383 | 0.9568 | -0.2017 | 0.1137 | 0.076168 | 0.3788 | NaN | -0.0707 | 0.0777 | 0.362659 | 0.7308 | -0.0038 | 0.1068 | 0.97125 | 0.9835 | -0.1565 | 0.1079 | 0.146674 | 0.6249 | NaN | -0.074 | 0.0588 | 0.208538 | 0.7091 | -0.0465 | 0.0849 | 0.583845 | 0.8371 | -0.115 | 0.0814 | 0.157663 | 0.5549 | NaN | -0.0881 | 0.0437 | 0.043647 | 0.3914 | -0.1405 | 0.0641 | 0.028476 | 0.2246 | -0.0327 | 0.06 | 0.586061 | 0.9975 | NaN | -0.0141 | 0.0355 | 0.691182 | 0.9708 | 0.0051 | 0.0541 | 0.92508 | 0.9977 | -0.037 | 0.047 | 0.431546 | 0.9967 | NaN | -0.0906 | 0.0433 | 0.036305 | 0.7271 | -0.1188 | 0.0639 | 0.062885 | 0.3895 | -0.0616 | 0.0597 | 0.301665 | 0.8042 |
| riboflavin | 376.1322 | 14.122794 | Cofactors and Vitamins | Riboflavin Metabolism | -0.0759 | 0.0762 | 0.319515 | 0.681 | 0.0586 | 0.1111 | 0.597577 | 0.8393 | -0.1914 | 0.107 | 0.073751 | 0.3735 | NaN | -0.0614 | 0.0706 | 0.384112 | 0.7434 | 0.0311 | 0.0977 | 0.749943 | 0.89 | -0.1512 | 0.1014 | 0.136041 | 0.6206 | NaN | -0.0197 | 0.0539 | 0.714133 | 0.9414 | 0.028 | 0.0777 | 0.718757 | 0.8816 | -0.0393 | 0.0783 | 0.615516 | 0.8637 | NaN | 0.0512 | 0.0404 | 0.205302 | 0.5151 | 0.0505 | 0.0594 | 0.395163 | 0.6734 | 0.033 | 0.0573 | 0.563998 | 0.9885 | NaN | 0.0373 | 0.0323 | 0.248904 | 0.9708 | 0.0243 | 0.0495 | 0.623605 | 0.9977 | 0.0594 | 0.0448 | 0.184752 | 0.9967 | NaN | 0.0166 | 0.0401 | 0.67771 | 0.8886 | -0.0252 | 0.0593 | 0.670889 | 0.8407 | 0.0431 | 0.0574 | 0.452467 | 0.8635 |
| thyroxine | 776.6865 | 16.140047 | Cofactors and Vitamins | Thyroxine Metabolism | 0.0382 | 0.0886 | 0.666602 | 0.8782 | 0.1169 | 0.1397 | 0.402738 | 0.7124 | -0.0224 | 0.1138 | 0.843802 | 0.9565 | NaN | 0.0365 | 0.0819 | 0.655783 | 0.9303 | 0.1391 | 0.1223 | 0.255393 | 0.6149 | -0.0328 | 0.1067 | 0.758205 | 0.9436 | NaN | 0.0396 | 0.0623 | 0.524909 | 0.8998 | 0.0716 | 0.0978 | 0.464161 | 0.7982 | 0.0096 | 0.0806 | 0.904951 | 0.9707 | NaN | -0.0074 | 0.0466 | 0.873731 | 0.9579 | -0.0483 | 0.0758 | 0.524147 | 0.7594 | 0.0261 | 0.0585 | 0.654899 | 0.9994 | NaN | -0.0079 | 0.0374 | 0.833593 | 0.9722 | 0.0253 | 0.0625 | 0.685876 | 0.9977 | -0.0326 | 0.0459 | 0.477472 | 0.9967 | NaN | -0.0457 | 0.0463 | 0.323625 | 0.7727 | -0.0547 | 0.0752 | 0.466694 | 0.7446 | -0.036 | 0.0585 | 0.537699 | 0.9105 |
| alpha-tocopherol | 430.3784 | 24.493536 | Cofactors and Vitamins | Tocopherol Metabolism | 0.0251 | 0.0867 | 0.772507 | 0.9192 | 0.2284 | 0.1316 | 0.082582 | 0.3252 | -0.1214 | 0.1124 | 0.280249 | 0.6622 | NaN | 0.0204 | 0.0802 | 0.798887 | 0.976 | 0.2023 | 0.1156 | 0.07999 | 0.441 | -0.1173 | 0.1054 | 0.265765 | 0.6818 | NaN | -0.017 | 0.0611 | 0.781331 | 0.9569 | 0.0638 | 0.0946 | 0.499994 | 0.807 | -0.0708 | 0.0799 | 0.375962 | 0.7398 | NaN | 0.0035 | 0.0456 | 0.939059 | 0.9731 | 0.0251 | 0.0729 | 0.730805 | 0.8663 | -0.0159 | 0.0584 | 0.785255 | 0.9994 | NaN | 0.0542 | 0.0364 | 0.136324 | 0.9708 | 0.1601 | 0.0573 | 0.00518 | 0.3177 | -0.0217 | 0.0458 | 0.6358 | 0.9967 | NaN | 0.0082 | 0.0453 | 0.856881 | 0.9644 | 0.0432 | 0.072 | 0.548354 | 0.7966 | -0.0199 | 0.0585 | 0.733549 | 0.968 |
| 4-pyridoxate | 183.0525 | 1.874988 | Cofactors and Vitamins | Vitamin B6 Metabolism | -0.0846 | 0.0839 | 0.313349 | 0.6791 | -0.1035 | 0.1269 | 0.414565 | 0.7219 | -0.0609 | 0.111 | 0.583519 | 0.8382 | NaN | -0.0669 | 0.0777 | 0.389059 | 0.7434 | -0.0889 | 0.1114 | 0.425137 | 0.7515 | -0.0408 | 0.1043 | 0.695489 | 0.9182 | NaN | -0.0529 | 0.0591 | 0.370995 | 0.8094 | -0.0845 | 0.0886 | 0.340067 | 0.7705 | -0.0233 | 0.0788 | 0.767134 | 0.9437 | NaN | 0.0245 | 0.0444 | 0.581174 | 0.8081 | 0.0655 | 0.0688 | 0.341591 | 0.6506 | -0.0095 | 0.0572 | 0.868042 | 0.9994 | NaN | 0.0812 | 0.0354 | 0.021916 | 0.8627 | 0.1279 | 0.0564 | 0.023309 | 0.6225 | 0.0503 | 0.0449 | 0.262661 | 0.9967 | NaN | 0.0221 | 0.0441 | 0.616678 | 0.8626 | 0.0264 | 0.0682 | 0.698613 | 0.8475 | 0.0164 | 0.0574 | 0.77499 | 0.9748 |
| pyridoxamine | 168.091 | 2.715419 | Cofactors and Vitamins | Vitamin B6 Metabolism | 0.0259 | 0.0813 | 0.749765 | 0.9192 | 0.0739 | 0.1136 | 0.51522 | 0.8001 | -0.013 | 0.1156 | 0.910585 | 0.9854 | NaN | 0.001 | 0.0753 | 0.988961 | 0.9933 | 0.0621 | 0.0997 | 0.53372 | 0.7797 | -0.0435 | 0.1087 | 0.688947 | 0.9182 | NaN | 0.0043 | 0.0572 | 0.940082 | 0.9968 | 0.0233 | 0.0796 | 0.770143 | 0.8988 | -0.0052 | 0.0819 | 0.949037 | 0.9766 | NaN | -0.0039 | 0.0428 | 0.928189 | 0.9722 | -0.0052 | 0.0612 | 0.931821 | 0.9554 | -0.0117 | 0.0594 | 0.844067 | 0.9994 | NaN | -0.0155 | 0.0343 | 0.651473 | 0.9708 | -0.0116 | 0.0508 | 0.820103 | 0.9977 | -0.0175 | 0.0467 | 0.707036 | 0.9967 | NaN | -0.007 | 0.0425 | 0.868808 | 0.9644 | -0.0304 | 0.0608 | 0.616778 | 0.8191 | 0.0103 | 0.0595 | 0.862839 | 0.9881 |
| biotin | 244.0928 | 4.970581 | Cofactors and Vitamins | Vitamin B7 metabolism | 0.0985 | 0.0841 | 0.241383 | 0.5927 | 0.195 | 0.1183 | 0.099173 | 0.3602 | -0.0079 | 0.1187 | 0.947156 | 0.9916 | NaN | 0.0949 | 0.0777 | 0.222195 | 0.5873 | 0.1974 | 0.1033 | 0.055978 | 0.4173 | -0.0181 | 0.1113 | 0.870535 | 0.9708 | NaN | 0.0531 | 0.0593 | 0.370423 | 0.8094 | 0.1433 | 0.0826 | 0.082981 | 0.549 | -0.0494 | 0.084 | 0.556821 | 0.8398 | NaN | 0.0841 | 0.044 | 0.055753 | 0.3989 | 0.0684 | 0.0645 | 0.288628 | 0.599 | 0.1172 | 0.0604 | 0.052337 | 0.8712 | NaN | 0.0861 | 0.0351 | 0.014051 | 0.7645 | 0.1163 | 0.0522 | 0.025828 | 0.6225 | 0.0538 | 0.0477 | 0.259746 | 0.9967 | NaN | 0.0933 | 0.0435 | 0.032178 | 0.7271 | 0.0835 | 0.0636 | 0.189218 | 0.5437 | 0.1154 | 0.0605 | 0.056433 | 0.702 |
| 5-methyltetrahydrofolate | 459.1865 | 3.632105 | Cofactors and Vitamins | Vitamin B9 Metabolism | -0.1504 | 0.0817 | 0.065704 | 0.3074 | -0.0293 | 0.1278 | 0.818511 | 0.9335 | -0.2308 | 0.1048 | 0.02765 | 0.288 | NaN | -0.1356 | 0.0756 | 0.073067 | 0.3627 | 0.0119 | 0.1124 | 0.915893 | 0.9682 | -0.2213 | 0.0982 | 0.024217 | 0.3518 | NaN | -0.0992 | 0.0576 | 0.085372 | 0.5364 | 0.0465 | 0.0895 | 0.603232 | 0.8395 | -0.1908 | 0.0737 | 0.009658 | 0.1838 | NaN | -0.0123 | 0.0437 | 0.779238 | 0.898 | -0.0434 | 0.0684 | 0.52605 | 0.7595 | 0.0044 | 0.0568 | 0.938062 | 0.9994 | NaN | -0.0494 | 0.0347 | 0.155023 | 0.9708 | -0.0049 | 0.0569 | 0.931815 | 0.9977 | -0.0812 | 0.0431 | 0.059138 | 0.9967 | NaN | -0.0483 | 0.0431 | 0.262009 | 0.7516 | -0.097 | 0.0674 | 0.150125 | 0.5225 | -0.02 | 0.0565 | 0.722921 | 0.968 |
| cis-aconitate | 174.0164 | 1.361663 | Energy | TCA Cycle | 0.0198 | 0.0873 | 0.820704 | 0.9399 | 0.1479 | 0.1277 | 0.246838 | 0.5516 | -0.0795 | 0.1176 | 0.49924 | 0.7965 | NaN | -0.0257 | 0.0811 | 0.751257 | 0.9649 | 0.0975 | 0.1129 | 0.387808 | 0.7136 | -0.1276 | 0.1105 | 0.24837 | 0.6818 | NaN | -0.0511 | 0.0615 | 0.405997 | 0.8406 | 0.0403 | 0.0904 | 0.655688 | 0.8516 | -0.1339 | 0.0826 | 0.105233 | 0.4845 | NaN | 0.021 | 0.0459 | 0.646943 | 0.846 | 0.1379 | 0.0675 | 0.04107 | 0.2513 | -0.0719 | 0.0602 | 0.2322 | 0.9622 | NaN | 0.0302 | 0.0368 | 0.411229 | 0.9708 | 0.0642 | 0.057 | 0.260066 | 0.9821 | 0.001 | 0.0477 | 0.983672 | 0.9967 | NaN | 0.0781 | 0.0453 | 0.084816 | 0.7508 | 0.1662 | 0.0663 | 0.012175 | 0.265 | 0.0077 | 0.0609 | 0.89897 | 0.9953 |
| citramalate | 148.0374 | 1.446943 | Energy | TCA Cycle | 0.0235 | 0.0889 | 0.791089 | 0.9232 | 0.0598 | 0.1265 | 0.636418 | 0.8649 | -0.0249 | 0.1237 | 0.840526 | 0.9565 | NaN | -0.0248 | 0.0826 | 0.764036 | 0.9671 | -0.0183 | 0.1121 | 0.870279 | 0.942 | -0.0659 | 0.1163 | 0.571048 | 0.8877 | NaN | 0.0035 | 0.0625 | 0.955453 | 0.997 | 0.0723 | 0.0882 | 0.412604 | 0.7881 | -0.0664 | 0.0875 | 0.448009 | 0.7876 | NaN | 0.0147 | 0.0467 | 0.753756 | 0.8904 | 0.0233 | 0.0679 | 0.73133 | 0.8663 | 0.0103 | 0.0636 | 0.871195 | 0.9994 | NaN | 0.0042 | 0.0375 | 0.911477 | 0.9722 | 0.0272 | 0.0563 | 0.629274 | 0.9977 | -0.0206 | 0.0499 | 0.679348 | 0.9967 | NaN | 0.0116 | 0.0464 | 0.80306 | 0.9482 | -0.0211 | 0.0675 | 0.754243 | 0.884 | 0.0448 | 0.0637 | 0.481717 | 0.8686 |
| trans-aconitate | 174.0161 | 1.145015 | Energy | TCA Cycle | -0.0721 | 0.0821 | 0.380159 | 0.7152 | 0.0113 | 0.113 | 0.920665 | 0.968 | -0.1583 | 0.1175 | 0.178074 | 0.5263 | NaN | -0.0914 | 0.0759 | 0.228083 | 0.5924 | 0.0275 | 0.0992 | 0.781345 | 0.9189 | -0.1971 | 0.1099 | 0.073003 | 0.5166 | NaN | -0.0854 | 0.0576 | 0.137826 | 0.6296 | 0.0175 | 0.0789 | 0.824396 | 0.9229 | -0.1945 | 0.0819 | 0.017518 | 0.2763 | NaN | -0.0349 | 0.0432 | 0.419241 | 0.7088 | 0.0023 | 0.0606 | 0.969745 | 0.9786 | -0.0779 | 0.0606 | 0.198701 | 0.9514 | NaN | 0.0478 | 0.0347 | 0.168381 | 0.9708 | 0.0884 | 0.0496 | 0.074956 | 0.6995 | 0.0033 | 0.0484 | 0.944866 | 0.9967 | NaN | 0.0163 | 0.0431 | 0.704756 | 0.9111 | 0.0148 | 0.0601 | 0.804976 | 0.9086 | 0.0166 | 0.0618 | 0.788632 | 0.9748 |
| citrate | 192.0271 | 0.984674 | Energy | TCA Cycle | -0.0172 | 0.0876 | 0.844406 | 0.9457 | 0.0218 | 0.1283 | 0.865104 | 0.9547 | -0.0506 | 0.1184 | 0.668997 | 0.8856 | NaN | -0.0556 | 0.0811 | 0.493158 | 0.7987 | 0.0765 | 0.1128 | 0.498058 | 0.7788 | -0.1256 | 0.1121 | 0.262338 | 0.6818 | NaN | -0.0656 | 0.0615 | 0.285927 | 0.7662 | 0.0476 | 0.0896 | 0.595264 | 0.8374 | -0.1581 | 0.0832 | 0.057369 | 0.4204 | NaN | 0.0213 | 0.046 | 0.643284 | 0.846 | 0.0389 | 0.0687 | 0.571804 | 0.7754 | 0.0028 | 0.061 | 0.963655 | 0.9994 | NaN | 0.0548 | 0.0368 | 0.136287 | 0.9708 | 0.1088 | 0.0562 | 0.052948 | 0.6733 | 0.0101 | 0.0479 | 0.832818 | 0.9967 | NaN | 0.0677 | 0.0456 | 0.137664 | 0.7516 | 0.0566 | 0.0681 | 0.40558 | 0.6982 | 0.0748 | 0.061 | 0.220304 | 0.7294 |
| isocitrate | 192.0271 | 0.942504 | Energy | TCA Cycle | -0.0634 | 0.0844 | 0.452378 | 0.7691 | 0.0735 | 0.1332 | 0.580775 | 0.8296 | -0.1409 | 0.1081 | 0.192603 | 0.5449 | NaN | -0.0334 | 0.0783 | 0.670199 | 0.9303 | 0.1012 | 0.1167 | 0.385995 | 0.7136 | -0.1148 | 0.1018 | 0.259607 | 0.6818 | NaN | 0.0061 | 0.0597 | 0.91829 | 0.9959 | 0.1385 | 0.0923 | 0.133545 | 0.5905 | -0.0904 | 0.0768 | 0.239415 | 0.6205 | NaN | -0.0267 | 0.0444 | 0.548075 | 0.7962 | -0.0222 | 0.0717 | 0.756549 | 0.8746 | -0.0191 | 0.0564 | 0.734962 | 0.9994 | NaN | 0.0168 | 0.0357 | 0.638426 | 0.9708 | 0.0205 | 0.0594 | 0.729951 | 0.9977 | 0.013 | 0.0445 | 0.770656 | 0.9967 | NaN | -0.0035 | 0.0442 | 0.937364 | 0.9776 | 0.0032 | 0.0711 | 0.963715 | 0.987 | -0.0008 | 0.0567 | 0.989173 | 0.996 |
| malate | 134.0217 | 0.867725 | Energy | TCA Cycle | -0.0055 | 0.0851 | 0.948903 | 0.9754 | 0.0813 | 0.1138 | 0.474957 | 0.7739 | -0.11 | 0.1255 | 0.381052 | 0.7082 | NaN | -0.0179 | 0.0787 | 0.820469 | 0.9803 | 0.0512 | 0.1002 | 0.609116 | 0.8385 | -0.1172 | 0.1176 | 0.319283 | 0.7194 | NaN | -0.0187 | 0.0598 | 0.754857 | 0.9454 | 0.0897 | 0.0792 | 0.257241 | 0.7102 | -0.1563 | 0.0881 | 0.075928 | 0.455 | NaN | -0.0589 | 0.0446 | 0.186321 | 0.5115 | -0.0471 | 0.0616 | 0.444512 | 0.7003 | -0.0679 | 0.0645 | 0.292567 | 0.9622 | NaN | 0.0152 | 0.0359 | 0.671418 | 0.9708 | 0.0615 | 0.0504 | 0.222135 | 0.9527 | -0.0429 | 0.0508 | 0.399018 | 0.9967 | NaN | -0.0293 | 0.0443 | 0.509297 | 0.8283 | -0.0567 | 0.0611 | 0.353454 | 0.6566 | 0.0064 | 0.0652 | 0.921992 | 0.996 |
| succinate | 118.027 | 1.295398 | Energy | TCA Cycle | 0.0224 | 0.0834 | 0.788225 | 0.9232 | 0.0922 | 0.1956 | 0.63725 | 0.8649 | 0.0014 | 0.0921 | 0.988282 | 0.9955 | NaN | 0.023 | 0.0772 | 0.765635 | 0.9671 | -0.0366 | 0.1735 | 0.833014 | 0.9389 | 0.012 | 0.0864 | 0.889094 | 0.9776 | NaN | 0.0163 | 0.0587 | 0.780763 | 0.9569 | 0.1142 | 0.1363 | 0.402018 | 0.7814 | -0.012 | 0.0652 | 0.85393 | 0.9569 | NaN | -0.0222 | 0.0439 | 0.613684 | 0.8244 | -0.0398 | 0.1053 | 0.705279 | 0.8608 | -0.0126 | 0.0473 | 0.789552 | 0.9994 | NaN | -0.0219 | 0.0352 | 0.534402 | 0.9708 | 0.056 | 0.087 | 0.519385 | 0.9977 | -0.0407 | 0.037 | 0.271755 | 0.9967 | NaN | -0.024 | 0.0436 | 0.582263 | 0.8527 | -0.0998 | 0.1044 | 0.338913 | 0.6496 | -0.0039 | 0.0474 | 0.935244 | 0.996 |
| hippurate | 179.0586 | 4.79845 | Exogenous | Benzoate Metabolism | -0.0762 | 0.084 | 0.364376 | 0.7078 | -0.199 | 0.117 | 0.089062 | 0.3414 | 0.0596 | 0.1186 | 0.615416 | 0.8557 | NaN | -0.0605 | 0.0778 | 0.436535 | 0.7723 | -0.1669 | 0.103 | 0.105115 | 0.4511 | 0.065 | 0.1112 | 0.558719 | 0.8762 | NaN | -0.0097 | 0.0594 | 0.8698 | 0.9805 | -0.0927 | 0.0831 | 0.264729 | 0.7133 | 0.0624 | 0.0839 | 0.457108 | 0.7916 | NaN | -0.0138 | 0.0443 | 0.755897 | 0.8904 | -0.0333 | 0.0645 | 0.605553 | 0.7902 | 0.0158 | 0.0611 | 0.795294 | 0.9994 | NaN | -0.0267 | 0.0355 | 0.452052 | 0.9708 | -0.0177 | 0.0536 | 0.741336 | 0.9977 | -0.0336 | 0.048 | 0.484086 | 0.9967 | NaN | 0.0011 | 0.0441 | 0.980629 | 0.9951 | -0.0503 | 0.0637 | 0.429517 | 0.7185 | 0.0594 | 0.0609 | 0.329506 | 0.8205 |
| benzoin | 212.1031 | 6.033384 | Exogenous | Drug | 0.0153 | 0.0836 | 0.854616 | 0.9457 | 0.1471 | 0.1242 | 0.235942 | 0.5379 | -0.0706 | 0.1119 | 0.527959 | 0.8099 | NaN | -0.0263 | 0.0776 | 0.734774 | 0.9589 | 0.0753 | 0.1103 | 0.494868 | 0.7769 | -0.1026 | 0.105 | 0.328465 | 0.7341 | NaN | -0.0924 | 0.0589 | 0.116858 | 0.5708 | -0.0105 | 0.0888 | 0.906191 | 0.9657 | -0.1566 | 0.0784 | 0.045653 | 0.3772 | NaN | 0.0172 | 0.0439 | 0.695481 | 0.855 | -0.0531 | 0.0681 | 0.435959 | 0.6955 | 0.0714 | 0.0578 | 0.216826 | 0.9519 | NaN | 0.0317 | 0.0352 | 0.367123 | 0.9708 | 0.0521 | 0.0556 | 0.349022 | 0.9977 | 0.0181 | 0.0454 | 0.690812 | 0.9967 | NaN | 0.0361 | 0.0436 | 0.40709 | 0.8117 | -0.0364 | 0.0675 | 0.589941 | 0.8122 | 0.094 | 0.0578 | 0.103686 | 0.7232 |
| guaifenesin | 198.0869 | 3.703858 | Exogenous | Drug | 0.0586 | 0.0778 | 0.451448 | 0.7691 | 0.2146 | 0.124 | 0.083589 | 0.3252 | -0.0204 | 0.0987 | 0.836094 | 0.9565 | NaN | 0.0301 | 0.0722 | 0.677025 | 0.9303 | 0.1373 | 0.1107 | 0.214826 | 0.5647 | -0.0362 | 0.0926 | 0.696354 | 0.9182 | NaN | -0.0106 | 0.055 | 0.847589 | 0.9805 | 0.0794 | 0.0887 | 0.3708 | 0.7724 | -0.0683 | 0.0698 | 0.328012 | 0.702 | NaN | 0.0523 | 0.0408 | 0.200164 | 0.5115 | 0.0088 | 0.0689 | 0.897901 | 0.9441 | 0.0841 | 0.0505 | 0.095799 | 0.8712 | NaN | 0.0054 | 0.0329 | 0.870444 | 0.9722 | 0.077 | 0.0559 | 0.168695 | 0.8945 | -0.0364 | 0.0397 | 0.359792 | 0.9967 | NaN | 0.0416 | 0.0406 | 0.304749 | 0.7695 | 0.0021 | 0.0684 | 0.975589 | 0.9954 | 0.0687 | 0.0507 | 0.175238 | 0.7294 |
| chlorpheniramine | 274.1192 | 13.793018 | Exogenous | Drug | 0.1355 | 0.0833 | 0.103666 | 0.3755 | 0.2966 | 0.1332 | 0.025997 | 0.2208 | 0.046 | 0.1053 | 0.66216 | 0.8853 | NaN | 0.0826 | 0.0778 | 0.288479 | 0.6553 | 0.1768 | 0.121 | 0.143953 | 0.4923 | 0.0144 | 0.0992 | 0.884611 | 0.9776 | NaN | -0.0052 | 0.0598 | 0.930029 | 0.9968 | 0.1725 | 0.0947 | 0.068417 | 0.5245 | -0.1084 | 0.0754 | 0.150467 | 0.5464 | NaN | 0.0661 | 0.0439 | 0.132357 | 0.4825 | 0.0342 | 0.0753 | 0.64921 | 0.8257 | 0.0816 | 0.0536 | 0.128374 | 0.9514 | NaN | 0.0175 | 0.0355 | 0.621627 | 0.9708 | 0.0458 | 0.062 | 0.460481 | 0.9977 | 0.0024 | 0.0426 | 0.955832 | 0.9967 | NaN | 0.0626 | 0.0436 | 0.151361 | 0.7516 | 0.0016 | 0.0753 | 0.983252 | 0.9974 | 0.0953 | 0.0535 | 0.074993 | 0.7232 |
| ibuprofen carboxylic acid | 236.1035 | 9.971766 | Exogenous | Drug | 0.1398 | 0.0841 | 0.096627 | 0.3653 | 0.2806 | 0.1331 | 0.035018 | 0.2428 | 0.0674 | 0.1076 | 0.530903 | 0.8099 | NaN | 0.0966 | 0.0784 | 0.217882 | 0.5867 | 0.1651 | 0.1205 | 0.170661 | 0.5189 | 0.0462 | 0.1011 | 0.647763 | 0.8939 | NaN | 0.0135 | 0.0602 | 0.8232 | 0.9805 | 0.1127 | 0.096 | 0.240401 | 0.6876 | -0.045 | 0.077 | 0.558729 | 0.8404 | NaN | 0.0571 | 0.0445 | 0.19964 | 0.5115 | 0.0344 | 0.0748 | 0.645503 | 0.8248 | 0.0689 | 0.055 | 0.210371 | 0.9514 | NaN | -0.007 | 0.036 | 0.845942 | 0.9722 | 0.0146 | 0.0621 | 0.81475 | 0.9977 | -0.0181 | 0.0436 | 0.679075 | 0.9967 | NaN | 0.0512 | 0.0442 | 0.246444 | 0.7516 | -0.0028 | 0.0748 | 0.970424 | 0.992 | 0.0823 | 0.0549 | 0.133974 | 0.7232 |
| salicyluric acid | 195.054 | 2.946303 | Exogenous | Drug | 0.0241 | 0.0872 | 0.781773 | 0.9211 | 0.0069 | 0.133 | 0.958836 | 0.974 | 0.0479 | 0.1144 | 0.675155 | 0.8876 | NaN | 0.0059 | 0.0807 | 0.941621 | 0.9933 | 0.0711 | 0.1171 | 0.543493 | 0.7852 | 0.0029 | 0.108 | 0.978252 | 0.9993 | NaN | 0.0321 | 0.0613 | 0.600298 | 0.9166 | 0.0273 | 0.0929 | 0.768844 | 0.8988 | 0.0355 | 0.081 | 0.661228 | 0.8899 | NaN | 0.0592 | 0.0457 | 0.194819 | 0.5115 | 0.0852 | 0.0709 | 0.229877 | 0.54 | 0.0419 | 0.0587 | 0.475066 | 0.9735 | NaN | -0.0083 | 0.0368 | 0.821866 | 0.9722 | -0.0271 | 0.0591 | 0.647131 | 0.9977 | 0.0071 | 0.0463 | 0.878639 | 0.9967 | NaN | 0.0657 | 0.0453 | 0.146879 | 0.7516 | 0.0509 | 0.0706 | 0.471129 | 0.7495 | 0.0781 | 0.0585 | 0.18179 | 0.7294 |
| tricarballylic acid | 176.0311 | 1.087867 | Exogenous | Food Component/Plant | 0.1154 | 0.0843 | 0.170957 | 0.4915 | 0.149 | 0.1377 | 0.279045 | 0.592 | 0.0953 | 0.1061 | 0.368972 | 0.7082 | NaN | 0.1442 | 0.0778 | 0.063926 | 0.3472 | 0.1888 | 0.1203 | 0.116495 | 0.4674 | 0.1168 | 0.0994 | 0.24005 | 0.6818 | NaN | 0.1118 | 0.0591 | 0.058324 | 0.4236 | 0.0672 | 0.0969 | 0.487814 | 0.8029 | 0.1276 | 0.0745 | 0.086797 | 0.4613 | NaN | 0.0701 | 0.0443 | 0.113771 | 0.4618 | 0.0426 | 0.0745 | 0.566877 | 0.7754 | 0.096 | 0.054 | 0.075203 | 0.8712 | NaN | 0.0675 | 0.0354 | 0.056857 | 0.9656 | 0.1846 | 0.0587 | 0.001668 | 0.2446 | -0.0014 | 0.0432 | 0.975023 | 0.9967 | NaN | 0.0694 | 0.044 | 0.114512 | 0.7516 | 0.0855 | 0.0733 | 0.243372 | 0.5776 | 0.0667 | 0.0545 | 0.22098 | 0.7294 |
| 2-acetyl-pyrrolidine | 113.0845 | 4.492652 | Exogenous | Food Component/Plant | 0.0039 | 0.0812 | 0.961688 | 0.9784 | -0.2082 | 0.1571 | 0.185078 | 0.4633 | 0.0623 | 0.0945 | 0.509686 | 0.8016 | NaN | 0.0071 | 0.0751 | 0.924199 | 0.9933 | -0.2339 | 0.1372 | 0.088131 | 0.4459 | 0.0687 | 0.0886 | 0.437913 | 0.8278 | NaN | 0.0114 | 0.0571 | 0.842201 | 0.9805 | -0.1652 | 0.1095 | 0.131419 | 0.5898 | 0.0686 | 0.0667 | 0.303758 | 0.6872 | NaN | 0.0277 | 0.0426 | 0.515207 | 0.7749 | -0.0477 | 0.0855 | 0.576992 | 0.7754 | 0.0584 | 0.0483 | 0.226663 | 0.9622 | NaN | 0.0198 | 0.0342 | 0.561915 | 0.9708 | 0.0126 | 0.0714 | 0.860195 | 0.9977 | 0.021 | 0.0382 | 0.582358 | 0.9967 | NaN | -0.0047 | 0.0423 | 0.911679 | 0.9724 | -0.083 | 0.0843 | 0.324887 | 0.6453 | 0.0251 | 0.0487 | 0.606287 | 0.9367 |
| 2-piperidinone | 99.0691 | 2.676115 | Exogenous | Food Component/Plant | -0.0474 | 0.0851 | 0.577473 | 0.8499 | 0.1022 | 0.1144 | 0.37165 | 0.6978 | -0.2197 | 0.1236 | 0.075523 | 0.3788 | NaN | -0.0792 | 0.0787 | 0.314287 | 0.6816 | 0.049 | 0.1012 | 0.627868 | 0.8459 | -0.2484 | 0.1154 | 0.031391 | 0.403 | NaN | 0.0081 | 0.06 | 0.892119 | 0.9865 | 0.0997 | 0.0796 | 0.210483 | 0.6538 | -0.1098 | 0.0889 | 0.21666 | 0.6205 | NaN | 0.0087 | 0.0448 | 0.847029 | 0.9461 | 0.0511 | 0.0615 | 0.405851 | 0.6798 | -0.0336 | 0.0653 | 0.606988 | 0.9994 | NaN | -0.0611 | 0.0357 | 0.086583 | 0.9708 | -0.0196 | 0.0514 | 0.702484 | 0.9977 | -0.1148 | 0.0497 | 0.020789 | 0.8197 | NaN | -0.0247 | 0.0444 | 0.578582 | 0.8527 | 0.025 | 0.0612 | 0.682869 | 0.8461 | -0.0797 | 0.0646 | 0.217835 | 0.7294 |
| 5-aminolevulinate | 131.0586 | 0.616781 | Exogenous | Food Component/Plant | -0.0761 | 0.084 | 0.36533 | 0.7078 | -0.078 | 0.1159 | 0.500923 | 0.7964 | -0.0889 | 0.1208 | 0.461647 | 0.7607 | NaN | -0.1015 | 0.0776 | 0.191233 | 0.548 | -0.1065 | 0.1015 | 0.294448 | 0.6731 | -0.1167 | 0.1132 | 0.302754 | 0.7081 | NaN | -0.0976 | 0.0589 | 0.097225 | 0.5647 | -0.0745 | 0.0808 | 0.356285 | 0.7705 | -0.1277 | 0.0849 | 0.132744 | 0.5272 | NaN | -0.0204 | 0.0443 | 0.645667 | 0.846 | -0.0134 | 0.0624 | 0.830538 | 0.9053 | -0.0248 | 0.0623 | 0.690115 | 0.9994 | NaN | 0.0241 | 0.0356 | 0.49874 | 0.9708 | 0.0358 | 0.0519 | 0.490318 | 0.9977 | 0.0093 | 0.0491 | 0.849195 | 0.9967 | NaN | 0.0011 | 0.0441 | 0.980344 | 0.9951 | 0.0001 | 0.062 | 0.99895 | 0.9991 | 0.0041 | 0.0625 | 0.947689 | 0.996 |
| 5-hydroxy-1,4-naphthoquinone | 174.0272 | 4.803483 | Exogenous | Food Component/Plant | 0.0907 | 0.0828 | 0.273226 | 0.6386 | 0.2613 | 0.1414 | 0.064562 | 0.2923 | -0.0109 | 0.1016 | 0.914366 | 0.9854 | NaN | 0.135 | 0.0766 | 0.077835 | 0.3769 | 0.1739 | 0.1262 | 0.167951 | 0.5189 | 0.0599 | 0.0969 | 0.536011 | 0.8742 | NaN | 0.0261 | 0.0586 | 0.65543 | 0.9288 | 0.2426 | 0.0974 | 0.012732 | 0.2845 | -0.0848 | 0.0719 | 0.23797 | 0.6205 | NaN | 0.0228 | 0.0437 | 0.601589 | 0.818 | -0.1388 | 0.0803 | 0.083984 | 0.313 | 0.0996 | 0.0517 | 0.054148 | 0.8712 | NaN | -0.0064 | 0.0351 | 0.855396 | 0.9722 | 0.0198 | 0.0652 | 0.761707 | 0.9977 | -0.0231 | 0.041 | 0.57385 | 0.9967 | NaN | -0.0039 | 0.0435 | 0.928387 | 0.9724 | -0.166 | 0.0796 | 0.037066 | 0.3022 | 0.0677 | 0.0521 | 0.193758 | 0.7294 |
| raffinose | 504.1699 | 0.718023 | Exogenous | Food Component/Plant | 0.1418 | 0.0874 | 0.104771 | 0.3755 | 0.3117 | 0.1324 | 0.018567 | 0.1898 | 0.0188 | 0.1145 | 0.869856 | 0.9655 | NaN | 0.0778 | 0.0819 | 0.342022 | 0.7098 | 0.1158 | 0.1258 | 0.357294 | 0.7021 | 0.0001 | 0.1075 | 0.999345 | 0.9993 | NaN | 0.0306 | 0.0623 | 0.624046 | 0.9285 | 0.092 | 0.0974 | 0.345097 | 0.7705 | -0.0043 | 0.0811 | 0.957549 | 0.9766 | NaN | 0.0984 | 0.0458 | 0.031568 | 0.3584 | 0.1761 | 0.0713 | 0.01356 | 0.1826 | 0.0371 | 0.0588 | 0.528007 | 0.9885 | NaN | 0.0038 | 0.0374 | 0.919313 | 0.9722 | 0.0704 | 0.0615 | 0.252098 | 0.9821 | -0.0413 | 0.0462 | 0.371028 | 0.9967 | NaN | 0.1087 | 0.0453 | 0.016381 | 0.7271 | 0.1689 | 0.071 | 0.017335 | 0.2658 | 0.0627 | 0.0587 | 0.285661 | 0.8004 |
| methyl-jasmonate | 224.141 | 16.080898 | Exogenous | Food Component/Plants | 0.0491 | 0.0827 | 0.552798 | 0.836 | 0.0579 | 0.1203 | 0.630199 | 0.8611 | 0.0678 | 0.1148 | 0.554944 | 0.8324 | NaN | 0.0665 | 0.0764 | 0.384585 | 0.7434 | 0.0708 | 0.1055 | 0.501702 | 0.7797 | 0.0802 | 0.1077 | 0.456033 | 0.8391 | NaN | 0.0313 | 0.0582 | 0.590859 | 0.9166 | 0.0991 | 0.0836 | 0.235922 | 0.6783 | -0.0494 | 0.0821 | 0.547357 | 0.8359 | NaN | -0.0787 | 0.0435 | 0.070608 | 0.3995 | -0.1693 | 0.0639 | 0.008035 | 0.1672 | 0.016 | 0.0592 | 0.7872 | 0.9994 | NaN | 0.0325 | 0.0348 | 0.350711 | 0.9708 | -0.004 | 0.0537 | 0.94048 | 0.9977 | 0.0664 | 0.046 | 0.14933 | 0.9967 | NaN | -0.04 | 0.0433 | 0.355349 | 0.7843 | -0.1458 | 0.0636 | 0.02191 | 0.2725 | 0.064 | 0.0589 | 0.277041 | 0.7924 |
| 1,3,7-trimethyluric acid | 210.0867 | 5.631745 | Exogenous | Xanthine Metabolism | 0.0667 | 0.0804 | 0.407029 | 0.7391 | 0.088 | 0.131 | 0.502053 | 0.7964 | 0.0543 | 0.1016 | 0.593004 | 0.8415 | NaN | 0.0275 | 0.0748 | 0.712678 | 0.9423 | 0.016 | 0.1161 | 0.890611 | 0.9565 | 0.0287 | 0.0956 | 0.764018 | 0.9436 | NaN | 0.0035 | 0.0569 | 0.950978 | 0.997 | 0.0509 | 0.0917 | 0.578432 | 0.8355 | -0.0133 | 0.0724 | 0.854172 | 0.9569 | NaN | -0.0242 | 0.0425 | 0.568433 | 0.8059 | 0.0247 | 0.0705 | 0.725689 | 0.8643 | -0.0662 | 0.0524 | 0.206027 | 0.9514 | NaN | -0.0114 | 0.0341 | 0.736994 | 0.9722 | 0.0265 | 0.0585 | 0.650082 | 0.9977 | -0.0319 | 0.0412 | 0.437758 | 0.9967 | NaN | -0.0195 | 0.0422 | 0.644023 | 0.8687 | -0.0059 | 0.0701 | 0.933383 | 0.9719 | -0.0355 | 0.0525 | 0.499377 | 0.8921 |
| 7-methylxanthine | 166.0541 | 2.619145 | Exogenous | Xanthine Metabolism | 0.002 | 0.0842 | 0.981014 | 0.993 | 0.0065 | 0.1293 | 0.959917 | 0.974 | -0.0116 | 0.11 | 0.9158 | 0.9854 | NaN | -0.0091 | 0.0779 | 0.907439 | 0.9933 | 0.0137 | 0.1135 | 0.903912 | 0.9651 | -0.0274 | 0.1032 | 0.790458 | 0.9535 | NaN | 0.0025 | 0.0592 | 0.965844 | 0.9971 | -0.0244 | 0.0903 | 0.786755 | 0.9143 | 0.0221 | 0.0779 | 0.776808 | 0.9437 | NaN | 0.0245 | 0.0442 | 0.579647 | 0.808 | -0.0694 | 0.0691 | 0.315454 | 0.6309 | 0.0921 | 0.0562 | 0.100948 | 0.8845 | NaN | 0 | 0.0355 | 0.999707 | 0.9997 | -0.008 | 0.0575 | 0.889074 | 0.9977 | 0.0042 | 0.0444 | 0.924487 | 0.9967 | NaN | -0.0052 | 0.0439 | 0.904873 | 0.9724 | -0.0414 | 0.0687 | 0.547187 | 0.7966 | 0.0194 | 0.0566 | 0.732034 | 0.968 |
| caffeine | 194.081 | 5.866517 | Exogenous | Xanthine Metabolism | 0.1183 | 0.0878 | 0.177522 | 0.5051 | 0.1338 | 0.1293 | 0.300622 | 0.6256 | 0.1204 | 0.1185 | 0.309385 | 0.6892 | NaN | 0.0846 | 0.0815 | 0.299075 | 0.6657 | 0.0424 | 0.1153 | 0.713454 | 0.8811 | 0.1034 | 0.1113 | 0.352909 | 0.767 | NaN | 0.0626 | 0.062 | 0.312653 | 0.782 | 0.0567 | 0.0909 | 0.532996 | 0.8173 | 0.0607 | 0.0843 | 0.471283 | 0.8005 | NaN | 0.0912 | 0.0459 | 0.047065 | 0.3914 | 0.0926 | 0.0691 | 0.180322 | 0.463 | 0.0966 | 0.0605 | 0.110397 | 0.8962 | NaN | 0.0112 | 0.0373 | 0.763301 | 0.9722 | -0.0313 | 0.0584 | 0.591377 | 0.9977 | 0.0467 | 0.048 | 0.330514 | 0.9967 | NaN | 0.082 | 0.0457 | 0.072445 | 0.7496 | 0.0547 | 0.0691 | 0.428648 | 0.7185 | 0.1097 | 0.0604 | 0.069282 | 0.7232 |
| paraxanthine | 180.0652 | 4.203445 | Exogenous | Xanthine Metabolism | 0.1102 | 0.0796 | 0.166484 | 0.4815 | 0.1221 | 0.1106 | 0.269884 | 0.5842 | 0.1277 | 0.1143 | 0.264121 | 0.6394 | NaN | 0.0834 | 0.0739 | 0.259172 | 0.6275 | 0.0203 | 0.0996 | 0.838475 | 0.9389 | 0.1306 | 0.1071 | 0.222898 | 0.6714 | NaN | 0.0577 | 0.0563 | 0.305342 | 0.782 | 0.042 | 0.0781 | 0.590433 | 0.8374 | 0.076 | 0.0813 | 0.349585 | 0.7227 | NaN | 0.1145 | 0.0413 | 0.005543 | 0.34 | 0.1177 | 0.0585 | 0.044077 | 0.2513 | 0.1138 | 0.0581 | 0.050183 | 0.8712 | NaN | 0.0442 | 0.0337 | 0.188695 | 0.9708 | 0.0601 | 0.0493 | 0.222642 | 0.9527 | 0.0331 | 0.0465 | 0.476508 | 0.9967 | NaN | 0.0953 | 0.0412 | 0.020694 | 0.7271 | 0.1057 | 0.0582 | 0.069519 | 0.3895 | 0.0871 | 0.0586 | 0.137398 | 0.7232 |
| theobromine | 180.065 | 3.297352 | Exogenous | Xanthine Metabolism | -0.2041 | 0.0855 | 0.016931 | 0.1377 | -0.2367 | 0.1341 | 0.077584 | 0.3149 | -0.1635 | 0.1111 | 0.141083 | 0.4985 | NaN | -0.149 | 0.0801 | 0.06278 | 0.3472 | -0.1768 | 0.1188 | 0.136644 | 0.4744 | -0.1134 | 0.1056 | 0.282833 | 0.6902 | NaN | -0.0574 | 0.0617 | 0.351981 | 0.793 | -0.0423 | 0.0972 | 0.663656 | 0.8559 | -0.0721 | 0.0797 | 0.365774 | 0.7396 | NaN | -0.0539 | 0.0459 | 0.240359 | 0.546 | -0.0995 | 0.0729 | 0.172584 | 0.4558 | -0.0137 | 0.0583 | 0.814107 | 0.9994 | NaN | -0.0321 | 0.0369 | 0.384974 | 0.9708 | -0.0093 | 0.0618 | 0.880701 | 0.9977 | -0.0455 | 0.0454 | 0.316576 | 0.9967 | NaN | -0.0464 | 0.0456 | 0.308876 | 0.7695 | -0.0756 | 0.0728 | 0.299182 | 0.6411 | -0.0208 | 0.0583 | 0.721464 | 0.968 |
| theophylline | 180.0652 | 4.276442 | Exogenous | Xanthine Metabolism | -0.0107 | 0.0808 | 0.894537 | 0.9586 | 0.0224 | 0.1085 | 0.836055 | 0.9436 | -0.029 | 0.1203 | 0.809319 | 0.9518 | NaN | -0.0233 | 0.0747 | 0.755132 | 0.9649 | -0.0531 | 0.0961 | 0.580455 | 0.8209 | -0.014 | 0.1129 | 0.901184 | 0.9812 | NaN | -0.0005 | 0.0569 | 0.992343 | 0.9992 | 0.0323 | 0.0757 | 0.670045 | 0.8602 | -0.0442 | 0.0851 | 0.603261 | 0.8637 | NaN | 0.0504 | 0.0424 | 0.235107 | 0.5455 | 0.0094 | 0.0582 | 0.872073 | 0.9311 | 0.109 | 0.0615 | 0.076121 | 0.8712 | NaN | -0.0006 | 0.0341 | 0.986129 | 0.9922 | 0.038 | 0.0481 | 0.430173 | 0.9977 | -0.045 | 0.0484 | 0.353108 | 0.9967 | NaN | 0.045 | 0.0421 | 0.285649 | 0.7695 | 0.0146 | 0.0577 | 0.799498 | 0.9086 | 0.0874 | 0.0617 | 0.156813 | 0.7294 |
| quinolin-2-ol | 145.053 | 7.731086 | Exogenous | Bacteria Metabolism | 0.071 | 0.074 | 0.337142 | 0.6908 | 0.1465 | 0.1176 | 0.212794 | 0.4978 | 0.0207 | 0.0942 | 0.826336 | 0.9565 | NaN | 0.0299 | 0.0689 | 0.664046 | 0.9303 | 0.0754 | 0.1047 | 0.471024 | 0.7643 | -0.0096 | 0.0887 | 0.913441 | 0.9876 | NaN | -0.0353 | 0.0526 | 0.50254 | 0.8921 | 0.0705 | 0.0829 | 0.394617 | 0.7775 | -0.1004 | 0.0671 | 0.134363 | 0.5298 | NaN | 0.0177 | 0.039 | 0.649817 | 0.846 | -0.0409 | 0.0646 | 0.52694 | 0.7595 | 0.0502 | 0.0482 | 0.298448 | 0.9622 | NaN | 0.0237 | 0.0313 | 0.448813 | 0.9708 | -0.0062 | 0.0533 | 0.90725 | 0.9977 | 0.0413 | 0.0379 | 0.275212 | 0.9967 | NaN | 0.026 | 0.0387 | 0.501115 | 0.8283 | -0.0562 | 0.0641 | 0.380551 | 0.6777 | 0.0737 | 0.0481 | 0.125273 | 0.7232 |
| honaucin A | 188.0495 | 0.965569 | Exogenous | Bacteria Metabolite | -0.0227 | 0.0851 | 0.78977 | 0.9232 | -0.0527 | 0.106 | 0.619293 | 0.8589 | 0.0089 | 0.1409 | 0.949755 | 0.9916 | NaN | -0.0594 | 0.0789 | 0.451179 | 0.7771 | -0.0643 | 0.093 | 0.48887 | 0.7759 | -0.0611 | 0.1333 | 0.646746 | 0.8939 | NaN | 0.0337 | 0.06 | 0.574189 | 0.9166 | 0.0265 | 0.0745 | 0.722137 | 0.8816 | 0.043 | 0.0998 | 0.66641 | 0.8903 | NaN | -0.036 | 0.0447 | 0.420914 | 0.7088 | -0.0531 | 0.0567 | 0.348705 | 0.6506 | -0.001 | 0.0724 | 0.98891 | 0.9994 | NaN | 0.0393 | 0.0359 | 0.273442 | 0.9708 | 0.0107 | 0.0473 | 0.820782 | 0.9977 | 0.086 | 0.0564 | 0.127268 | 0.9967 | NaN | -0.0272 | 0.0444 | 0.539783 | 0.8373 | -0.0549 | 0.0562 | 0.32829 | 0.6453 | 0.0244 | 0.0725 | 0.736512 | 0.968 |
| trimethylamine | 59.074 | 0.696045 | Exogenous | Bacteria Metabolite | -0.0676 | 0.0869 | 0.43619 | 0.7644 | -0.0858 | 0.162 | 0.596222 | 0.8393 | -0.042 | 0.1035 | 0.685026 | 0.8959 | NaN | -0.0665 | 0.0803 | 0.407622 | 0.7538 | 0.0059 | 0.1434 | 0.967083 | 0.9835 | -0.062 | 0.0971 | 0.523142 | 0.8742 | NaN | -0.0843 | 0.0609 | 0.166255 | 0.6546 | -0.0982 | 0.1129 | 0.384538 | 0.7775 | -0.0939 | 0.0729 | 0.198242 | 0.614 | NaN | -0.0291 | 0.0457 | 0.523767 | 0.7793 | -0.0441 | 0.0869 | 0.612111 | 0.7932 | -0.0108 | 0.0532 | 0.839587 | 0.9994 | NaN | -0.0177 | 0.0367 | 0.630457 | 0.9708 | 0.017 | 0.0724 | 0.814658 | 0.9977 | -0.031 | 0.0417 | 0.457678 | 0.9967 | NaN | 0.0043 | 0.0455 | 0.923841 | 0.9724 | 0.0215 | 0.0865 | 0.803366 | 0.9086 | 0.0066 | 0.0534 | 0.901469 | 0.9953 |
| N-cyclohexylformamide | 127.099 | 7.931769 | Exogenous | Bacteria Metabolism | 0.0195 | 0.0874 | 0.823752 | 0.9405 | 0.0252 | 0.1344 | 0.851272 | 0.9493 | 0.0071 | 0.1143 | 0.950296 | 0.9916 | NaN | -0.0098 | 0.081 | 0.904037 | 0.9933 | 0.0119 | 0.118 | 0.919426 | 0.9686 | -0.0288 | 0.1075 | 0.789176 | 0.9535 | NaN | 0.0248 | 0.0615 | 0.68657 | 0.9341 | 0.0394 | 0.0938 | 0.67448 | 0.8638 | 0.0083 | 0.0809 | 0.918683 | 0.9752 | NaN | -0.0279 | 0.046 | 0.543694 | 0.7928 | -0.1145 | 0.0717 | 0.110294 | 0.3735 | 0.0385 | 0.0587 | 0.511746 | 0.9885 | NaN | 0.0303 | 0.0368 | 0.409867 | 0.9708 | 0.0289 | 0.0598 | 0.628777 | 0.9977 | 0.0292 | 0.0461 | 0.526276 | 0.9967 | NaN | -0.0355 | 0.0456 | 0.436089 | 0.8178 | -0.089 | 0.0713 | 0.21183 | 0.5528 | 0.0055 | 0.0588 | 0.925925 | 0.996 |
| phenylephrine | 167.0945 | 0.944446 | Exogenous | Drug | -0.021 | 0.0869 | 0.809359 | 0.9369 | -0.1102 | 0.1382 | 0.42527 | 0.7255 | 0.0713 | 0.113 | 0.52848 | 0.8099 | NaN | -0.0519 | 0.0804 | 0.518926 | 0.8279 | -0.1072 | 0.1212 | 0.376605 | 0.7136 | 0.0322 | 0.1067 | 0.762509 | 0.9436 | NaN | -0.0153 | 0.0611 | 0.802094 | 0.971 | -0.0883 | 0.0965 | 0.359906 | 0.7705 | 0.0438 | 0.0801 | 0.584588 | 0.8601 | NaN | 0.059 | 0.0456 | 0.195983 | 0.5115 | -0.0815 | 0.0739 | 0.270335 | 0.5824 | 0.1488 | 0.0566 | 0.008556 | 0.8712 | NaN | 0.0327 | 0.0366 | 0.372024 | 0.9708 | 0.0142 | 0.062 | 0.818608 | 0.9977 | 0.0539 | 0.0455 | 0.235878 | 0.9967 | NaN | 0.0435 | 0.0453 | 0.336988 | 0.7759 | -0.0908 | 0.0732 | 0.21497 | 0.5528 | 0.1305 | 0.057 | 0.022096 | 0.6979 |
| debrisoquin | 175.1106 | 3.15226 | Exogenous | Drug | 0.0547 | 0.0853 | 0.521152 | 0.8173 | 0.2063 | 0.1328 | 0.120245 | 0.3728 | -0.0309 | 0.1099 | 0.778619 | 0.9425 | NaN | 0.003 | 0.0794 | 0.969552 | 0.9933 | 0.0968 | 0.1195 | 0.417948 | 0.7466 | -0.065 | 0.1033 | 0.528986 | 0.8742 | NaN | -0.0524 | 0.0604 | 0.385807 | 0.8287 | 0.1178 | 0.0936 | 0.207914 | 0.6538 | -0.1673 | 0.0772 | 0.030298 | 0.3354 | NaN | 0.0502 | 0.0447 | 0.261949 | 0.5828 | 0.0231 | 0.0731 | 0.752027 | 0.8746 | 0.0697 | 0.0564 | 0.216231 | 0.9519 | NaN | 0.0079 | 0.036 | 0.826272 | 0.9722 | 0.0104 | 0.0607 | 0.863266 | 0.9977 | 0.007 | 0.0444 | 0.874238 | 0.9967 | NaN | 0.0608 | 0.0443 | 0.1702 | 0.7516 | 0.0175 | 0.0725 | 0.809874 | 0.9093 | 0.0913 | 0.0563 | 0.104956 | 0.7232 |
| diethyl-2-methyl-3-oxosuccinate | 202.0845 | 3.062651 | Exogenous | Food Component/Plant | 0.0735 | 0.0849 | 0.387028 | 0.7203 | 0.1921 | 0.1412 | 0.173677 | 0.45 | 0.0263 | 0.1064 | 0.804639 | 0.9511 | NaN | 0.0303 | 0.079 | 0.701523 | 0.9341 | 0.1928 | 0.1236 | 0.118766 | 0.4674 | -0.0233 | 0.1007 | 0.817063 | 0.9616 | NaN | -0.0255 | 0.0602 | 0.672058 | 0.9288 | 0.1524 | 0.0985 | 0.121578 | 0.577 | -0.1154 | 0.0758 | 0.127809 | 0.5265 | NaN | 0.0244 | 0.0447 | 0.586087 | 0.8129 | -0.0299 | 0.0778 | 0.700808 | 0.8597 | 0.0449 | 0.0546 | 0.410997 | 0.9735 | NaN | 0.0265 | 0.0358 | 0.459893 | 0.9708 | 0.0729 | 0.0633 | 0.249515 | 0.9821 | 0.0055 | 0.043 | 0.897719 | 0.9967 | NaN | 0.0286 | 0.0444 | 0.519516 | 0.8373 | -0.0632 | 0.0773 | 0.413856 | 0.7051 | 0.0721 | 0.0544 | 0.18532 | 0.7294 |
| pinitol | 194.0788 | 0.882718 | Exogenous | Food Component/Plant | -0.0646 | 0.0845 | 0.44434 | 0.7689 | -0.1044 | 0.1243 | 0.401147 | 0.7124 | -0.0405 | 0.1146 | 0.723643 | 0.9022 | NaN | -0.0326 | 0.0784 | 0.677263 | 0.9303 | -0.0595 | 0.1097 | 0.587226 | 0.8258 | -0.0153 | 0.1077 | 0.887394 | 0.9776 | NaN | -0.1103 | 0.0591 | 0.061992 | 0.4387 | -0.0549 | 0.0871 | 0.52818 | 0.8173 | -0.1736 | 0.0805 | 0.030991 | 0.3354 | NaN | -0.0624 | 0.0442 | 0.158648 | 0.5033 | -0.1221 | 0.0657 | 0.063224 | 0.2837 | -0.002 | 0.059 | 0.973508 | 0.9994 | NaN | 0.0026 | 0.0357 | 0.942766 | 0.9797 | -0.0125 | 0.0557 | 0.822115 | 0.9977 | 0.0123 | 0.0464 | 0.791219 | 0.9967 | NaN | -0.0294 | 0.0441 | 0.505419 | 0.8283 | -0.0932 | 0.0657 | 0.155631 | 0.5303 | 0.0314 | 0.0591 | 0.595472 | 0.9367 |
| 4-nitrophenol | 139.027 | 7.010404 | Exogenous | Pesticide Metabolism | -0.0238 | 0.0827 | 0.77318 | 0.9192 | 0.0313 | 0.1119 | 0.779744 | 0.9222 | -0.0793 | 0.1217 | 0.514528 | 0.8041 | NaN | -0.0409 | 0.0764 | 0.593036 | 0.8776 | -0.0032 | 0.0985 | 0.974091 | 0.9835 | -0.0958 | 0.114 | 0.400741 | 0.8015 | NaN | -0.0365 | 0.0581 | 0.530321 | 0.9005 | 0.0303 | 0.0781 | 0.698361 | 0.8816 | -0.1317 | 0.0856 | 0.123761 | 0.5215 | NaN | -0.0068 | 0.0435 | 0.875727 | 0.9579 | -0.0201 | 0.0601 | 0.73784 | 0.8684 | 0.0246 | 0.0629 | 0.695503 | 0.9994 | NaN | 0.0039 | 0.0349 | 0.911544 | 0.9722 | -0.0191 | 0.0498 | 0.702176 | 0.9977 | 0.0282 | 0.0494 | 0.567991 | 0.9967 | NaN | 0.0006 | 0.0431 | 0.988831 | 0.9972 | -0.0417 | 0.0596 | 0.484253 | 0.7613 | 0.0613 | 0.063 | 0.330285 | 0.8205 |
| estradiol valerate | 356.2358 | 21.2267 | Exogenous | Synthetic estrodiol | -0.0191 | 0.0833 | 0.818343 | 0.9391 | -0.1551 | 0.1245 | 0.212841 | 0.4978 | 0.098 | 0.1104 | 0.374712 | 0.7082 | NaN | -0.0224 | 0.0771 | 0.771505 | 0.9675 | -0.0262 | 0.1129 | 0.816337 | 0.9349 | 0.052 | 0.1045 | 0.619016 | 0.8939 | NaN | -0.0176 | 0.0586 | 0.764263 | 0.9502 | -0.023 | 0.0886 | 0.795473 | 0.9217 | -0.0059 | 0.0791 | 0.940669 | 0.9766 | NaN | -0.105 | 0.0434 | 0.015456 | 0.3584 | -0.1562 | 0.0654 | 0.016868 | 0.2 | -0.0716 | 0.0574 | 0.211995 | 0.9514 | NaN | 0.0044 | 0.0351 | 0.900238 | 0.9722 | -0.0419 | 0.056 | 0.453614 | 0.9977 | 0.0439 | 0.0446 | 0.324745 | 0.9967 | NaN | -0.0729 | 0.0433 | 0.092065 | 0.7516 | -0.1616 | 0.0647 | 0.012482 | 0.265 | -0.0067 | 0.0573 | 0.906926 | 0.9953 |
| phytanate | 312.3016 | 23.236364 | Lipid | Branched Chain Fatty Acid | -0.0155 | 0.086 | 0.856746 | 0.9457 | -0.1318 | 0.1215 | 0.277831 | 0.592 | 0.1158 | 0.1201 | 0.334927 | 0.7038 | NaN | 0.0122 | 0.0797 | 0.877798 | 0.9933 | -0.0455 | 0.1084 | 0.674594 | 0.87 | 0.1163 | 0.1126 | 0.301381 | 0.7079 | NaN | 0.0253 | 0.0605 | 0.676402 | 0.9288 | 0.0406 | 0.087 | 0.640468 | 0.8476 | 0.0055 | 0.0861 | 0.94941 | 0.9766 | NaN | -0.0643 | 0.045 | 0.153415 | 0.4947 | -0.1234 | 0.0643 | 0.055081 | 0.2691 | 0.0035 | 0.0623 | 0.955174 | 0.9994 | NaN | 0.0283 | 0.0362 | 0.435308 | 0.9708 | 0.002 | 0.0548 | 0.970951 | 0.9977 | 0.0569 | 0.0485 | 0.240698 | 0.9967 | NaN | -0.0336 | 0.0448 | 0.453357 | 0.8178 | -0.1128 | 0.064 | 0.077978 | 0.3895 | 0.0512 | 0.062 | 0.409086 | 0.8463 |
| Cer 35:0 | 569.5027 | 24.040377 | Lipid | Ceramide | 0.01 | 0.0851 | 0.906235 | 0.9586 | -0.1721 | 0.1294 | 0.183349 | 0.4621 | 0.147 | 0.1103 | 0.182424 | 0.5263 | NaN | 0.0125 | 0.0787 | 0.873367 | 0.9933 | -0.0476 | 0.117 | 0.683832 | 0.8726 | 0.111 | 0.1042 | 0.286347 | 0.6902 | NaN | 0.0655 | 0.0598 | 0.273246 | 0.7604 | 0.0328 | 0.0935 | 0.725393 | 0.8816 | 0.0923 | 0.0784 | 0.238949 | 0.6205 | NaN | -0.082 | 0.0445 | 0.065809 | 0.3995 | -0.1303 | 0.0688 | 0.058144 | 0.2743 | -0.0469 | 0.0581 | 0.418971 | 0.9735 | NaN | -0.0309 | 0.0358 | 0.387859 | 0.9708 | -0.1012 | 0.0573 | 0.077296 | 0.6995 | 0.022 | 0.0452 | 0.626674 | 0.9967 | NaN | -0.0564 | 0.0443 | 0.202843 | 0.7516 | -0.1226 | 0.0684 | 0.072921 | 0.3895 | -0.007 | 0.0579 | 0.903766 | 0.9953 |
| Cer 36:0 | 583.5183 | 24.290825 | Lipid | Ceramide | -0.0287 | 0.0842 | 0.733011 | 0.916 | -0.1654 | 0.1202 | 0.168597 | 0.4411 | 0.0691 | 0.117 | 0.554443 | 0.8324 | NaN | 0.0192 | 0.0783 | 0.806791 | 0.9803 | -0.0705 | 0.1078 | 0.513543 | 0.7797 | 0.106 | 0.1098 | 0.334177 | 0.7438 | NaN | 0.0002 | 0.0593 | 0.997624 | 0.9992 | -0.0692 | 0.085 | 0.415911 | 0.7889 | 0.0739 | 0.0827 | 0.371417 | 0.7398 | NaN | -0.0473 | 0.0442 | 0.284115 | 0.5896 | -0.0819 | 0.0648 | 0.205936 | 0.5052 | -0.0272 | 0.0604 | 0.653102 | 0.9994 | NaN | -0.0267 | 0.0355 | 0.451943 | 0.9708 | -0.0956 | 0.0532 | 0.072575 | 0.6995 | 0.0346 | 0.0472 | 0.464222 | 0.9967 | NaN | -0.0364 | 0.0439 | 0.407406 | 0.8117 | -0.0872 | 0.0641 | 0.173609 | 0.5384 | 0.0028 | 0.0604 | 0.962618 | 0.996 |
| Cer 37:0 | 597.5333 | 24.592678 | Lipid | Ceramide | -0.0107 | 0.0878 | 0.902694 | 0.9586 | -0.2936 | 0.1352 | 0.02985 | 0.2362 | 0.1603 | 0.1121 | 0.15276 | 0.5142 | NaN | 0.059 | 0.0819 | 0.471551 | 0.7817 | -0.1347 | 0.125 | 0.281176 | 0.6549 | 0.2002 | 0.1049 | 0.056253 | 0.4962 | NaN | 0.0171 | 0.0618 | 0.781834 | 0.9569 | -0.0728 | 0.0991 | 0.462645 | 0.7981 | 0.0728 | 0.0803 | 0.365007 | 0.7396 | NaN | -0.0504 | 0.046 | 0.273698 | 0.5828 | -0.1749 | 0.0725 | 0.015801 | 0.1982 | 0.0349 | 0.0586 | 0.551319 | 0.9885 | NaN | 0.0036 | 0.037 | 0.922277 | 0.9722 | -0.0896 | 0.0618 | 0.147196 | 0.8645 | 0.0635 | 0.0455 | 0.162783 | 0.9967 | NaN | -0.0382 | 0.0457 | 0.403301 | 0.8117 | -0.1801 | 0.0717 | 0.011967 | 0.265 | 0.0581 | 0.0583 | 0.318967 | 0.8169 |
| Cer 38:0 | 611.5497 | 24.956318 | Lipid | Ceramide | 0.1314 | 0.0825 | 0.111365 | 0.3866 | -0.0369 | 0.1257 | 0.769261 | 0.9222 | 0.2369 | 0.1084 | 0.028905 | 0.2924 | NaN | 0.1462 | 0.0762 | 0.054871 | 0.3365 | 0.0673 | 0.1119 | 0.547627 | 0.7852 | 0.2255 | 0.1017 | 0.026553 | 0.3692 | NaN | 0.0998 | 0.0581 | 0.085518 | 0.5364 | 0.0468 | 0.0881 | 0.595301 | 0.8374 | 0.149 | 0.0777 | 0.055034 | 0.4161 | NaN | -0.0328 | 0.0442 | 0.458215 | 0.7396 | -0.0811 | 0.067 | 0.226102 | 0.5371 | -0.0007 | 0.0587 | 0.9911 | 0.9994 | NaN | 0.0129 | 0.0352 | 0.714284 | 0.971 | -0.0524 | 0.0557 | 0.347249 | 0.9977 | 0.0634 | 0.045 | 0.158712 | 0.9967 | NaN | -0.0146 | 0.0438 | 0.739517 | 0.9202 | -0.0592 | 0.0666 | 0.374337 | 0.6709 | 0.0177 | 0.0585 | 0.762273 | 0.9745 |
| Cer 40:0 | 639.5812 | 25.886269 | Lipid | Ceramide | 0.0203 | 0.0841 | 0.8096 | 0.9369 | -0.1989 | 0.1257 | 0.113544 | 0.3717 | 0.1988 | 0.1096 | 0.0696 | 0.3664 | NaN | -0.0011 | 0.0778 | 0.988768 | 0.9933 | -0.1228 | 0.112 | 0.272795 | 0.6408 | 0.145 | 0.1044 | 0.164918 | 0.6552 | NaN | 0.0437 | 0.0591 | 0.459658 | 0.863 | -0.0303 | 0.0905 | 0.738146 | 0.8816 | 0.0987 | 0.0788 | 0.21059 | 0.6205 | NaN | -0.0869 | 0.044 | 0.048574 | 0.3914 | -0.1409 | 0.0668 | 0.034979 | 0.2355 | -0.0432 | 0.0588 | 0.46246 | 0.9735 | NaN | -0.0241 | 0.0354 | 0.496509 | 0.9708 | -0.09 | 0.0562 | 0.109273 | 0.7937 | 0.0292 | 0.0454 | 0.519793 | 0.9967 | NaN | -0.0467 | 0.0438 | 0.286539 | 0.7695 | -0.1193 | 0.0668 | 0.074064 | 0.3895 | 0.0127 | 0.0583 | 0.827513 | 0.9785 |
| Cer 41:0 | 653.5953 | 26.49853 | Lipid | Ceramide | 0.052 | 0.0836 | 0.53399 | 0.8257 | -0.2104 | 0.1261 | 0.095213 | 0.3536 | 0.2492 | 0.1072 | 0.020147 | 0.251 | NaN | 0.0445 | 0.0774 | 0.565069 | 0.8617 | -0.1175 | 0.1131 | 0.298744 | 0.6731 | 0.2088 | 0.1017 | 0.040033 | 0.4527 | NaN | 0.0841 | 0.0587 | 0.151483 | 0.6546 | -0.0096 | 0.0917 | 0.916299 | 0.9695 | 0.1518 | 0.0771 | 0.048795 | 0.3839 | NaN | -0.1056 | 0.0439 | 0.016219 | 0.3584 | -0.1898 | 0.0658 | 0.003936 | 0.1608 | -0.0384 | 0.0589 | 0.514163 | 0.9885 | NaN | -0.0398 | 0.0353 | 0.259451 | 0.9708 | -0.125 | 0.0556 | 0.02465 | 0.6225 | 0.0261 | 0.0454 | 0.565639 | 0.9967 | NaN | -0.0667 | 0.0437 | 0.127308 | 0.7516 | -0.1582 | 0.0662 | 0.016861 | 0.2658 | 0.0065 | 0.0584 | 0.910855 | 0.996 |
| Cer 42:0 | 667.6126 | 27.104397 | Lipid | Ceramide | 0.0131 | 0.0848 | 0.876918 | 0.9457 | -0.2574 | 0.1248 | 0.039223 | 0.2428 | 0.2334 | 0.1108 | 0.03515 | 0.3207 | NaN | 0.0121 | 0.0784 | 0.87695 | 0.9933 | -0.1628 | 0.1123 | 0.147115 | 0.4937 | 0.1961 | 0.1048 | 0.061397 | 0.4962 | NaN | 0.0508 | 0.0596 | 0.393654 | 0.8313 | -0.07 | 0.0909 | 0.441062 | 0.7964 | 0.1369 | 0.0796 | 0.085401 | 0.4613 | NaN | -0.1325 | 0.0441 | 0.002636 | 0.2657 | -0.2043 | 0.0652 | 0.001739 | 0.12 | -0.0704 | 0.0605 | 0.244399 | 0.9622 | NaN | -0.0326 | 0.0357 | 0.360878 | 0.9708 | -0.1122 | 0.0561 | 0.045446 | 0.6733 | 0.0314 | 0.0464 | 0.49917 | 0.9967 | NaN | -0.0766 | 0.0441 | 0.082457 | 0.7508 | -0.1603 | 0.0661 | 0.01539 | 0.2658 | -0.0042 | 0.0599 | 0.943651 | 0.996 |
| Cer 43:0 | 681.6278 | 27.911722 | Lipid | Ceramide | 0.0045 | 0.0858 | 0.958614 | 0.9784 | -0.2535 | 0.124 | 0.040839 | 0.2428 | 0.2276 | 0.1141 | 0.046054 | 0.3531 | NaN | 0.0073 | 0.0793 | 0.926634 | 0.9933 | -0.1791 | 0.1106 | 0.105429 | 0.4511 | 0.1996 | 0.1075 | 0.063272 | 0.4962 | NaN | 0.0471 | 0.0603 | 0.434869 | 0.8511 | -0.0796 | 0.0899 | 0.375698 | 0.775 | 0.1423 | 0.0816 | 0.081045 | 0.4613 | NaN | -0.1428 | 0.0444 | 0.001304 | 0.2657 | -0.2117 | 0.0644 | 0.001014 | 0.08 | -0.0778 | 0.0619 | 0.208934 | 0.9514 | NaN | -0.0353 | 0.0361 | 0.327956 | 0.9708 | -0.1109 | 0.0557 | 0.046375 | 0.6733 | 0.029 | 0.0476 | 0.543214 | 0.9967 | NaN | -0.0916 | 0.0445 | 0.039479 | 0.7271 | -0.1699 | 0.0653 | 0.009261 | 0.265 | -0.0188 | 0.0615 | 0.759993 | 0.9745 |
| Cer 44:0 | 695.6444 | 28.868212 | Lipid | Ceramide | -0.0081 | 0.0862 | 0.925041 | 0.9635 | -0.2563 | 0.1258 | 0.041557 | 0.2428 | 0.2067 | 0.1145 | 0.071169 | 0.3706 | NaN | -0.007 | 0.0797 | 0.929735 | 0.9933 | -0.1869 | 0.112 | 0.095088 | 0.4459 | 0.1779 | 0.1079 | 0.099286 | 0.5686 | NaN | 0.0324 | 0.0607 | 0.593511 | 0.9166 | -0.0919 | 0.0909 | 0.311739 | 0.7581 | 0.1206 | 0.082 | 0.141186 | 0.5393 | NaN | -0.1506 | 0.0445 | 0.000714 | 0.2657 | -0.216 | 0.0653 | 0.000944 | 0.08 | -0.0896 | 0.0616 | 0.145803 | 0.9514 | NaN | -0.0384 | 0.0363 | 0.289004 | 0.9708 | -0.1084 | 0.0566 | 0.055384 | 0.6733 | 0.0192 | 0.0476 | 0.686294 | 0.9967 | NaN | -0.0934 | 0.0447 | 0.036437 | 0.7271 | -0.1665 | 0.0664 | 0.012183 | 0.265 | -0.0264 | 0.0613 | 0.666728 | 0.9564 |
| Cer d38:1 (2OH) | 609.5342 | 24.481514 | Lipid | Ceramide | 0.1643 | 0.0835 | 0.048928 | 0.2597 | 0.0337 | 0.1308 | 0.796912 | 0.9222 | 0.2469 | 0.1065 | 0.02046 | 0.251 | NaN | 0.1709 | 0.077 | 0.026477 | 0.2284 | 0.1274 | 0.1154 | 0.26943 | 0.637 | 0.2297 | 0.1001 | 0.02168 | 0.3375 | NaN | 0.1516 | 0.0583 | 0.009321 | 0.166 | 0.14 | 0.0909 | 0.123498 | 0.577 | 0.1669 | 0.076 | 0.028171 | 0.3354 | NaN | -0.0759 | 0.0452 | 0.093175 | 0.4393 | -0.1231 | 0.0698 | 0.077642 | 0.304 | -0.0467 | 0.0586 | 0.425582 | 0.9735 | NaN | 0.0103 | 0.0359 | 0.773792 | 0.9722 | -0.0239 | 0.0582 | 0.682088 | 0.9977 | 0.0362 | 0.0449 | 0.420702 | 0.9967 | NaN | -0.0551 | 0.0448 | 0.21875 | 0.7516 | -0.0969 | 0.0694 | 0.162471 | 0.5359 | -0.0271 | 0.0585 | 0.643539 | 0.9483 |
| Cer d40:1 (2OH) | 637.5656 | 25.195412 | Lipid | Ceramide | 0.0353 | 0.0857 | 0.680436 | 0.8796 | -0.167 | 0.1286 | 0.194189 | 0.4734 | 0.1953 | 0.1117 | 0.08026 | 0.3886 | NaN | 0.0328 | 0.0793 | 0.679204 | 0.9303 | -0.0863 | 0.1146 | 0.451488 | 0.7607 | 0.1643 | 0.1054 | 0.119007 | 0.6083 | NaN | 0.0605 | 0.0602 | 0.314662 | 0.782 | -0.009 | 0.092 | 0.922199 | 0.9721 | 0.1128 | 0.0799 | 0.15783 | 0.5549 | NaN | -0.0834 | 0.045 | 0.063913 | 0.3995 | -0.1367 | 0.0682 | 0.044894 | 0.2513 | -0.0404 | 0.0597 | 0.498885 | 0.988 | NaN | -0.0152 | 0.0362 | 0.674387 | 0.9708 | -0.064 | 0.0576 | 0.266052 | 0.9821 | 0.0248 | 0.0463 | 0.591718 | 0.9967 | NaN | -0.0488 | 0.0448 | 0.275738 | 0.7695 | -0.1093 | 0.0682 | 0.108986 | 0.4527 | 0.0007 | 0.0594 | 0.991157 | 0.996 |
| Cer d42:1 (2OH) | 665.5972 | 26.210842 | Lipid | Ceramide | 0.0145 | 0.0859 | 0.865549 | 0.9457 | -0.2453 | 0.1279 | 0.055143 | 0.2818 | 0.2199 | 0.1116 | 0.048841 | 0.3542 | NaN | 0.0037 | 0.0795 | 0.962574 | 0.9933 | -0.1564 | 0.1146 | 0.172436 | 0.5201 | 0.174 | 0.106 | 0.100637 | 0.5686 | NaN | 0.0502 | 0.0604 | 0.406384 | 0.8406 | -0.052 | 0.0931 | 0.576652 | 0.8355 | 0.1216 | 0.0802 | 0.129718 | 0.5265 | NaN | -0.1023 | 0.0449 | 0.02274 | 0.3584 | -0.1617 | 0.0681 | 0.017651 | 0.2 | -0.0527 | 0.0604 | 0.382832 | 0.9735 | NaN | -0.0314 | 0.0362 | 0.384938 | 0.9708 | -0.1203 | 0.0571 | 0.034925 | 0.6466 | 0.038 | 0.0464 | 0.41345 | 0.9967 | NaN | -0.0604 | 0.0448 | 0.17728 | 0.7516 | -0.142 | 0.0681 | 0.037146 | 0.3022 | 0.0074 | 0.0598 | 0.900909 | 0.9953 |
| Cer d43:1 (2OH) | 679.6125 | 26.850416 | Lipid | Ceramide | 0.0078 | 0.0877 | 0.929131 | 0.9641 | -0.2468 | 0.1296 | 0.056897 | 0.2819 | 0.2133 | 0.1151 | 0.063784 | 0.3614 | NaN | 0.0014 | 0.0811 | 0.986012 | 0.9933 | -0.1778 | 0.1152 | 0.122771 | 0.4674 | 0.1771 | 0.1087 | 0.103394 | 0.5745 | NaN | 0.0626 | 0.0616 | 0.30941 | 0.782 | -0.0568 | 0.0941 | 0.546293 | 0.8202 | 0.145 | 0.0819 | 0.076659 | 0.455 | NaN | -0.1087 | 0.0457 | 0.017482 | 0.3584 | -0.1611 | 0.0691 | 0.019726 | 0.2134 | -0.0605 | 0.0619 | 0.328381 | 0.9622 | NaN | -0.0327 | 0.0369 | 0.375586 | 0.9708 | -0.1266 | 0.0576 | 0.02801 | 0.6225 | 0.0414 | 0.0476 | 0.384399 | 0.9967 | NaN | -0.064 | 0.0456 | 0.160405 | 0.7516 | -0.1426 | 0.069 | 0.038868 | 0.3022 | 0.0052 | 0.0614 | 0.932163 | 0.996 |
| Cer d44:1 (2OH) | 693.6285 | 27.404913 | Lipid | Ceramide | -0.0379 | 0.0859 | 0.659426 | 0.8782 | -0.3022 | 0.1236 | 0.014517 | 0.1742 | 0.1815 | 0.1146 | 0.113167 | 0.4498 | NaN | -0.0315 | 0.0794 | 0.691984 | 0.9341 | -0.1982 | 0.112 | 0.076782 | 0.4408 | 0.1477 | 0.1082 | 0.172119 | 0.6598 | NaN | 0.0221 | 0.0606 | 0.714925 | 0.9414 | -0.1126 | 0.0905 | 0.213476 | 0.6538 | 0.1198 | 0.0815 | 0.141654 | 0.5393 | NaN | -0.1064 | 0.0447 | 0.017163 | 0.3584 | -0.1603 | 0.067 | 0.016779 | 0.2 | -0.0574 | 0.061 | 0.346501 | 0.9622 | NaN | -0.0346 | 0.0361 | 0.338908 | 0.9708 | -0.1333 | 0.0557 | 0.0168 | 0.5917 | 0.0453 | 0.047 | 0.33537 | 0.9967 | NaN | -0.0591 | 0.0447 | 0.185356 | 0.7516 | -0.1353 | 0.0673 | 0.044296 | 0.3175 | 0.0089 | 0.0605 | 0.883283 | 0.993 |
| Cer t34:0(2OH) | 571.4738 | 23.930481 | Lipid | Ceramide | 0.0422 | 0.0836 | 0.614068 | 0.8736 | -0.1525 | 0.127 | 0.229772 | 0.5285 | 0.2019 | 0.1082 | 0.062134 | 0.3614 | NaN | 0.035 | 0.0773 | 0.650759 | 0.9303 | -0.0363 | 0.1145 | 0.751313 | 0.89 | 0.1563 | 0.1028 | 0.128585 | 0.6104 | NaN | 0.081 | 0.0587 | 0.1675 | 0.6546 | 0.0572 | 0.0917 | 0.532836 | 0.8173 | 0.1059 | 0.0778 | 0.173656 | 0.5775 | NaN | -0.0853 | 0.0439 | 0.052291 | 0.3914 | -0.1502 | 0.0669 | 0.02467 | 0.2177 | -0.0374 | 0.0582 | 0.519712 | 0.9885 | NaN | -0.0272 | 0.0353 | 0.441659 | 0.9708 | -0.0709 | 0.0566 | 0.210517 | 0.9357 | 0.0096 | 0.0452 | 0.831315 | 0.9967 | NaN | -0.0535 | 0.0437 | 0.221098 | 0.7516 | -0.1231 | 0.0669 | 0.065708 | 0.3895 | -0.0002 | 0.0579 | 0.997816 | 0.9978 |
| Cer t38:0(2OH) | 627.5368 | 25.20021 | Lipid | Ceramide | 0.08 | 0.0837 | 0.338966 | 0.6908 | -0.133 | 0.1231 | 0.279907 | 0.592 | 0.2526 | 0.1101 | 0.021854 | 0.2567 | NaN | 0.0845 | 0.0773 | 0.27444 | 0.6455 | -0.0524 | 0.1096 | 0.632935 | 0.8459 | 0.2296 | 0.1036 | 0.026755 | 0.3692 | NaN | 0.0969 | 0.0586 | 0.098208 | 0.5647 | 0.0455 | 0.0882 | 0.605734 | 0.8395 | 0.144 | 0.0794 | 0.069886 | 0.4434 | NaN | -0.0868 | 0.0443 | 0.049719 | 0.3914 | -0.1762 | 0.064 | 0.00588 | 0.1623 | -0.0086 | 0.06 | 0.88599 | 0.9994 | NaN | 0.003 | 0.0354 | 0.932019 | 0.9744 | -0.0409 | 0.0551 | 0.458242 | 0.9977 | 0.0427 | 0.0463 | 0.356821 | 0.9967 | NaN | -0.0495 | 0.044 | 0.259844 | 0.7516 | -0.1335 | 0.0644 | 0.038252 | 0.3022 | 0.0244 | 0.0596 | 0.68227 | 0.9564 |
| Cer t40:0(2OH) | 655.5675 | 26.20871 | Lipid | Ceramide | 0.0129 | 0.0866 | 0.881141 | 0.9481 | -0.2645 | 0.1293 | 0.040773 | 0.2428 | 0.2252 | 0.1119 | 0.044078 | 0.3531 | NaN | 0.0009 | 0.0801 | 0.990763 | 0.9933 | -0.1772 | 0.1158 | 0.125771 | 0.4744 | 0.1792 | 0.1062 | 0.091569 | 0.5595 | NaN | 0.056 | 0.0609 | 0.357201 | 0.7983 | -0.0555 | 0.0946 | 0.557192 | 0.8202 | 0.1329 | 0.0802 | 0.097616 | 0.4716 | NaN | -0.0888 | 0.0453 | 0.049928 | 0.3914 | -0.1671 | 0.069 | 0.015476 | 0.1982 | -0.0251 | 0.0604 | 0.677792 | 0.9994 | NaN | -0.0211 | 0.0365 | 0.563323 | 0.9708 | -0.104 | 0.0584 | 0.074811 | 0.6995 | 0.0424 | 0.0465 | 0.36215 | 0.9967 | NaN | -0.0551 | 0.0451 | 0.222007 | 0.7516 | -0.1452 | 0.0691 | 0.035535 | 0.3022 | 0.0176 | 0.0599 | 0.768737 | 0.9748 |
| Cer t41:0(2OH) | 669.5838 | 26.84795 | Lipid | Ceramide | -0.0165 | 0.0861 | 0.847812 | 0.9457 | -0.2947 | 0.1219 | 0.015667 | 0.1765 | 0.2269 | 0.1155 | 0.049415 | 0.3542 | NaN | -0.0159 | 0.0796 | 0.84126 | 0.9933 | -0.2086 | 0.1095 | 0.056751 | 0.4173 | 0.1913 | 0.1091 | 0.079656 | 0.5496 | NaN | 0.0369 | 0.0606 | 0.542515 | 0.9012 | -0.0921 | 0.0898 | 0.305222 | 0.7522 | 0.1395 | 0.0826 | 0.091287 | 0.4613 | NaN | -0.0992 | 0.0449 | 0.027091 | 0.3584 | -0.1678 | 0.0657 | 0.010618 | 0.1724 | -0.0348 | 0.0623 | 0.576114 | 0.9888 | NaN | -0.0285 | 0.0362 | 0.432244 | 0.9708 | -0.1111 | 0.0556 | 0.045502 | 0.6733 | 0.0435 | 0.048 | 0.363949 | 0.9967 | NaN | -0.0604 | 0.0448 | 0.177548 | 0.7516 | -0.1504 | 0.0657 | 0.022028 | 0.2725 | 0.0234 | 0.0617 | 0.703729 | 0.9666 |
| Cer t42:0(2OH) | 683.5993 | 27.302876 | Lipid | Ceramide | -0.0227 | 0.0849 | 0.788982 | 0.9232 | -0.3115 | 0.1216 | 0.010404 | 0.1606 | 0.2188 | 0.1124 | 0.051657 | 0.3614 | NaN | -0.0116 | 0.0786 | 0.883006 | 0.9933 | -0.1847 | 0.1118 | 0.0985 | 0.4459 | 0.1844 | 0.1062 | 0.082517 | 0.5555 | NaN | 0.0403 | 0.0599 | 0.500942 | 0.8921 | -0.091 | 0.0904 | 0.313996 | 0.7586 | 0.1414 | 0.0802 | 0.077979 | 0.4579 | NaN | -0.0993 | 0.0442 | 0.024751 | 0.3584 | -0.176 | 0.0656 | 0.007276 | 0.1672 | -0.0345 | 0.0606 | 0.568659 | 0.9885 | NaN | -0.0249 | 0.0358 | 0.487086 | 0.9708 | -0.1131 | 0.0557 | 0.042246 | 0.6733 | 0.0485 | 0.0466 | 0.29806 | 0.9967 | NaN | -0.0595 | 0.0442 | 0.177758 | 0.7516 | -0.1493 | 0.066 | 0.02356 | 0.2725 | 0.0173 | 0.0601 | 0.77286 | 0.9748 |
| PE-Cer d34:1 | 660.5193 | 23.983944 | Lipid | Ceramide phosphoethanolamines | 0.004 | 0.0856 | 0.962728 | 0.9784 | -0.2064 | 0.1262 | 0.101976 | 0.3627 | 0.1805 | 0.1129 | 0.109998 | 0.4472 | NaN | -0.007 | 0.0792 | 0.930013 | 0.9933 | -0.1342 | 0.1124 | 0.232276 | 0.5936 | 0.1385 | 0.107 | 0.195291 | 0.6714 | NaN | 0.0263 | 0.0602 | 0.661773 | 0.9288 | -0.049 | 0.0907 | 0.589145 | 0.8374 | 0.0812 | 0.0812 | 0.316786 | 0.6914 | NaN | -0.0836 | 0.0448 | 0.061906 | 0.3995 | -0.1082 | 0.068 | 0.11188 | 0.3743 | -0.0611 | 0.0601 | 0.309237 | 0.9622 | NaN | -0.0322 | 0.036 | 0.372023 | 0.9708 | -0.0978 | 0.0563 | 0.082572 | 0.7247 | 0.022 | 0.0466 | 0.637727 | 0.9967 | NaN | -0.0362 | 0.0446 | 0.417619 | 0.8132 | -0.0771 | 0.0681 | 0.25806 | 0.5937 | 0.0011 | 0.0598 | 0.98489 | 0.996 |
| PE-Cer d34:2 | 658.5018 | 23.675238 | Lipid | Ceramide phosphoethanolamines | -0.0338 | 0.0801 | 0.672984 | 0.8782 | -0.2007 | 0.119 | 0.091576 | 0.3462 | 0.1063 | 0.1059 | 0.31575 | 0.6905 | NaN | -0.0466 | 0.0741 | 0.529795 | 0.8356 | -0.1274 | 0.1061 | 0.229658 | 0.5924 | 0.0645 | 0.1002 | 0.519748 | 0.8742 | NaN | 0.0488 | 0.0566 | 0.388151 | 0.8305 | 0.0151 | 0.0872 | 0.862287 | 0.9388 | 0.081 | 0.075 | 0.28034 | 0.6728 | NaN | -0.0831 | 0.0418 | 0.0469 | 0.3914 | -0.0766 | 0.0648 | 0.236691 | 0.5536 | -0.0946 | 0.0552 | 0.086299 | 0.8712 | NaN | -0.0287 | 0.0337 | 0.394877 | 0.9708 | -0.0606 | 0.0538 | 0.259982 | 0.9821 | -0.0011 | 0.0432 | 0.979752 | 0.9967 | NaN | -0.0487 | 0.0417 | 0.242572 | 0.7516 | -0.0618 | 0.0645 | 0.338266 | 0.6496 | -0.0405 | 0.0553 | 0.463906 | 0.8635 |
| PE-Cer d36:2 | 686.5345 | 23.691633 | Lipid | Ceramide phosphoethanolamines | 0.0162 | 0.0852 | 0.84898 | 0.9457 | -0.0464 | 0.133 | 0.727306 | 0.9045 | 0.106 | 0.1129 | 0.347692 | 0.7082 | NaN | 0.0045 | 0.0789 | 0.954206 | 0.9933 | -0.013 | 0.1169 | 0.911628 | 0.9659 | 0.0779 | 0.1063 | 0.463731 | 0.8416 | NaN | 0.0542 | 0.0599 | 0.366049 | 0.8082 | 0.1197 | 0.0936 | 0.200761 | 0.6538 | 0.0175 | 0.0807 | 0.828413 | 0.9496 | NaN | -0.0436 | 0.0448 | 0.330349 | 0.6376 | -0.0764 | 0.0709 | 0.281773 | 0.5914 | -0.021 | 0.0587 | 0.719978 | 0.9994 | NaN | -0.0052 | 0.0359 | 0.885382 | 0.9722 | -0.0009 | 0.0592 | 0.987529 | 0.9977 | -0.0011 | 0.046 | 0.980738 | 0.9967 | NaN | -0.0227 | 0.0445 | 0.610544 | 0.8587 | -0.0553 | 0.0705 | 0.432722 | 0.7216 | 0.002 | 0.0587 | 0.973453 | 0.996 |
| DG 36:0 | 646.5518 | 29.627296 | Lipid | Diacylglycerol | 0.0718 | 0.0906 | 0.427904 | 0.7595 | 0.1272 | 0.1673 | 0.447202 | 0.748 | 0.068 | 0.1077 | 0.527734 | 0.8099 | NaN | 0.0654 | 0.0838 | 0.435252 | 0.7723 | 0.1047 | 0.1469 | 0.47624 | 0.7664 | 0.0611 | 0.101 | 0.545187 | 0.8748 | NaN | 0.0348 | 0.0638 | 0.585359 | 0.9166 | 0.0612 | 0.1172 | 0.601819 | 0.8395 | 0.015 | 0.0766 | 0.845048 | 0.9539 | NaN | 0.0041 | 0.0478 | 0.931814 | 0.9723 | 0.0368 | 0.0901 | 0.682853 | 0.849 | -0.0003 | 0.0556 | 0.994999 | 0.9994 | NaN | 0.0155 | 0.0383 | 0.685651 | 0.9708 | -0.0391 | 0.075 | 0.602674 | 0.9977 | 0.0385 | 0.0434 | 0.375314 | 0.9967 | NaN | 0.0012 | 0.0474 | 0.980391 | 0.9951 | 0.0001 | 0.0896 | 0.999135 | 0.9991 | 0.0082 | 0.0556 | 0.883169 | 0.993 |
| DG 38:3 | 668.5383 | 27.205564 | Lipid | Diacylglycerol | 0.1832 | 0.0882 | 0.037813 | 0.2244 | 0.0652 | 0.1304 | 0.616899 | 0.8589 | 0.2947 | 0.118 | 0.012502 | 0.1816 | NaN | 0.153 | 0.0819 | 0.061684 | 0.3472 | 0.1237 | 0.1144 | 0.279478 | 0.6537 | 0.2311 | 0.1131 | 0.041057 | 0.4527 | NaN | 0.1053 | 0.0625 | 0.092049 | 0.5584 | 0.0965 | 0.0907 | 0.287499 | 0.7347 | 0.1057 | 0.0875 | 0.226817 | 0.6205 | NaN | -0.0256 | 0.0477 | 0.591416 | 0.8141 | -0.0881 | 0.0701 | 0.208965 | 0.5104 | 0.0409 | 0.0641 | 0.523834 | 0.9885 | NaN | 0.0541 | 0.0376 | 0.150785 | 0.9708 | 0.0369 | 0.058 | 0.524129 | 0.9977 | 0.0722 | 0.0495 | 0.144943 | 0.9967 | NaN | 0.0052 | 0.0471 | 0.911933 | 0.9724 | -0.0901 | 0.0695 | 0.19486 | 0.5437 | 0.0969 | 0.0629 | 0.123325 | 0.7232 |
| 15R-PGE2 methyl ester, 15-acetate | 408.2501 | 17.902542 | Lipid | Eicosanoid | 0.0252 | 0.0818 | 0.758414 | 0.9192 | 0.1208 | 0.1598 | 0.449562 | 0.7497 | -0.018 | 0.0964 | 0.852079 | 0.9565 | NaN | 0.0428 | 0.0757 | 0.571528 | 0.8691 | 0.1856 | 0.1399 | 0.184407 | 0.5358 | -0.0022 | 0.0905 | 0.980894 | 0.9993 | NaN | 0.0274 | 0.0576 | 0.633472 | 0.9288 | 0.1677 | 0.1107 | 0.129903 | 0.5878 | -0.0013 | 0.0683 | 0.985228 | 0.9961 | NaN | 0.0355 | 0.043 | 0.408084 | 0.7018 | -0.1002 | 0.0865 | 0.246577 | 0.5603 | 0.0677 | 0.0494 | 0.170514 | 0.9514 | NaN | 0.0281 | 0.0345 | 0.415508 | 0.9708 | -0.0417 | 0.0716 | 0.561012 | 0.9977 | 0.0548 | 0.0387 | 0.156984 | 0.9967 | NaN | 0.0262 | 0.0427 | 0.539268 | 0.8373 | -0.0975 | 0.0858 | 0.255718 | 0.5931 | 0.0585 | 0.0495 | 0.237604 | 0.7365 |
| leukotriene B4 | 336.2348 | 22.004122 | Lipid | Eicosanoid | -0.0699 | 0.0847 | 0.40921 | 0.7406 | 0.188 | 0.1434 | 0.189688 | 0.4657 | -0.1977 | 0.1028 | 0.054422 | 0.3614 | NaN | -0.07 | 0.0783 | 0.371283 | 0.7361 | 0.08 | 0.1284 | 0.533396 | 0.7797 | -0.1781 | 0.0967 | 0.065406 | 0.4962 | NaN | -0.0463 | 0.0596 | 0.437802 | 0.8511 | 0.0005 | 0.1028 | 0.996119 | 0.9998 | -0.0883 | 0.0744 | 0.235026 | 0.6205 | NaN | -0.0495 | 0.0445 | 0.265715 | 0.5828 | -0.0701 | 0.0791 | 0.375365 | 0.6609 | -0.029 | 0.0546 | 0.594919 | 0.9994 | NaN | -0.0582 | 0.0355 | 0.101542 | 0.9708 | -0.0027 | 0.0651 | 0.966549 | 0.9977 | -0.092 | 0.0415 | 0.026849 | 0.8504 | NaN | -0.0408 | 0.0442 | 0.35607 | 0.7843 | -0.0227 | 0.0781 | 0.771002 | 0.8941 | -0.0443 | 0.0544 | 0.41563 | 0.8487 |
| FA 9:0 | 158.1307 | 18.327808 | Lipid | Fatty Acid | 0.0416 | 0.0862 | 0.629776 | 0.8777 | 0.1825 | 0.132 | 0.166842 | 0.4386 | -0.058 | 0.1119 | 0.604457 | 0.8469 | NaN | 0.0074 | 0.08 | 0.926102 | 0.9933 | 0.0736 | 0.1186 | 0.535035 | 0.7797 | -0.0679 | 0.1049 | 0.517387 | 0.8742 | NaN | -0.0909 | 0.061 | 0.136494 | 0.6296 | 0.0349 | 0.0942 | 0.710992 | 0.8816 | -0.1795 | 0.0783 | 0.021901 | 0.3181 | NaN | 0.0603 | 0.0452 | 0.182106 | 0.5115 | 0.1322 | 0.0703 | 0.059863 | 0.2766 | 0.0085 | 0.0577 | 0.883608 | 0.9994 | NaN | -0.0039 | 0.0364 | 0.91567 | 0.9722 | 0.0098 | 0.06 | 0.870068 | 0.9977 | -0.0148 | 0.0453 | 0.744523 | 0.9967 | NaN | 0.0594 | 0.0448 | 0.184857 | 0.7516 | 0.0694 | 0.0709 | 0.32785 | 0.6453 | 0.0522 | 0.0578 | 0.366918 | 0.8297 |
| FA 12:0 | 200.1775 | 21.715498 | Lipid | Fatty Acid | -0.024 | 0.0834 | 0.773624 | 0.9192 | -0.0451 | 0.127 | 0.72244 | 0.9045 | 0.0055 | 0.1098 | 0.960327 | 0.9916 | NaN | 0.0298 | 0.0777 | 0.701335 | 0.9341 | 0.0229 | 0.1122 | 0.838452 | 0.9389 | 0.0543 | 0.1037 | 0.600233 | 0.8877 | NaN | -0.0667 | 0.0586 | 0.255085 | 0.7568 | 0.0683 | 0.0892 | 0.444074 | 0.7964 | -0.1721 | 0.0778 | 0.02706 | 0.3354 | NaN | -0.0572 | 0.0437 | 0.190399 | 0.5115 | -0.1107 | 0.0673 | 0.100026 | 0.3495 | -0.016 | 0.0565 | 0.776338 | 0.9994 | NaN | 0.0357 | 0.0351 | 0.310083 | 0.9708 | 0.0339 | 0.0566 | 0.548606 | 0.9977 | 0.0391 | 0.0442 | 0.377099 | 0.9967 | NaN | -0.0108 | 0.0435 | 0.803866 | 0.9482 | -0.086 | 0.0671 | 0.199942 | 0.5437 | 0.0465 | 0.0564 | 0.409358 | 0.8463 |
| FA 14:0 | 228.2091 | 22.407074 | Lipid | Fatty Acid | 0.1284 | 0.0826 | 0.120117 | 0.4018 | 0.0094 | 0.1257 | 0.940147 | 0.9682 | 0.2142 | 0.1078 | 0.04695 | 0.3542 | NaN | 0.1325 | 0.0763 | 0.082395 | 0.3825 | 0.053 | 0.1105 | 0.631446 | 0.8459 | 0.2043 | 0.1011 | 0.04328 | 0.4527 | NaN | 0.0767 | 0.0583 | 0.188741 | 0.6946 | 0.1252 | 0.0876 | 0.153212 | 0.6041 | 0.0407 | 0.0796 | 0.609323 | 0.8637 | NaN | -0.0247 | 0.0442 | 0.575219 | 0.8059 | -0.0949 | 0.0671 | 0.156887 | 0.4339 | 0.0329 | 0.0573 | 0.56631 | 0.9885 | NaN | 0.0292 | 0.0351 | 0.406375 | 0.9708 | 0.021 | 0.0559 | 0.707015 | 0.9977 | 0.0367 | 0.0449 | 0.413985 | 0.9967 | NaN | -0.0009 | 0.0437 | 0.984463 | 0.9971 | -0.0632 | 0.0667 | 0.343808 | 0.6499 | 0.0504 | 0.0571 | 0.378103 | 0.8297 |
| FA 15:0 | 242.2245 | 22.619587 | Lipid | Fatty Acid | 0.0778 | 0.0809 | 0.336494 | 0.6908 | 0.0094 | 0.1162 | 0.935672 | 0.9682 | 0.1311 | 0.1118 | 0.241135 | 0.6106 | NaN | 0.0948 | 0.0748 | 0.204771 | 0.5669 | 0.0746 | 0.1024 | 0.466367 | 0.7643 | 0.1282 | 0.1048 | 0.221422 | 0.6714 | NaN | 0.0875 | 0.0567 | 0.122773 | 0.5898 | 0.1252 | 0.081 | 0.121963 | 0.577 | 0.0506 | 0.08 | 0.527076 | 0.826 | NaN | -0.0445 | 0.0429 | 0.298557 | 0.6019 | -0.1012 | 0.0619 | 0.101996 | 0.3541 | 0.0143 | 0.0582 | 0.805927 | 0.9994 | NaN | 0.0097 | 0.0343 | 0.776125 | 0.9722 | -0.0099 | 0.0517 | 0.847658 | 0.9977 | 0.0264 | 0.0456 | 0.562428 | 0.9967 | NaN | -0.0093 | 0.0425 | 0.82681 | 0.9529 | -0.0734 | 0.0616 | 0.232991 | 0.5691 | 0.0549 | 0.0579 | 0.34312 | 0.8286 |
| FA 16:0 | 256.2406 | 22.803902 | Lipid | Fatty Acid | 0.1444 | 0.0835 | 0.083718 | 0.3439 | -0.0153 | 0.1261 | 0.903541 | 0.9573 | 0.2686 | 0.109 | 0.013679 | 0.1936 | NaN | 0.1346 | 0.0772 | 0.081444 | 0.3825 | 0.0412 | 0.1111 | 0.710895 | 0.8811 | 0.2358 | 0.1029 | 0.022009 | 0.3375 | NaN | 0.1085 | 0.0587 | 0.064641 | 0.4439 | 0.1165 | 0.0882 | 0.186845 | 0.652 | 0.1046 | 0.0804 | 0.193373 | 0.6065 | NaN | -0.0284 | 0.0448 | 0.526628 | 0.7799 | -0.1005 | 0.0671 | 0.133861 | 0.4016 | 0.0358 | 0.0591 | 0.544913 | 0.9885 | NaN | 0.0095 | 0.0357 | 0.791254 | 0.9722 | -0.0024 | 0.0561 | 0.966007 | 0.9977 | 0.0211 | 0.0465 | 0.649413 | 0.9967 | NaN | -0.0075 | 0.0444 | 0.865295 | 0.9644 | -0.0755 | 0.0667 | 0.258147 | 0.5937 | 0.0526 | 0.0589 | 0.371986 | 0.8297 |
| FA 18:0 | 284.2719 | 23.144428 | Lipid | Fatty Acid | 0.1497 | 0.0822 | 0.068767 | 0.3125 | 0.0473 | 0.1276 | 0.710792 | 0.902 | 0.2226 | 0.1058 | 0.035434 | 0.3207 | NaN | 0.1282 | 0.0762 | 0.09252 | 0.3985 | 0.036 | 0.112 | 0.748018 | 0.89 | 0.1974 | 0.0997 | 0.047778 | 0.4577 | NaN | 0.1171 | 0.0578 | 0.04283 | 0.3813 | 0.1451 | 0.0885 | 0.101199 | 0.577 | 0.0987 | 0.0769 | 0.199111 | 0.614 | NaN | -0.0119 | 0.0442 | 0.787383 | 0.9001 | -0.0639 | 0.0685 | 0.351483 | 0.6511 | 0.0286 | 0.0566 | 0.613779 | 0.9994 | NaN | 0.0125 | 0.0352 | 0.723493 | 0.971 | -0.0107 | 0.0569 | 0.850302 | 0.9977 | 0.0307 | 0.0443 | 0.488295 | 0.9967 | NaN | 0.0046 | 0.0437 | 0.916858 | 0.9724 | -0.0451 | 0.068 | 0.507679 | 0.7783 | 0.0433 | 0.0564 | 0.442627 | 0.8627 |
| FA 19:0 | 298.2865 | 23.328478 | Lipid | Fatty Acid | 0.038 | 0.0836 | 0.649741 | 0.8782 | -0.0227 | 0.1254 | 0.856187 | 0.9521 | 0.1129 | 0.1117 | 0.312329 | 0.6896 | NaN | 0.0492 | 0.0773 | 0.524528 | 0.832 | 0.0096 | 0.1102 | 0.930618 | 0.9707 | 0.1155 | 0.1047 | 0.27004 | 0.6818 | NaN | 0.0118 | 0.0589 | 0.840797 | 0.9805 | 0.0408 | 0.0877 | 0.641968 | 0.8476 | -0.0102 | 0.0804 | 0.899068 | 0.9707 | NaN | 0.0117 | 0.044 | 0.791056 | 0.9022 | -0.0606 | 0.067 | 0.365393 | 0.659 | 0.0721 | 0.0573 | 0.208556 | 0.9514 | NaN | 0.0651 | 0.035 | 0.062687 | 0.9656 | 0.0758 | 0.0555 | 0.171763 | 0.8945 | 0.0632 | 0.045 | 0.160231 | 0.9967 | NaN | 0.0193 | 0.0436 | 0.658429 | 0.8716 | -0.0409 | 0.0666 | 0.539441 | 0.7906 | 0.0699 | 0.0574 | 0.223403 | 0.7294 |
| FA 20:0 | 312.303 | 23.478868 | Lipid | Fatty Acid | 0.009 | 0.0845 | 0.915098 | 0.9586 | -0.2021 | 0.1258 | 0.108323 | 0.3717 | 0.182 | 0.1106 | 0.099852 | 0.4331 | NaN | 0.0022 | 0.0781 | 0.97751 | 0.9933 | -0.1083 | 0.1129 | 0.33715 | 0.6996 | 0.1402 | 0.1047 | 0.180872 | 0.6637 | NaN | 0.0467 | 0.0594 | 0.432065 | 0.8488 | 0.0315 | 0.0922 | 0.732718 | 0.8816 | 0.061 | 0.08 | 0.445768 | 0.7876 | NaN | -0.0871 | 0.0442 | 0.048764 | 0.3914 | -0.1513 | 0.0667 | 0.023311 | 0.2149 | -0.0345 | 0.0588 | 0.557547 | 0.9885 | NaN | 0.0067 | 0.0356 | 0.851838 | 0.9722 | -0.0343 | 0.0573 | 0.548966 | 0.9977 | 0.0416 | 0.0455 | 0.359519 | 0.9967 | NaN | -0.0404 | 0.044 | 0.359411 | 0.7862 | -0.1201 | 0.0669 | 0.072622 | 0.3895 | 0.025 | 0.0583 | 0.667777 | 0.9564 |
| FA 22:0 | 340.3339 | 24.054163 | Lipid | Fatty Acid | -0.0369 | 0.0873 | 0.672683 | 0.8782 | -0.0602 | 0.132 | 0.64852 | 0.8671 | -0.0052 | 0.116 | 0.964183 | 0.9916 | NaN | -0.0919 | 0.081 | 0.256674 | 0.6275 | -0.1678 | 0.1164 | 0.149366 | 0.4937 | -0.0495 | 0.1093 | 0.650976 | 0.8939 | NaN | -0.0279 | 0.0614 | 0.650162 | 0.9288 | 0.0063 | 0.0926 | 0.945712 | 0.9762 | -0.0654 | 0.0821 | 0.426105 | 0.7865 | NaN | 0.0023 | 0.046 | 0.959907 | 0.9867 | 0.0051 | 0.071 | 0.942873 | 0.9603 | 0.0124 | 0.0596 | 0.834731 | 0.9994 | NaN | 0.0028 | 0.0368 | 0.940245 | 0.9793 | 0.0776 | 0.0587 | 0.186087 | 0.9357 | -0.0522 | 0.0466 | 0.263513 | 0.9967 | NaN | 0.0056 | 0.0456 | 0.901657 | 0.9724 | 0.0073 | 0.0704 | 0.917685 | 0.9654 | 0.013 | 0.0597 | 0.827812 | 0.9785 |
| FA 24:0 | 368.3658 | 24.705492 | Lipid | Fatty Acid | 0.0481 | 0.0866 | 0.578688 | 0.8499 | -0.0355 | 0.1219 | 0.770951 | 0.9222 | 0.1112 | 0.1256 | 0.375742 | 0.7082 | NaN | 0.0488 | 0.08 | 0.542192 | 0.8388 | -0.0995 | 0.1072 | 0.353499 | 0.7021 | 0.1343 | 0.1176 | 0.253477 | 0.6818 | NaN | 0.0321 | 0.0609 | 0.598749 | 0.9166 | -0.0173 | 0.0852 | 0.839259 | 0.9257 | 0.0603 | 0.0892 | 0.499339 | 0.8203 | NaN | 0.0422 | 0.0455 | 0.353221 | 0.6617 | 0.0055 | 0.0655 | 0.933329 | 0.9554 | 0.1062 | 0.064 | 0.09699 | 0.8712 | NaN | -0.0008 | 0.0366 | 0.981879 | 0.9915 | 0.0004 | 0.0543 | 0.994469 | 0.9977 | -0.0087 | 0.0512 | 0.865578 | 0.9967 | NaN | 0.0282 | 0.0452 | 0.5324 | 0.8373 | -0.0069 | 0.0649 | 0.915252 | 0.9654 | 0.0821 | 0.0644 | 0.202456 | 0.7294 |
| FA 25:0 | 382.3813 | 24.61329 | Lipid | Fatty Acid | 0.0238 | 0.0863 | 0.782593 | 0.9211 | -0.1556 | 0.1202 | 0.195551 | 0.4734 | 0.2246 | 0.1203 | 0.061913 | 0.3614 | NaN | 0.0003 | 0.0799 | 0.996945 | 0.9969 | -0.139 | 0.1055 | 0.187839 | 0.5388 | 0.1842 | 0.1138 | 0.105439 | 0.5745 | NaN | 0.0599 | 0.0606 | 0.323101 | 0.782 | 0.1286 | 0.0884 | 0.145647 | 0.5917 | 0.0221 | 0.0889 | 0.803495 | 0.9477 | NaN | -0.0391 | 0.0454 | 0.389173 | 0.6828 | -0.1402 | 0.0634 | 0.027106 | 0.2227 | 0.0572 | 0.0634 | 0.36621 | 0.9622 | NaN | -0.0159 | 0.0364 | 0.661428 | 0.9708 | -0.0462 | 0.054 | 0.392802 | 0.9977 | 0.0217 | 0.0501 | 0.664715 | 0.9967 | NaN | -0.014 | 0.045 | 0.755059 | 0.9221 | -0.1216 | 0.0633 | 0.05491 | 0.3608 | 0.092 | 0.0628 | 0.142701 | 0.7232 |
| FA 26:0 | 396.3969 | 25.627758 | Lipid | Fatty Acid | -0.0042 | 0.0828 | 0.959988 | 0.9784 | -0.1754 | 0.1073 | 0.10208 | 0.3627 | 0.2203 | 0.1259 | 0.080221 | 0.3886 | NaN | -0.0476 | 0.0768 | 0.535819 | 0.8366 | -0.228 | 0.0931 | 0.014319 | 0.2909 | 0.1674 | 0.1195 | 0.161465 | 0.6552 | NaN | -0.0367 | 0.0582 | 0.528619 | 0.9005 | -0.1153 | 0.0753 | 0.125884 | 0.5791 | 0.0508 | 0.0919 | 0.580086 | 0.8571 | NaN | 0.0176 | 0.0435 | 0.686254 | 0.8515 | -0.0328 | 0.059 | 0.578761 | 0.7754 | 0.1049 | 0.0652 | 0.107719 | 0.8962 | NaN | 0.0087 | 0.0349 | 0.802465 | 0.9722 | 0.0066 | 0.0493 | 0.893052 | 0.9977 | 0.0127 | 0.0523 | 0.809014 | 0.9967 | NaN | 0.0356 | 0.0431 | 0.409067 | 0.8117 | -0.0285 | 0.0586 | 0.626872 | 0.8191 | 0.137 | 0.0646 | 0.033808 | 0.6979 |
| FA 28:0 | 424.39 | 23.17103 | Lipid | Fatty Acid | -0.0976 | 0.0825 | 0.236857 | 0.588 | -0.3103 | 0.1344 | 0.02094 | 0.2028 | 0.0406 | 0.1035 | 0.694839 | 0.8959 | NaN | -0.1465 | 0.0763 | 0.054832 | 0.3365 | -0.2472 | 0.1192 | 0.038039 | 0.395 | -0.0374 | 0.0992 | 0.705981 | 0.9257 | NaN | -0.032 | 0.0584 | 0.583651 | 0.9166 | -0.0395 | 0.1005 | 0.694498 | 0.8793 | -0.0342 | 0.0736 | 0.641906 | 0.8795 | NaN | -0.1013 | 0.0429 | 0.018317 | 0.3584 | -0.1561 | 0.073 | 0.03263 | 0.2309 | -0.0668 | 0.0532 | 0.209215 | 0.9514 | NaN | -0.0039 | 0.035 | 0.911784 | 0.9722 | -0.0279 | 0.0631 | 0.658895 | 0.9977 | 0.0121 | 0.0418 | 0.773057 | 0.9967 | NaN | -0.059 | 0.043 | 0.169834 | 0.7516 | -0.1349 | 0.0731 | 0.064847 | 0.3895 | -0.0128 | 0.0534 | 0.809941 | 0.9748 |
| FA 14:1 | 226.1935 | 22.031717 | Lipid | Fatty Acid | 0.1787 | 0.0839 | 0.033136 | 0.2202 | 0.1244 | 0.1184 | 0.293702 | 0.6164 | 0.2148 | 0.1184 | 0.069477 | 0.3664 | NaN | 0.2418 | 0.0772 | 0.001745 | 0.0458 | 0.2005 | 0.1034 | 0.052561 | 0.4173 | 0.2797 | 0.1105 | 0.011384 | 0.2167 | NaN | 0.0814 | 0.0598 | 0.173143 | 0.6546 | 0.1896 | 0.0812 | 0.019516 | 0.3282 | -0.0308 | 0.0885 | 0.727578 | 0.9305 | NaN | -0.0372 | 0.0455 | 0.413859 | 0.7088 | -0.0974 | 0.0647 | 0.132495 | 0.4016 | 0.0223 | 0.0628 | 0.722768 | 0.9994 | NaN | 0.0389 | 0.0359 | 0.279335 | 0.9708 | 0.0342 | 0.0531 | 0.519553 | 0.9977 | 0.0418 | 0.0489 | 0.393394 | 0.9967 | NaN | -0.0141 | 0.045 | 0.753971 | 0.9221 | -0.0883 | 0.0642 | 0.169142 | 0.5381 | 0.0591 | 0.0623 | 0.342849 | 0.8286 |
| FA 16:1 | 254.225 | 22.542202 | Lipid | Fatty Acid | 0.1383 | 0.0844 | 0.101026 | 0.3718 | -0.0176 | 0.1269 | 0.889751 | 0.9558 | 0.259 | 0.1106 | 0.019183 | 0.251 | NaN | 0.1656 | 0.0778 | 0.033257 | 0.27 | 0.1079 | 0.1133 | 0.340542 | 0.702 | 0.2519 | 0.1035 | 0.014985 | 0.2668 | NaN | 0.0937 | 0.0595 | 0.115079 | 0.5674 | 0.1658 | 0.0889 | 0.062205 | 0.5028 | 0.0408 | 0.0832 | 0.624282 | 0.868 | NaN | -0.0482 | 0.0453 | 0.287149 | 0.5937 | -0.1403 | 0.067 | 0.036295 | 0.2414 | 0.0333 | 0.0597 | 0.576795 | 0.9888 | NaN | 0.0215 | 0.036 | 0.549343 | 0.9708 | 0.0069 | 0.0565 | 0.902688 | 0.9977 | 0.0352 | 0.0467 | 0.451192 | 0.9967 | NaN | -0.0187 | 0.0448 | 0.676454 | 0.8886 | -0.1 | 0.0669 | 0.135425 | 0.4951 | 0.0529 | 0.0594 | 0.373371 | 0.8297 |
| FA 17:1 | 268.2396 | 22.72618 | Lipid | Fatty Acid | 0.2108 | 0.0818 | 0.009957 | 0.1037 | 0.1831 | 0.1173 | 0.1185 | 0.3717 | 0.2456 | 0.1134 | 0.030356 | 0.294 | NaN | 0.1956 | 0.0757 | 0.009748 | 0.126 | 0.2668 | 0.1017 | 0.008689 | 0.2398 | 0.1898 | 0.1083 | 0.079553 | 0.5496 | NaN | 0.1085 | 0.0584 | 0.063229 | 0.4418 | 0.2124 | 0.0801 | 0.008003 | 0.2454 | -0.0047 | 0.0859 | 0.956043 | 0.9766 | NaN | 0.0193 | 0.0445 | 0.665005 | 0.846 | -0.0363 | 0.0652 | 0.577583 | 0.7754 | 0.0835 | 0.0598 | 0.162283 | 0.9514 | NaN | 0.0583 | 0.0352 | 0.09719 | 0.9708 | 0.0453 | 0.0531 | 0.393153 | 0.9977 | 0.0708 | 0.0469 | 0.131474 | 0.9967 | NaN | 0.0591 | 0.0437 | 0.17627 | 0.7516 | -0.0066 | 0.0643 | 0.91776 | 0.9654 | 0.1298 | 0.0587 | 0.027101 | 0.6979 |
| FA 18:1 | 282.2566 | 22.883368 | Lipid | Fatty Acid | 0.1036 | 0.0854 | 0.224996 | 0.5723 | -0.0248 | 0.1299 | 0.848732 | 0.9493 | 0.2056 | 0.1112 | 0.064574 | 0.3614 | NaN | 0.1256 | 0.0788 | 0.111035 | 0.4199 | 0.089 | 0.1156 | 0.441462 | 0.7563 | 0.1966 | 0.1043 | 0.059385 | 0.4962 | NaN | 0.0763 | 0.0601 | 0.203915 | 0.7091 | 0.1358 | 0.0911 | 0.135868 | 0.5905 | 0.0337 | 0.0818 | 0.680097 | 0.8981 | NaN | -0.055 | 0.0454 | 0.225526 | 0.5407 | -0.1266 | 0.0688 | 0.065682 | 0.2844 | 0.0047 | 0.0593 | 0.9362 | 0.9994 | NaN | 0.0065 | 0.0363 | 0.858037 | 0.9722 | 0.0121 | 0.0578 | 0.833594 | 0.9977 | 0.0045 | 0.0465 | 0.922129 | 0.9967 | NaN | -0.0265 | 0.045 | 0.555992 | 0.8505 | -0.0924 | 0.0686 | 0.177875 | 0.5427 | 0.0283 | 0.059 | 0.631721 | 0.9483 |
| FA 19:1 | 296.2718 | 23.05411 | Lipid | Fatty Acid | 0.105 | 0.0822 | 0.201426 | 0.554 | 0.1946 | 0.1175 | 0.097554 | 0.3566 | 0.036 | 0.1138 | 0.751671 | 0.9282 | NaN | 0.096 | 0.076 | 0.206807 | 0.5679 | 0.195 | 0.1027 | 0.05745 | 0.4173 | 0.0181 | 0.1068 | 0.865804 | 0.9708 | NaN | 0.0506 | 0.0581 | 0.383363 | 0.8287 | 0.1784 | 0.0812 | 0.028032 | 0.3439 | -0.0792 | 0.081 | 0.328101 | 0.702 | NaN | -0.0092 | 0.0437 | 0.832366 | 0.9396 | -0.0449 | 0.0657 | 0.493853 | 0.7368 | 0.0333 | 0.0584 | 0.568542 | 0.9885 | NaN | 0.0147 | 0.0349 | 0.674238 | 0.9708 | 0.0256 | 0.0537 | 0.63388 | 0.9977 | 0.0037 | 0.046 | 0.93637 | 0.9967 | NaN | -0.0056 | 0.0433 | 0.89703 | 0.9724 | -0.0451 | 0.0651 | 0.48822 | 0.7613 | 0.0361 | 0.0585 | 0.536676 | 0.9105 |
| FA 20:1 | 310.2876 | 23.21554 | Lipid | Fatty Acid | 0.0945 | 0.0865 | 0.274931 | 0.6386 | -0.068 | 0.1288 | 0.597513 | 0.8393 | 0.2331 | 0.1141 | 0.041184 | 0.3497 | NaN | 0.1223 | 0.0799 | 0.125926 | 0.4437 | 0.0779 | 0.1162 | 0.502458 | 0.7797 | 0.2192 | 0.1071 | 0.040707 | 0.4527 | NaN | 0.0752 | 0.0609 | 0.216497 | 0.7113 | 0.1547 | 0.0914 | 0.090533 | 0.5507 | 0.0176 | 0.0852 | 0.836294 | 0.9506 | NaN | -0.0805 | 0.0459 | 0.07961 | 0.4034 | -0.1739 | 0.0672 | 0.009673 | 0.1687 | 0.0028 | 0.0613 | 0.963444 | 0.9994 | NaN | -0.0053 | 0.0367 | 0.886169 | 0.9722 | -0.0458 | 0.0572 | 0.42382 | 0.9977 | 0.0307 | 0.0477 | 0.519944 | 0.9967 | NaN | -0.0437 | 0.0456 | 0.337824 | 0.7759 | -0.1502 | 0.0671 | 0.025185 | 0.278 | 0.0491 | 0.0607 | 0.418213 | 0.8487 |
| FA 22:1 | 338.319 | 23.61596 | Lipid | Fatty Acid | 0.0144 | 0.0862 | 0.866968 | 0.9457 | -0.1191 | 0.1199 | 0.320815 | 0.6425 | 0.1718 | 0.1215 | 0.157222 | 0.5166 | NaN | 0.0287 | 0.0798 | 0.718992 | 0.945 | 0.0035 | 0.1084 | 0.974548 | 0.9835 | 0.1381 | 0.1146 | 0.227914 | 0.6764 | NaN | 0.0515 | 0.0606 | 0.395122 | 0.8313 | 0.0795 | 0.0861 | 0.356221 | 0.7705 | 0.0301 | 0.0879 | 0.732055 | 0.9305 | NaN | -0.0611 | 0.0453 | 0.177256 | 0.5115 | -0.1107 | 0.0636 | 0.081935 | 0.3119 | -0.006 | 0.0639 | 0.92512 | 0.9994 | NaN | 0.0166 | 0.0363 | 0.646864 | 0.9708 | 0.018 | 0.0541 | 0.739171 | 0.9977 | 0.0212 | 0.0499 | 0.671213 | 0.9967 | NaN | -0.0303 | 0.045 | 0.501294 | 0.8283 | -0.0846 | 0.0636 | 0.183096 | 0.5427 | 0.0298 | 0.0636 | 0.63888 | 0.9483 |
| FA 24:1 | 366.3504 | 24.114376 | Lipid | Fatty Acid | 0.007 | 0.0841 | 0.933952 | 0.9665 | -0.0609 | 0.1238 | 0.622871 | 0.8596 | 0.0689 | 0.113 | 0.542224 | 0.8195 | NaN | 0.0267 | 0.0778 | 0.731875 | 0.9573 | 0.0055 | 0.1095 | 0.959967 | 0.9835 | 0.0715 | 0.106 | 0.499911 | 0.8733 | NaN | 0.0184 | 0.0591 | 0.755721 | 0.9454 | 0.0771 | 0.0873 | 0.377483 | 0.775 | -0.0278 | 0.0807 | 0.730557 | 0.9305 | NaN | -0.0548 | 0.0441 | 0.213779 | 0.5222 | -0.1038 | 0.0657 | 0.114244 | 0.3784 | -0.0122 | 0.0584 | 0.833863 | 0.9994 | NaN | 0.007 | 0.0354 | 0.844155 | 0.9722 | 0.0338 | 0.0553 | 0.540637 | 0.9977 | -0.013 | 0.0459 | 0.776295 | 0.9967 | NaN | -0.033 | 0.0438 | 0.451238 | 0.8178 | -0.0659 | 0.0656 | 0.315295 | 0.6453 | -0.004 | 0.0584 | 0.945383 | 0.996 |
| FA 25:1 | 380.3652 | 24.144978 | Lipid | Fatty Acid | -0.0454 | 0.0872 | 0.602207 | 0.8708 | -0.1891 | 0.1203 | 0.116108 | 0.3717 | 0.1338 | 0.1244 | 0.282177 | 0.6628 | NaN | -0.0431 | 0.0806 | 0.593085 | 0.8776 | -0.2045 | 0.1049 | 0.051341 | 0.4173 | 0.1442 | 0.1165 | 0.215856 | 0.6714 | NaN | 0.0395 | 0.0616 | 0.521782 | 0.8998 | 0.0799 | 0.089 | 0.369756 | 0.7724 | 0.0193 | 0.0892 | 0.829219 | 0.9496 | NaN | -0.081 | 0.0455 | 0.075193 | 0.3995 | -0.1777 | 0.0628 | 0.004658 | 0.161 | 0.0151 | 0.0646 | 0.814858 | 0.9994 | NaN | -0.046 | 0.0366 | 0.209386 | 0.9708 | -0.048 | 0.0545 | 0.377994 | 0.9977 | -0.0386 | 0.0509 | 0.4488 | 0.9967 | NaN | -0.0582 | 0.0453 | 0.198977 | 0.7516 | -0.1649 | 0.0626 | 0.008459 | 0.265 | 0.0508 | 0.0644 | 0.429569 | 0.8591 |
| FA 26:1 | 394.3815 | 24.47697 | Lipid | Fatty Acid | 0.0008 | 0.084 | 0.992273 | 0.9959 | -0.1786 | 0.1214 | 0.141139 | 0.4144 | 0.19 | 0.1142 | 0.096143 | 0.4331 | NaN | -0.0223 | 0.0778 | 0.774662 | 0.9675 | -0.1464 | 0.1069 | 0.170824 | 0.5189 | 0.145 | 0.1083 | 0.180595 | 0.6637 | NaN | 0.0616 | 0.0591 | 0.297425 | 0.782 | 0.0541 | 0.0888 | 0.541916 | 0.8173 | 0.0829 | 0.0822 | 0.313395 | 0.6892 | NaN | -0.072 | 0.044 | 0.101632 | 0.4561 | -0.1391 | 0.0643 | 0.030629 | 0.2296 | -0.0166 | 0.0607 | 0.784445 | 0.9994 | NaN | -0.0259 | 0.0354 | 0.464274 | 0.9708 | -0.0387 | 0.0549 | 0.481052 | 0.9977 | -0.0083 | 0.0475 | 0.86202 | 0.9967 | NaN | -0.045 | 0.0438 | 0.303475 | 0.7695 | -0.1143 | 0.0644 | 0.075876 | 0.3895 | 0.0154 | 0.0604 | 0.798486 | 0.9748 |
| FA 12:2 | 196.1463 | 20.184414 | Lipid | Fatty Acid | -0.1047 | 0.0866 | 0.227055 | 0.5749 | -0.1104 | 0.1204 | 0.359242 | 0.6909 | -0.1088 | 0.1241 | 0.38073 | 0.7082 | NaN | -0.0031 | 0.0823 | 0.96958 | 0.9933 | -0.0491 | 0.1067 | 0.645641 | 0.8459 | 0.0201 | 0.1218 | 0.868667 | 0.9708 | NaN | -0.0511 | 0.0612 | 0.403727 | 0.8406 | 0.0542 | 0.0859 | 0.528301 | 0.8173 | -0.1712 | 0.0869 | 0.048742 | 0.3839 | NaN | -0.09 | 0.0453 | 0.046878 | 0.3914 | -0.1589 | 0.0629 | 0.01151 | 0.1777 | -0.0054 | 0.0643 | 0.933466 | 0.9994 | NaN | -0.0515 | 0.0365 | 0.158366 | 0.9708 | -0.0736 | 0.0533 | 0.167379 | 0.8945 | -0.0331 | 0.0503 | 0.510908 | 0.9967 | NaN | -0.0888 | 0.0449 | 0.048186 | 0.7271 | -0.191 | 0.0615 | 0.001901 | 0.2424 | 0.0253 | 0.0645 | 0.694764 | 0.9612 |
| FA 14:2 | 224.1775 | 21.617804 | Lipid | Fatty Acid | 0.0252 | 0.0885 | 0.775679 | 0.9192 | -0.0328 | 0.1309 | 0.802127 | 0.9244 | 0.0505 | 0.12 | 0.674162 | 0.8876 | NaN | 0.1393 | 0.0834 | 0.094636 | 0.3988 | 0.091 | 0.1168 | 0.435638 | 0.7515 | 0.1676 | 0.1151 | 0.145337 | 0.6249 | NaN | -0.0173 | 0.0623 | 0.780692 | 0.9569 | 0.1153 | 0.0919 | 0.20924 | 0.6538 | -0.1357 | 0.0859 | 0.114207 | 0.5043 | NaN | -0.0872 | 0.0464 | 0.060025 | 0.3995 | -0.1814 | 0.0684 | 0.007987 | 0.1672 | -0.0066 | 0.0618 | 0.914926 | 0.9994 | NaN | -0.025 | 0.0373 | 0.502176 | 0.9708 | -0.0635 | 0.0579 | 0.273083 | 0.9834 | 0.0024 | 0.0486 | 0.959865 | 0.9967 | NaN | -0.065 | 0.0461 | 0.158356 | 0.7516 | -0.1798 | 0.0678 | 0.007984 | 0.265 | 0.0307 | 0.0618 | 0.618905 | 0.9449 |
| FA 16:2 | 252.2091 | 22.278397 | Lipid | Fatty Acid | 0.1418 | 0.0821 | 0.084076 | 0.3439 | 0.0321 | 0.1241 | 0.796163 | 0.9222 | 0.2133 | 0.1084 | 0.049062 | 0.3542 | NaN | 0.1707 | 0.0757 | 0.024087 | 0.2243 | 0.1485 | 0.11 | 0.176885 | 0.5254 | 0.2139 | 0.1014 | 0.034867 | 0.4277 | NaN | 0.0675 | 0.0582 | 0.246064 | 0.7548 | 0.1654 | 0.0861 | 0.054639 | 0.4944 | -0.0083 | 0.0812 | 0.918678 | 0.9752 | NaN | -0.0437 | 0.0441 | 0.322326 | 0.6354 | -0.1417 | 0.0659 | 0.031662 | 0.2309 | 0.0351 | 0.0576 | 0.542263 | 0.9885 | NaN | 0.0271 | 0.035 | 0.438694 | 0.9708 | 0.0171 | 0.0552 | 0.756569 | 0.9977 | 0.0347 | 0.0451 | 0.441806 | 0.9967 | NaN | -0.01 | 0.0436 | 0.819103 | 0.9499 | -0.1138 | 0.0657 | 0.083034 | 0.3918 | 0.073 | 0.0569 | 0.199909 | 0.7294 |
| FA 18:2 | 280.2409 | 22.678688 | Lipid | Fatty Acid | 0.1086 | 0.086 | 0.206667 | 0.5592 | -0.0608 | 0.1291 | 0.637687 | 0.8649 | 0.245 | 0.1126 | 0.029538 | 0.2924 | NaN | 0.1108 | 0.0795 | 0.163304 | 0.5093 | 0.0368 | 0.1149 | 0.749045 | 0.89 | 0.2142 | 0.1062 | 0.043786 | 0.4527 | NaN | 0.0805 | 0.0605 | 0.183517 | 0.6891 | 0.1214 | 0.0913 | 0.183483 | 0.652 | 0.0522 | 0.0836 | 0.532531 | 0.826 | NaN | -0.0516 | 0.0458 | 0.260159 | 0.5828 | -0.1377 | 0.0681 | 0.043083 | 0.2513 | 0.0238 | 0.0605 | 0.694285 | 0.9994 | NaN | 0.0126 | 0.0365 | 0.730008 | 0.971 | -0.0005 | 0.0576 | 0.993603 | 0.9977 | 0.0259 | 0.0474 | 0.583934 | 0.9967 | NaN | -0.019 | 0.0454 | 0.675144 | 0.8886 | -0.1054 | 0.068 | 0.120983 | 0.4626 | 0.0556 | 0.06 | 0.354311 | 0.8297 |
| FA 20:2 | 308.2719 | 22.989353 | Lipid | Fatty Acid | 0.1678 | 0.0834 | 0.044202 | 0.2416 | 0.1229 | 0.1241 | 0.322042 | 0.6425 | 0.2078 | 0.1114 | 0.062137 | 0.3614 | NaN | 0.1856 | 0.0768 | 0.015678 | 0.1841 | 0.2109 | 0.1085 | 0.051944 | 0.4173 | 0.2001 | 0.1044 | 0.055337 | 0.4962 | NaN | 0.1117 | 0.0589 | 0.0578 | 0.4236 | 0.1997 | 0.085 | 0.018856 | 0.3282 | 0.0359 | 0.0819 | 0.661428 | 0.8899 | NaN | -0.0384 | 0.0451 | 0.395049 | 0.685 | -0.0963 | 0.0677 | 0.154909 | 0.4339 | 0.0152 | 0.0593 | 0.797794 | 0.9994 | NaN | 0.0233 | 0.0358 | 0.515003 | 0.9708 | 0.001 | 0.0558 | 0.985603 | 0.9977 | 0.0417 | 0.0461 | 0.365318 | 0.9967 | NaN | -0.0075 | 0.0446 | 0.867279 | 0.9644 | -0.0704 | 0.0671 | 0.293908 | 0.6411 | 0.0487 | 0.0588 | 0.407817 | 0.8463 |
| FA 22:2 | 336.3035 | 23.333275 | Lipid | Fatty Acid | 0.0244 | 0.0866 | 0.77819 | 0.9198 | -0.1055 | 0.127 | 0.406113 | 0.7124 | 0.1563 | 0.1169 | 0.18131 | 0.5263 | NaN | 0.0345 | 0.0801 | 0.666609 | 0.9303 | 0.0046 | 0.1138 | 0.967952 | 0.9835 | 0.1264 | 0.1102 | 0.25114 | 0.6818 | NaN | 0.0273 | 0.0609 | 0.653449 | 0.9288 | 0.07 | 0.0904 | 0.439191 | 0.7964 | -0.0129 | 0.0851 | 0.879275 | 0.9674 | NaN | -0.07 | 0.0455 | 0.123425 | 0.4681 | -0.1466 | 0.0667 | 0.027988 | 0.2239 | 0.0052 | 0.0612 | 0.932954 | 0.9994 | NaN | 0.0115 | 0.0365 | 0.752129 | 0.9722 | -0.0047 | 0.0569 | 0.933863 | 0.9977 | 0.0293 | 0.0479 | 0.540715 | 0.9967 | NaN | -0.0273 | 0.0452 | 0.546553 | 0.8404 | -0.1132 | 0.0668 | 0.090152 | 0.4046 | 0.054 | 0.0608 | 0.374485 | 0.8297 |
| FA 24:2 | 364.335 | 23.7592 | Lipid | Fatty Acid | 0.0419 | 0.0856 | 0.62405 | 0.8777 | -0.1307 | 0.129 | 0.310774 | 0.6377 | 0.1937 | 0.1126 | 0.085566 | 0.4003 | NaN | 0.0632 | 0.0792 | 0.424711 | 0.7661 | -0.025 | 0.1155 | 0.828661 | 0.9389 | 0.1815 | 0.1057 | 0.085944 | 0.5595 | NaN | 0.0659 | 0.0601 | 0.272539 | 0.7604 | 0.0872 | 0.0927 | 0.347049 | 0.7705 | 0.0462 | 0.0821 | 0.573453 | 0.8532 | NaN | -0.062 | 0.045 | 0.168728 | 0.5068 | -0.1385 | 0.0681 | 0.041846 | 0.2513 | 0.0105 | 0.0597 | 0.860238 | 0.9994 | NaN | 0.0128 | 0.0361 | 0.722989 | 0.971 | -0.008 | 0.058 | 0.889709 | 0.9977 | 0.0325 | 0.0465 | 0.484455 | 0.9967 | NaN | -0.0253 | 0.0447 | 0.5713 | 0.8527 | -0.1083 | 0.0681 | 0.111462 | 0.4558 | 0.0495 | 0.0592 | 0.402785 | 0.8463 |
| FA 25:2 | 378.3497 | 23.828726 | Lipid | Fatty Acid | -0.045 | 0.0832 | 0.588406 | 0.857 | -0.2567 | 0.1182 | 0.029953 | 0.2362 | 0.1909 | 0.1151 | 0.097342 | 0.4331 | NaN | -0.074 | 0.077 | 0.336694 | 0.704 | -0.1946 | 0.1051 | 0.064216 | 0.4408 | 0.1216 | 0.1104 | 0.270826 | 0.6818 | NaN | 0.0423 | 0.0588 | 0.472142 | 0.8716 | 0.0283 | 0.0896 | 0.752193 | 0.8872 | 0.0633 | 0.0833 | 0.44781 | 0.7876 | NaN | -0.0931 | 0.0433 | 0.031734 | 0.3584 | -0.1795 | 0.0625 | 0.004077 | 0.1608 | -0.0129 | 0.0611 | 0.833159 | 0.9994 | NaN | -0.0289 | 0.0351 | 0.408921 | 0.9708 | -0.068 | 0.0543 | 0.21057 | 0.9357 | 0.0124 | 0.0477 | 0.795572 | 0.9967 | NaN | -0.0606 | 0.0432 | 0.161196 | 0.7516 | -0.1444 | 0.0631 | 0.022161 | 0.2725 | 0.0185 | 0.0608 | 0.761521 | 0.9745 |
| FA 26:2 | 392.3645 | 23.924543 | Lipid | Fatty Acid | -0.0839 | 0.084 | 0.318151 | 0.6807 | -0.3148 | 0.1159 | 0.006587 | 0.1275 | 0.177 | 0.1181 | 0.133784 | 0.4827 | NaN | -0.0872 | 0.0777 | 0.261582 | 0.6287 | -0.2331 | 0.1041 | 0.025159 | 0.3387 | 0.1319 | 0.1118 | 0.238109 | 0.6818 | NaN | 0.0065 | 0.0596 | 0.913474 | 0.9946 | 0.004 | 0.0907 | 0.964767 | 0.988 | 0.0113 | 0.086 | 0.895961 | 0.9707 | NaN | -0.1211 | 0.0435 | 0.005391 | 0.34 | -0.2116 | 0.0611 | 0.000537 | 0.08 | -0.0323 | 0.0624 | 0.604924 | 0.9994 | NaN | -0.0275 | 0.0355 | 0.438907 | 0.9708 | -0.0732 | 0.0545 | 0.179487 | 0.9259 | 0.0206 | 0.0486 | 0.67117 | 0.9967 | NaN | -0.082 | 0.0436 | 0.059894 | 0.7347 | -0.1823 | 0.0618 | 0.00318 | 0.2424 | 0.0173 | 0.0621 | 0.780883 | 0.9748 |
| FA 14:3 | 222.1618 | 20.25606 | Lipid | Fatty Acid | 0.0727 | 0.082 | 0.375549 | 0.7099 | -0.016 | 0.1222 | 0.896102 | 0.9568 | 0.1429 | 0.109 | 0.189846 | 0.543 | NaN | -0.0017 | 0.0771 | 0.982469 | 0.9933 | -0.1977 | 0.1102 | 0.072875 | 0.4408 | 0.0984 | 0.1033 | 0.340777 | 0.7555 | NaN | -0.0132 | 0.0581 | 0.819824 | 0.9805 | -0.0677 | 0.0853 | 0.427166 | 0.7964 | 0.0267 | 0.0786 | 0.733812 | 0.9305 | NaN | 0.0541 | 0.043 | 0.208442 | 0.5183 | 0.0813 | 0.0653 | 0.213201 | 0.5139 | 0.0352 | 0.0567 | 0.534716 | 0.9885 | NaN | 0.0313 | 0.0346 | 0.366156 | 0.9708 | 0.0446 | 0.0543 | 0.411016 | 0.9977 | 0.0221 | 0.0446 | 0.620299 | 0.9967 | NaN | 0.0526 | 0.0427 | 0.217998 | 0.7516 | 0.0754 | 0.0648 | 0.244848 | 0.5776 | 0.0372 | 0.0568 | 0.512468 | 0.8952 |
| FA 16:3 | 250.1933 | 22.076328 | Lipid | Fatty Acid | 0.1444 | 0.0862 | 0.093985 | 0.3603 | 0.1768 | 0.1245 | 0.155667 | 0.4298 | 0.1005 | 0.119 | 0.398383 | 0.7258 | NaN | 0.2466 | 0.0801 | 0.00207 | 0.0476 | 0.2667 | 0.1082 | 0.013722 | 0.2909 | 0.2126 | 0.1133 | 0.060669 | 0.4962 | NaN | 0.0676 | 0.0611 | 0.269114 | 0.7604 | 0.2514 | 0.0844 | 0.002881 | 0.173 | -0.1053 | 0.0863 | 0.222187 | 0.6205 | NaN | -0.0761 | 0.0463 | 0.100707 | 0.4561 | -0.1668 | 0.069 | 0.015626 | 0.1982 | -0.0002 | 0.0616 | 0.998014 | 0.9994 | NaN | 0.0117 | 0.0369 | 0.750341 | 0.9722 | 0.0248 | 0.0565 | 0.660599 | 0.9977 | -0.0033 | 0.0484 | 0.946072 | 0.9967 | NaN | -0.063 | 0.046 | 0.170353 | 0.7516 | -0.1759 | 0.0683 | 0.010021 | 0.265 | 0.0282 | 0.0615 | 0.646311 | 0.9483 |
| FA 20:3 | 306.2562 | 22.806253 | Lipid | Fatty Acid | 0.1091 | 0.0854 | 0.201044 | 0.554 | -0.0284 | 0.1288 | 0.825475 | 0.9363 | 0.2238 | 0.1117 | 0.045187 | 0.3531 | NaN | 0.0966 | 0.079 | 0.221102 | 0.5873 | 0.0576 | 0.1141 | 0.613694 | 0.8425 | 0.1786 | 0.106 | 0.092237 | 0.5595 | NaN | 0.0621 | 0.0602 | 0.302589 | 0.782 | 0.1047 | 0.0903 | 0.24661 | 0.6984 | 0.0293 | 0.0829 | 0.723369 | 0.9305 | NaN | -0.0633 | 0.0455 | 0.164005 | 0.5058 | -0.1251 | 0.0682 | 0.066596 | 0.2844 | -0.0093 | 0.0601 | 0.877585 | 0.9994 | NaN | 0.0033 | 0.0363 | 0.928436 | 0.9725 | -0.0099 | 0.0573 | 0.863547 | 0.9977 | 0.0164 | 0.0468 | 0.725484 | 0.9967 | NaN | -0.0184 | 0.045 | 0.683046 | 0.8913 | -0.0898 | 0.068 | 0.186596 | 0.5437 | 0.0428 | 0.0594 | 0.471586 | 0.8648 |
| FA 22:3 | 334.2871 | 23.009287 | Lipid | Fatty Acid | 0.0762 | 0.085 | 0.370022 | 0.7078 | -0.0169 | 0.1223 | 0.889973 | 0.9558 | 0.1578 | 0.1168 | 0.176413 | 0.5263 | NaN | 0.0548 | 0.0788 | 0.486764 | 0.7926 | 0.0652 | 0.1082 | 0.54675 | 0.7852 | 0.094 | 0.1114 | 0.398811 | 0.8005 | NaN | 0.0815 | 0.0596 | 0.171814 | 0.6546 | 0.1654 | 0.0856 | 0.053304 | 0.4904 | 0.0072 | 0.0847 | 0.932007 | 0.9766 | NaN | -0.0604 | 0.045 | 0.179562 | 0.5115 | -0.126 | 0.0647 | 0.051427 | 0.2572 | 0.0074 | 0.0611 | 0.903311 | 0.9994 | NaN | 0.0351 | 0.0358 | 0.327392 | 0.9708 | -0.0016 | 0.0544 | 0.97617 | 0.9977 | 0.0686 | 0.0473 | 0.146726 | 0.9967 | NaN | -0.0297 | 0.0446 | 0.505024 | 0.8283 | -0.1065 | 0.0644 | 0.097977 | 0.4327 | 0.0463 | 0.0608 | 0.446233 | 0.8627 |
| FA 26:3 | 390.3503 | 23.76976 | Lipid | Fatty Acid | 0.0145 | 0.0835 | 0.862068 | 0.9457 | -0.2467 | 0.1261 | 0.050447 | 0.2757 | 0.2324 | 0.1078 | 0.031096 | 0.2959 | NaN | -0.0187 | 0.0774 | 0.808954 | 0.9803 | -0.1875 | 0.1118 | 0.093546 | 0.4459 | 0.171 | 0.1034 | 0.098221 | 0.5686 | NaN | 0.034 | 0.0587 | 0.562765 | 0.911 | 0.0594 | 0.095 | 0.531722 | 0.8173 | 0.0255 | 0.0807 | 0.752314 | 0.9374 | NaN | -0.071 | 0.0438 | 0.104748 | 0.4581 | -0.2253 | 0.065 | 0.000529 | 0.08 | 0.0466 | 0.0575 | 0.417822 | 0.9735 | NaN | -0.0174 | 0.0352 | 0.621285 | 0.9708 | -0.1088 | 0.0566 | 0.054529 | 0.6733 | 0.0551 | 0.0448 | 0.218916 | 0.9967 | NaN | -0.0395 | 0.0435 | 0.363796 | 0.7902 | -0.1875 | 0.0658 | 0.004369 | 0.2424 | 0.0733 | 0.057 | 0.198753 | 0.7294 |
| FA 13:4 | 206.0786 | 1.517414 | Lipid | Fatty Acid | 0.1511 | 0.0921 | 0.100908 | 0.3718 | 0.2058 | 0.1251 | 0.100015 | 0.3608 | 0.0766 | 0.1343 | 0.568504 | 0.8352 | NaN | 0.1283 | 0.0853 | 0.13273 | 0.4462 | 0.1305 | 0.1115 | 0.241934 | 0.6051 | 0.0806 | 0.1259 | 0.52204 | 0.8742 | NaN | -0.0027 | 0.0661 | 0.967733 | 0.9971 | 0.0615 | 0.0896 | 0.492999 | 0.8029 | -0.0683 | 0.0961 | 0.476815 | 0.8049 | NaN | 0.1253 | 0.0479 | 0.008946 | 0.3584 | 0.119 | 0.0672 | 0.076439 | 0.3014 | 0.1248 | 0.0681 | 0.066967 | 0.8712 | NaN | 0.062 | 0.0389 | 0.111097 | 0.9708 | 0.1013 | 0.0558 | 0.06932 | 0.6957 | 0.0182 | 0.0544 | 0.738156 | 0.9967 | NaN | 0.1066 | 0.0478 | 0.025754 | 0.7271 | 0.0703 | 0.0677 | 0.298648 | 0.6411 | 0.1423 | 0.068 | 0.03637 | 0.6979 |
| FA 15:4 | 234.1102 | 4.254336 | Lipid | Fatty Acid | 0.0346 | 0.0919 | 0.706581 | 0.9008 | 0.1125 | 0.1306 | 0.388877 | 0.7038 | -0.0332 | 0.1274 | 0.794286 | 0.948 | NaN | -0.0116 | 0.0854 | 0.891998 | 0.9933 | 0.0452 | 0.1157 | 0.695706 | 0.8728 | -0.0745 | 0.1198 | 0.533845 | 0.8742 | NaN | -0.0697 | 0.0649 | 0.282496 | 0.7662 | -0.008 | 0.0924 | 0.931064 | 0.9734 | -0.1306 | 0.0899 | 0.146352 | 0.5464 | NaN | 0.0975 | 0.0479 | 0.04189 | 0.3914 | 0.1339 | 0.069 | 0.052183 | 0.2572 | 0.0642 | 0.0655 | 0.326764 | 0.9622 | NaN | 0.0441 | 0.0386 | 0.254062 | 0.9708 | 0.0346 | 0.0584 | 0.55372 | 0.9977 | 0.0525 | 0.0514 | 0.306916 | 0.9967 | NaN | 0.0862 | 0.0476 | 0.070382 | 0.7496 | 0.0599 | 0.0695 | 0.389185 | 0.6842 | 0.1128 | 0.0653 | 0.083829 | 0.7232 |
| FA 16:4 | 248.1258 | 4.832441 | Lipid | Fatty Acid | 0.0074 | 0.0901 | 0.934961 | 0.9665 | 0.126 | 0.1216 | 0.299908 | 0.6256 | -0.1292 | 0.1321 | 0.328161 | 0.6994 | NaN | -0.0277 | 0.0835 | 0.739806 | 0.9612 | 0.0202 | 0.1092 | 0.853125 | 0.9418 | -0.1283 | 0.1238 | 0.300062 | 0.7079 | NaN | -0.1075 | 0.0635 | 0.090328 | 0.556 | 0.0347 | 0.0858 | 0.686177 | 0.8747 | -0.2615 | 0.0914 | 0.004224 | 0.1228 | NaN | 0.0743 | 0.0472 | 0.11533 | 0.4618 | 0.075 | 0.0652 | 0.249701 | 0.5603 | 0.0621 | 0.0688 | 0.367031 | 0.9622 | NaN | 0.0187 | 0.038 | 0.622368 | 0.9708 | 0.0325 | 0.0545 | 0.550539 | 0.9977 | 0.0036 | 0.0539 | 0.946984 | 0.9967 | NaN | 0.0726 | 0.0468 | 0.121363 | 0.7516 | 0.0209 | 0.0653 | 0.74958 | 0.884 | 0.1295 | 0.0688 | 0.059771 | 0.702 |
| FA 18:4 | 276.1573 | 10.004185 | Lipid | Fatty Acid | -0.021 | 0.0856 | 0.80652 | 0.9369 | 0.1832 | 0.1212 | 0.130675 | 0.3899 | -0.2057 | 0.1212 | 0.089656 | 0.4159 | NaN | -0.0051 | 0.0792 | 0.948795 | 0.9933 | 0.1275 | 0.1074 | 0.235358 | 0.5987 | -0.1501 | 0.1153 | 0.193119 | 0.6714 | NaN | 0.0291 | 0.0603 | 0.629718 | 0.9288 | 0.1179 | 0.0851 | 0.165751 | 0.6267 | -0.028 | 0.0887 | 0.751918 | 0.9374 | NaN | -0.0081 | 0.045 | 0.856327 | 0.9469 | 0.0456 | 0.0662 | 0.491565 | 0.7353 | -0.0881 | 0.0629 | 0.161586 | 0.9514 | NaN | 0.0077 | 0.0361 | 0.83108 | 0.9722 | 0.0195 | 0.0552 | 0.724029 | 0.9977 | 0.0008 | 0.0504 | 0.987901 | 0.9967 | NaN | -0.022 | 0.0446 | 0.622586 | 0.8641 | 0.0068 | 0.0662 | 0.918092 | 0.9654 | -0.0713 | 0.0634 | 0.260542 | 0.7654 |
| FA 20:4 | 304.241 | 22.665243 | Lipid | Fatty Acid | 0.0318 | 0.0844 | 0.706586 | 0.9008 | -0.1169 | 0.1293 | 0.365999 | 0.695 | 0.1596 | 0.1099 | 0.146285 | 0.5047 | NaN | 0.0124 | 0.0782 | 0.874401 | 0.9933 | -0.0382 | 0.1149 | 0.739635 | 0.89 | 0.1074 | 0.1045 | 0.304201 | 0.7085 | NaN | 0.0653 | 0.0593 | 0.27035 | 0.7604 | 0.0717 | 0.0923 | 0.437695 | 0.7964 | 0.0604 | 0.079 | 0.443935 | 0.7876 | NaN | -0.0859 | 0.0443 | 0.052459 | 0.3914 | -0.1361 | 0.0682 | 0.046099 | 0.2513 | -0.0431 | 0.0581 | 0.457698 | 0.9735 | NaN | 0.0095 | 0.0356 | 0.790384 | 0.9722 | 0.0061 | 0.0581 | 0.915883 | 0.9977 | 0.0162 | 0.0452 | 0.720872 | 0.9967 | NaN | -0.0497 | 0.0441 | 0.259653 | 0.7516 | -0.0912 | 0.0684 | 0.182584 | 0.5427 | -0.0139 | 0.058 | 0.810782 | 0.9748 |
| FA 22:4 | 332.2713 | 22.904213 | Lipid | Fatty Acid | -0.0238 | 0.0822 | 0.771662 | 0.9192 | 0.1021 | 0.1387 | 0.461371 | 0.758 | -0.0645 | 0.1027 | 0.529737 | 0.8099 | NaN | -0.0124 | 0.076 | 0.870305 | 0.9933 | 0.1177 | 0.1215 | 0.332506 | 0.6989 | -0.0596 | 0.0963 | 0.536036 | 0.8742 | NaN | -0.0103 | 0.0578 | 0.85899 | 0.9805 | 0.0665 | 0.097 | 0.493072 | 0.8029 | -0.0638 | 0.0726 | 0.379273 | 0.7398 | NaN | 0.0128 | 0.0432 | 0.767575 | 0.8919 | 0.0379 | 0.0746 | 0.611199 | 0.7932 | 0.0124 | 0.0531 | 0.814525 | 0.9994 | NaN | -0.0235 | 0.0346 | 0.49717 | 0.9708 | -0.0147 | 0.0621 | 0.813404 | 0.9977 | -0.0282 | 0.0415 | 0.496622 | 0.9967 | NaN | 0.0209 | 0.0429 | 0.626272 | 0.8643 | -0.0017 | 0.0743 | 0.981993 | 0.9974 | 0.0431 | 0.0532 | 0.417555 | 0.8487 |
| FA 24:4 | 360.3031 | 23.212015 | Lipid | Fatty Acid | 0.0103 | 0.0819 | 0.900376 | 0.9586 | -0.0478 | 0.1204 | 0.69163 | 0.892 | 0.081 | 0.1138 | 0.476636 | 0.7784 | NaN | 0.0173 | 0.0757 | 0.818855 | 0.9803 | 0.0211 | 0.1065 | 0.843324 | 0.9389 | 0.055 | 0.107 | 0.607352 | 0.8893 | NaN | 0.0241 | 0.0576 | 0.675587 | 0.9288 | 0.0828 | 0.0848 | 0.328532 | 0.7705 | -0.0524 | 0.0816 | 0.521383 | 0.826 | NaN | -0.0566 | 0.043 | 0.18796 | 0.5115 | -0.0707 | 0.0642 | 0.270881 | 0.5824 | -0.0201 | 0.0589 | 0.733 | 0.9994 | NaN | -0.0172 | 0.0345 | 0.617568 | 0.9708 | -0.0309 | 0.0535 | 0.563763 | 0.9977 | -0.0073 | 0.0462 | 0.873849 | 0.9967 | NaN | -0.0191 | 0.0427 | 0.654384 | 0.8716 | -0.0767 | 0.0636 | 0.227936 | 0.5642 | 0.0502 | 0.0585 | 0.390804 | 0.8329 |
| FA 26:4 | 388.3348 | 23.58473 | Lipid | Fatty Acid | -0.0132 | 0.0823 | 0.872742 | 0.9457 | -0.1029 | 0.1265 | 0.416301 | 0.7226 | 0.0714 | 0.108 | 0.508687 | 0.8016 | NaN | -0.022 | 0.0761 | 0.772187 | 0.9675 | -0.0229 | 0.1124 | 0.838306 | 0.9389 | 0.0297 | 0.102 | 0.770672 | 0.9454 | NaN | 0.0195 | 0.0579 | 0.736936 | 0.9415 | 0.0596 | 0.09 | 0.507569 | 0.8105 | -0.0176 | 0.0771 | 0.819902 | 0.9488 | NaN | -0.0649 | 0.0431 | 0.131771 | 0.4825 | -0.1007 | 0.0673 | 0.134752 | 0.4021 | -0.028 | 0.0559 | 0.616394 | 0.9994 | NaN | 0.0032 | 0.0347 | 0.92723 | 0.9725 | 0.0059 | 0.0568 | 0.916914 | 0.9977 | 0.0035 | 0.0438 | 0.936607 | 0.9967 | NaN | -0.0285 | 0.0429 | 0.506598 | 0.8283 | -0.0702 | 0.0672 | 0.296288 | 0.6411 | 0.0103 | 0.0558 | 0.853089 | 0.9811 |
| FA 20:5 | 302.2251 | 22.461945 | Lipid | Fatty Acid | 0.1468 | 0.0872 | 0.092156 | 0.3578 | 0.1488 | 0.136 | 0.274202 | 0.5912 | 0.1512 | 0.1126 | 0.179454 | 0.5263 | NaN | 0.101 | 0.0812 | 0.213939 | 0.5835 | 0.1791 | 0.1189 | 0.131929 | 0.4744 | 0.0821 | 0.1079 | 0.446611 | 0.8364 | NaN | 0.0656 | 0.0618 | 0.288566 | 0.7695 | 0.209 | 0.0934 | 0.025223 | 0.3282 | -0.0411 | 0.0825 | 0.618036 | 0.8637 | NaN | -0.0086 | 0.0466 | 0.852863 | 0.9461 | -0.0545 | 0.0744 | 0.464061 | 0.7154 | 0.0291 | 0.0587 | 0.62006 | 0.9994 | NaN | 0.0197 | 0.0372 | 0.59641 | 0.9708 | 0.0308 | 0.0611 | 0.614052 | 0.9977 | 0.0123 | 0.0462 | 0.790355 | 0.9967 | NaN | 0.0182 | 0.0461 | 0.693094 | 0.8981 | -0.0252 | 0.0736 | 0.731625 | 0.8666 | 0.0528 | 0.0585 | 0.367246 | 0.8297 |
| FA 21:5 | 316.2604 | 21.114538 | Lipid | Fatty Acid | 0.0537 | 0.0829 | 0.51682 | 0.8173 | -0.109 | 0.1307 | 0.404347 | 0.7124 | 0.1382 | 0.1079 | 0.200372 | 0.549 | NaN | 0.0689 | 0.0766 | 0.368421 | 0.7361 | -0.0111 | 0.1166 | 0.923834 | 0.9689 | 0.1269 | 0.1013 | 0.210357 | 0.6714 | NaN | -0.0552 | 0.0587 | 0.346857 | 0.793 | -0.0328 | 0.0919 | 0.721379 | 0.8816 | -0.0906 | 0.0797 | 0.255559 | 0.644 | NaN | -0.0463 | 0.0437 | 0.289606 | 0.5965 | -0.087 | 0.0698 | 0.212676 | 0.5139 | -0.0118 | 0.0566 | 0.834201 | 0.9994 | NaN | 0.0212 | 0.035 | 0.543493 | 0.9708 | 0.0207 | 0.0587 | 0.723718 | 0.9977 | 0.0192 | 0.0442 | 0.663158 | 0.9967 | NaN | -0.0162 | 0.0434 | 0.709062 | 0.9124 | -0.0688 | 0.0694 | 0.321817 | 0.6453 | 0.0255 | 0.0563 | 0.650564 | 0.95 |
| FA 22:5 | 330.2556 | 22.778202 | Lipid | Fatty Acid | 0.0497 | 0.0843 | 0.555761 | 0.8382 | 0.0956 | 0.1288 | 0.457723 | 0.7565 | 0.0396 | 0.1114 | 0.72217 | 0.9022 | NaN | 0.0437 | 0.078 | 0.574923 | 0.8719 | 0.128 | 0.1127 | 0.256219 | 0.6149 | 0.0174 | 0.1047 | 0.868088 | 0.9708 | NaN | 0.0292 | 0.0594 | 0.622805 | 0.9285 | 0.1313 | 0.0893 | 0.1412 | 0.5905 | -0.0543 | 0.0793 | 0.493489 | 0.8203 | NaN | -0.0698 | 0.0444 | 0.115926 | 0.4618 | -0.0781 | 0.0697 | 0.262409 | 0.5771 | -0.0563 | 0.0573 | 0.326438 | 0.9622 | NaN | -0.0009 | 0.0356 | 0.978927 | 0.9915 | 0.0133 | 0.0576 | 0.817827 | 0.9977 | -0.0098 | 0.0451 | 0.827127 | 0.9967 | NaN | -0.044 | 0.0441 | 0.318366 | 0.7708 | -0.0574 | 0.0691 | 0.406046 | 0.6982 | -0.0285 | 0.0575 | 0.619637 | 0.9449 |
| FA 24:5 | 358.2875 | 23.041843 | Lipid | Fatty Acid | 0.0808 | 0.0817 | 0.322742 | 0.6826 | 0.0503 | 0.1227 | 0.681975 | 0.8879 | 0.112 | 0.1098 | 0.30773 | 0.6892 | NaN | 0.0932 | 0.0755 | 0.216989 | 0.5867 | 0.1807 | 0.1087 | 0.096558 | 0.4459 | 0.081 | 0.1035 | 0.433914 | 0.8249 | NaN | 0.0464 | 0.0576 | 0.420675 | 0.8456 | 0.146 | 0.085 | 0.085799 | 0.549 | -0.0504 | 0.0796 | 0.526866 | 0.826 | NaN | -0.0403 | 0.0433 | 0.352182 | 0.6617 | -0.0892 | 0.0658 | 0.175515 | 0.457 | 0.0153 | 0.057 | 0.788245 | 0.9994 | NaN | -0.0092 | 0.0347 | 0.790714 | 0.9722 | -0.0393 | 0.0547 | 0.47223 | 0.9977 | 0.0125 | 0.0448 | 0.779656 | 0.9967 | NaN | -0.0202 | 0.0429 | 0.637259 | 0.8685 | -0.084 | 0.0653 | 0.198593 | 0.5437 | 0.042 | 0.0568 | 0.459592 | 0.8635 |
| FA 26:5 | 386.3387 | 22.630043 | Lipid | Fatty Acid | -0.1369 | 0.085 | 0.107254 | 0.3795 | -0.2259 | 0.1194 | 0.058527 | 0.2819 | -0.0187 | 0.1214 | 0.877656 | 0.9689 | NaN | -0.1564 | 0.0784 | 0.045993 | 0.3214 | -0.2178 | 0.1044 | 0.036954 | 0.395 | -0.0594 | 0.1142 | 0.603069 | 0.8877 | NaN | -0.0746 | 0.0601 | 0.214643 | 0.7098 | -0.0683 | 0.0862 | 0.428432 | 0.7964 | -0.0968 | 0.0858 | 0.259657 | 0.6468 | NaN | -0.0794 | 0.0447 | 0.075589 | 0.3995 | -0.112 | 0.0646 | 0.083123 | 0.313 | -0.0354 | 0.0623 | 0.570427 | 0.9885 | NaN | -0.0199 | 0.0362 | 0.583227 | 0.9708 | -0.0379 | 0.0548 | 0.489905 | 0.9977 | 0.0005 | 0.0491 | 0.99226 | 0.9967 | NaN | -0.0596 | 0.0445 | 0.181045 | 0.7516 | -0.1013 | 0.0644 | 0.115616 | 0.4593 | -0.01 | 0.0625 | 0.873183 | 0.993 |
| FA 28:5 | 414.3696 | 22.880224 | Lipid | Fatty Acid | -0.0713 | 0.0826 | 0.387536 | 0.7203 | -0.2467 | 0.123 | 0.044887 | 0.2535 | 0.0884 | 0.1101 | 0.422092 | 0.7447 | NaN | -0.0469 | 0.0765 | 0.540281 | 0.8388 | -0.0985 | 0.1138 | 0.386516 | 0.7136 | 0.0663 | 0.1035 | 0.521935 | 0.8742 | NaN | 0.031 | 0.0586 | 0.597224 | 0.9166 | 0.063 | 0.0932 | 0.498573 | 0.807 | 0.0093 | 0.0786 | 0.905618 | 0.9707 | NaN | -0.127 | 0.0426 | 0.002888 | 0.2657 | -0.2162 | 0.0636 | 0.000682 | 0.08 | -0.0527 | 0.0571 | 0.355625 | 0.9622 | NaN | -0.0472 | 0.0347 | 0.174241 | 0.9708 | -0.1062 | 0.0553 | 0.054766 | 0.6733 | -0.0004 | 0.0448 | 0.992442 | 0.9967 | NaN | -0.088 | 0.0427 | 0.039341 | 0.7271 | -0.1742 | 0.0645 | 0.006933 | 0.265 | -0.0173 | 0.0571 | 0.762646 | 0.9745 |
| FA 30:5 | 442.3994 | 22.915 | Lipid | Fatty Acid | -0.1437 | 0.0854 | 0.092517 | 0.3578 | -0.3483 | 0.1202 | 0.003768 | 0.104 | 0.0779 | 0.1198 | 0.515673 | 0.8041 | NaN | -0.1291 | 0.0791 | 0.102727 | 0.408 | -0.214 | 0.1115 | 0.055069 | 0.4173 | 0.0373 | 0.1131 | 0.741268 | 0.9385 | NaN | -0.05 | 0.0608 | 0.410552 | 0.8406 | -0.0506 | 0.0932 | 0.587234 | 0.8374 | -0.0577 | 0.0859 | 0.501276 | 0.8211 | NaN | -0.1337 | 0.0443 | 0.002512 | 0.2657 | -0.2129 | 0.0643 | 0.00092 | 0.08 | -0.0635 | 0.0619 | 0.305009 | 0.9622 | NaN | -0.0272 | 0.0364 | 0.455933 | 0.9708 | -0.0539 | 0.0577 | 0.349856 | 0.9977 | 0.0008 | 0.0486 | 0.986818 | 0.9967 | NaN | -0.0921 | 0.0445 | 0.038309 | 0.7271 | -0.1792 | 0.0651 | 0.005912 | 0.265 | -0.0138 | 0.062 | 0.823875 | 0.978 |
| FA 20:6 | 300.235 | 21.899794 | Lipid | Fatty Acid | -0.1189 | 0.0844 | 0.158716 | 0.4783 | -0.1636 | 0.1158 | 0.157778 | 0.4333 | -0.0369 | 0.1248 | 0.767624 | 0.9398 | NaN | -0.0787 | 0.0785 | 0.316117 | 0.6816 | -0.1187 | 0.1023 | 0.246128 | 0.6081 | 0.0109 | 0.1177 | 0.92615 | 0.9876 | NaN | -0.0415 | 0.0598 | 0.488138 | 0.8893 | 0.0196 | 0.0838 | 0.815162 | 0.9217 | -0.0911 | 0.0881 | 0.301503 | 0.6849 | NaN | -0.077 | 0.0443 | 0.082049 | 0.407 | -0.1299 | 0.0614 | 0.034233 | 0.2355 | -0.0307 | 0.0641 | 0.631875 | 0.9994 | NaN | -0.0609 | 0.0355 | 0.08641 | 0.9708 | -0.0756 | 0.0517 | 0.143745 | 0.8645 | -0.0398 | 0.0503 | 0.428637 | 0.9967 | NaN | -0.0635 | 0.0441 | 0.149699 | 0.7516 | -0.1301 | 0.0608 | 0.032393 | 0.2981 | 0.0028 | 0.0643 | 0.965345 | 0.996 |
| FA 22:6 | 328.2413 | 22.651737 | Lipid | Fatty Acid | -0.0261 | 0.0864 | 0.762646 | 0.9192 | -0.1401 | 0.1356 | 0.301489 | 0.6256 | 0.0568 | 0.1108 | 0.608026 | 0.8492 | NaN | 0.0103 | 0.0802 | 0.897965 | 0.9933 | -0.0045 | 0.1224 | 0.970448 | 0.9835 | 0.0619 | 0.1039 | 0.550989 | 0.8762 | NaN | -0.0257 | 0.0608 | 0.672635 | 0.9288 | 0.0599 | 0.0971 | 0.537344 | 0.8173 | -0.0848 | 0.0793 | 0.285386 | 0.6732 | NaN | -0.0718 | 0.0452 | 0.1122 | 0.4618 | -0.1695 | 0.0711 | 0.017077 | 0.2 | -0.0021 | 0.0571 | 0.970662 | 0.9994 | NaN | -0.0214 | 0.0364 | 0.556239 | 0.9708 | -0.0348 | 0.0608 | 0.5673 | 0.9977 | -0.0114 | 0.0449 | 0.800114 | 0.9967 | NaN | -0.0405 | 0.045 | 0.367712 | 0.7929 | -0.1418 | 0.071 | 0.04593 | 0.3209 | 0.0301 | 0.0571 | 0.597353 | 0.9367 |
| FA 28:6 | 412.356 | 22.890285 | Lipid | Fatty Acid | -0.085 | 0.0894 | 0.341553 | 0.6908 | -0.2276 | 0.1238 | 0.066024 | 0.2948 | 0.0917 | 0.1278 | 0.473208 | 0.7751 | NaN | -0.1074 | 0.0826 | 0.193274 | 0.548 | -0.2154 | 0.1084 | 0.046887 | 0.4173 | 0.0529 | 0.1205 | 0.66066 | 0.9005 | NaN | -0.0047 | 0.0633 | 0.940347 | 0.9968 | 0.0719 | 0.0929 | 0.439164 | 0.7964 | -0.058 | 0.0917 | 0.527367 | 0.826 | NaN | -0.0693 | 0.0468 | 0.13898 | 0.4828 | -0.1826 | 0.065 | 0.004959 | 0.161 | 0.038 | 0.0658 | 0.564009 | 0.9885 | NaN | -0.0398 | 0.0377 | 0.290416 | 0.9708 | -0.0994 | 0.0555 | 0.073346 | 0.6995 | 0.0267 | 0.0518 | 0.606294 | 0.9967 | NaN | -0.0862 | 0.0463 | 0.062894 | 0.7496 | -0.1834 | 0.0644 | 0.004391 | 0.2424 | 0.0067 | 0.0661 | 0.919426 | 0.996 |
| FA 29:6 | 426.3724 | 22.978584 | Lipid | Fatty Acid | -0.1062 | 0.0871 | 0.222549 | 0.5715 | -0.2346 | 0.1242 | 0.058966 | 0.2819 | 0.0441 | 0.1217 | 0.717186 | 0.9018 | NaN | -0.1274 | 0.0804 | 0.113143 | 0.422 | -0.191 | 0.1096 | 0.081475 | 0.441 | -0.0064 | 0.115 | 0.955694 | 0.9893 | NaN | -0.0234 | 0.0618 | 0.704714 | 0.9414 | 0.0085 | 0.0919 | 0.926287 | 0.9721 | -0.0446 | 0.0866 | 0.60648 | 0.8637 | NaN | -0.0992 | 0.0454 | 0.02909 | 0.3584 | -0.1442 | 0.0665 | 0.030103 | 0.2296 | -0.0624 | 0.0626 | 0.318767 | 0.9622 | NaN | -0.0151 | 0.037 | 0.682058 | 0.9708 | -0.0642 | 0.0566 | 0.256835 | 0.9821 | 0.035 | 0.0491 | 0.475971 | 0.9967 | NaN | -0.066 | 0.0454 | 0.146355 | 0.7516 | -0.1163 | 0.0667 | 0.081145 | 0.3895 | -0.0218 | 0.0628 | 0.728491 | 0.968 |
| FA 30:6 | 440.3876 | 23.740631 | Lipid | Fatty Acid | -0.0266 | 0.086 | 0.75666 | 0.9192 | -0.2581 | 0.123 | 0.035863 | 0.2428 | 0.2374 | 0.1189 | 0.045822 | 0.3531 | NaN | -0.0459 | 0.0795 | 0.563613 | 0.8617 | -0.1964 | 0.1092 | 0.072161 | 0.4408 | 0.182 | 0.1132 | 0.107979 | 0.577 | NaN | 0.0012 | 0.0605 | 0.984604 | 0.9992 | -0.0585 | 0.0901 | 0.515999 | 0.8105 | 0.0581 | 0.0874 | 0.505997 | 0.8218 | NaN | -0.0661 | 0.045 | 0.141702 | 0.4833 | -0.1365 | 0.0665 | 0.040037 | 0.2511 | -0.0029 | 0.0638 | 0.963185 | 0.9994 | NaN | -0.0223 | 0.0362 | 0.538236 | 0.9708 | -0.0339 | 0.0571 | 0.552526 | 0.9977 | -0.0035 | 0.05 | 0.943933 | 0.9967 | NaN | -0.0479 | 0.0448 | 0.284999 | 0.7695 | -0.1027 | 0.0669 | 0.124517 | 0.4644 | 0.0026 | 0.0639 | 0.967545 | 0.996 |
| AC 2:0 | 203.116 | 0.914417 | Lipid | Fatty Acid Metabolism (also BCAA Metabolism) | -0.0412 | 0.0876 | 0.638236 | 0.8782 | 0.1133 | 0.1296 | 0.381875 | 0.698 | -0.1539 | 0.1201 | 0.199881 | 0.549 | NaN | 0.0599 | 0.0827 | 0.469089 | 0.7817 | 0.2408 | 0.1138 | 0.034249 | 0.3858 | -0.0677 | 0.1157 | 0.558748 | 0.8762 | NaN | 0.0079 | 0.0617 | 0.8985 | 0.99 | 0.1018 | 0.0903 | 0.259623 | 0.7102 | -0.1036 | 0.0852 | 0.224426 | 0.6205 | NaN | -0.0741 | 0.0458 | 0.105408 | 0.4581 | -0.0822 | 0.0704 | 0.243244 | 0.5571 | -0.0444 | 0.0624 | 0.476184 | 0.9735 | NaN | -0.0254 | 0.0369 | 0.490587 | 0.9708 | 0.0051 | 0.0581 | 0.930266 | 0.9977 | -0.0574 | 0.0487 | 0.238769 | 0.9967 | NaN | -0.0624 | 0.0455 | 0.170153 | 0.7516 | -0.0631 | 0.0698 | 0.366143 | 0.6653 | -0.0477 | 0.0624 | 0.444744 | 0.8627 |
| AC 6:0 | 259.1784 | 7.03923 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1325 | 0.0904 | 0.142474 | 0.4418 | 0.2865 | 0.1304 | 0.028003 | 0.2307 | -0.0059 | 0.1236 | 0.962179 | 0.9916 | NaN | 0.233 | 0.0839 | 0.005504 | 0.0887 | 0.4084 | 0.1116 | 0.000252 | 0.0464 | 0.0842 | 0.1179 | 0.475218 | 0.8435 | NaN | 0.0259 | 0.0643 | 0.687472 | 0.9341 | 0.1632 | 0.0927 | 0.07848 | 0.549 | -0.1076 | 0.0875 | 0.218509 | 0.6205 | NaN | -0.0165 | 0.0482 | 0.731556 | 0.8817 | -0.0086 | 0.0743 | 0.907569 | 0.9488 | -0.0107 | 0.0635 | 0.8665 | 0.9994 | NaN | 0.0229 | 0.0384 | 0.551369 | 0.9708 | 0.0831 | 0.0598 | 0.164451 | 0.89 | -0.0312 | 0.0498 | 0.531147 | 0.9967 | NaN | -0.0125 | 0.0478 | 0.794369 | 0.9482 | -0.02 | 0.0739 | 0.787131 | 0.9029 | 0.0009 | 0.0636 | 0.98855 | 0.996 |
| AC 8:0 | 287.21 | 11.700219 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0328 | 0.0896 | 0.714609 | 0.9027 | 0.0088 | 0.1452 | 0.951416 | 0.974 | -0.0621 | 0.1133 | 0.583524 | 0.8382 | NaN | 0.0649 | 0.0844 | 0.442137 | 0.7757 | 0.1946 | 0.1303 | 0.135104 | 0.4744 | 0.0065 | 0.1079 | 0.951719 | 0.9893 | NaN | -0.0701 | 0.0629 | 0.265514 | 0.7604 | -0.0152 | 0.1015 | 0.880965 | 0.9516 | -0.1153 | 0.0798 | 0.148142 | 0.5464 | NaN | -0.0348 | 0.0471 | 0.459712 | 0.7398 | -0.0422 | 0.0778 | 0.587493 | 0.7765 | -0.0211 | 0.0583 | 0.717621 | 0.9994 | NaN | -0.003 | 0.0378 | 0.937583 | 0.9783 | 0.013 | 0.0646 | 0.840252 | 0.9977 | -0.0154 | 0.0459 | 0.737572 | 0.9967 | NaN | -0.0347 | 0.0467 | 0.4575 | 0.8226 | -0.059 | 0.0771 | 0.444277 | 0.7321 | -0.0142 | 0.0585 | 0.807855 | 0.9748 |
| AC 10:0 | 315.2413 | 15.299243 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.101 | 0.0902 | 0.262717 | 0.6259 | -0.0768 | 0.1429 | 0.590687 | 0.836 | -0.1165 | 0.1153 | 0.311999 | 0.6896 | NaN | 0.0112 | 0.0859 | 0.895884 | 0.9933 | 0.1342 | 0.1308 | 0.304894 | 0.6814 | -0.0356 | 0.1107 | 0.74752 | 0.9421 | NaN | -0.1144 | 0.0631 | 0.069978 | 0.4654 | -0.0893 | 0.0995 | 0.369555 | 0.7724 | -0.1384 | 0.081 | 0.087398 | 0.4613 | NaN | -0.0358 | 0.0476 | 0.451442 | 0.7308 | -0.0379 | 0.0767 | 0.621374 | 0.8019 | -0.0277 | 0.0597 | 0.643154 | 0.9994 | NaN | -0.0106 | 0.0382 | 0.781054 | 0.9722 | 0.0027 | 0.0638 | 0.966092 | 0.9977 | -0.0209 | 0.0469 | 0.655398 | 0.9967 | NaN | -0.0368 | 0.0472 | 0.435769 | 0.8178 | -0.0494 | 0.076 | 0.515311 | 0.7783 | -0.0243 | 0.0598 | 0.684389 | 0.9564 |
| AC 11:0 | 329.2544 | 16.329609 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1429 | 0.0949 | 0.132106 | 0.4315 | 0.0219 | 0.1481 | 0.882419 | 0.9558 | 0.2301 | 0.1222 | 0.059716 | 0.3614 | NaN | 0.1604 | 0.0875 | 0.066875 | 0.3516 | 0.1137 | 0.1306 | 0.384029 | 0.7136 | 0.23 | 0.1143 | 0.044288 | 0.4527 | NaN | 0.0108 | 0.0677 | 0.873051 | 0.9815 | -0.0471 | 0.1036 | 0.649262 | 0.8476 | 0.0655 | 0.0892 | 0.462627 | 0.7968 | NaN | 0.066 | 0.0501 | 0.187346 | 0.5115 | 0.0497 | 0.0793 | 0.530889 | 0.7612 | 0.0657 | 0.0642 | 0.306591 | 0.9622 | NaN | 0.0632 | 0.0401 | 0.114456 | 0.9708 | 0.0461 | 0.0657 | 0.482937 | 0.9977 | 0.0809 | 0.05 | 0.105622 | 0.9967 | NaN | 0.0939 | 0.0494 | 0.057168 | 0.7339 | 0.0709 | 0.0785 | 0.366517 | 0.6653 | 0.104 | 0.0636 | 0.101935 | 0.7232 |
| AC 12:0 | 343.2717 | 17.918053 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0412 | 0.0865 | 0.633912 | 0.8777 | 0.0342 | 0.1275 | 0.788693 | 0.9222 | -0.0902 | 0.1168 | 0.439979 | 0.7481 | NaN | 0.0505 | 0.0814 | 0.535404 | 0.8366 | 0.2184 | 0.1144 | 0.056265 | 0.4173 | -0.0289 | 0.111 | 0.794557 | 0.9535 | NaN | -0.0852 | 0.0606 | 0.160255 | 0.6546 | -0.043 | 0.0893 | 0.629787 | 0.8438 | -0.1334 | 0.082 | 0.104018 | 0.4845 | NaN | -0.033 | 0.0454 | 0.466955 | 0.7407 | -0.0297 | 0.0684 | 0.664702 | 0.8415 | -0.0258 | 0.0602 | 0.668564 | 0.9994 | NaN | 0.01 | 0.0365 | 0.783783 | 0.9722 | 0.0291 | 0.0567 | 0.60804 | 0.9977 | -0.0065 | 0.0474 | 0.891592 | 0.9967 | NaN | -0.0208 | 0.0451 | 0.644542 | 0.8687 | -0.024 | 0.0679 | 0.723873 | 0.8612 | -0.0115 | 0.0604 | 0.849539 | 0.9809 |
| AC 14:0 | 371.3022 | 19.886253 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0142 | 0.0851 | 0.8674 | 0.9457 | 0.0377 | 0.1239 | 0.761105 | 0.9222 | -0.0038 | 0.1175 | 0.97391 | 0.994 | NaN | 0.0891 | 0.0794 | 0.261943 | 0.6287 | 0.1708 | 0.11 | 0.120601 | 0.4674 | 0.0479 | 0.1109 | 0.66571 | 0.9007 | NaN | -0.0522 | 0.0599 | 0.383934 | 0.8287 | -0.0014 | 0.0867 | 0.986688 | 0.9998 | -0.1238 | 0.0832 | 0.136486 | 0.5306 | NaN | -0.049 | 0.0447 | 0.273162 | 0.5828 | -0.0729 | 0.0664 | 0.272223 | 0.5824 | -0.0095 | 0.0604 | 0.875331 | 0.9994 | NaN | 0.0298 | 0.0358 | 0.404488 | 0.9708 | 0.0583 | 0.0548 | 0.287589 | 0.9834 | 0.0024 | 0.0475 | 0.959396 | 0.9967 | NaN | -0.014 | 0.0444 | 0.752463 | 0.9221 | -0.0441 | 0.066 | 0.503688 | 0.7764 | 0.0258 | 0.0605 | 0.669909 | 0.9564 |
| AC 16:0 | 399.335 | 21.273067 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1028 | 0.0878 | 0.2416 | 0.5927 | 0.0404 | 0.1311 | 0.757836 | 0.9222 | 0.16 | 0.1184 | 0.176596 | 0.5263 | NaN | 0.1338 | 0.0811 | 0.098997 | 0.4077 | 0.1708 | 0.1162 | 0.141747 | 0.489 | 0.1521 | 0.1111 | 0.170721 | 0.6598 | NaN | 0.0629 | 0.0619 | 0.309412 | 0.782 | 0.0944 | 0.0913 | 0.300964 | 0.7517 | 0.0189 | 0.0857 | 0.825613 | 0.9495 | NaN | -0.0286 | 0.0466 | 0.539344 | 0.7918 | -0.074 | 0.0703 | 0.292499 | 0.6018 | 0.0275 | 0.0618 | 0.656771 | 0.9994 | NaN | 0.0375 | 0.0371 | 0.312215 | 0.9708 | 0.0473 | 0.0582 | 0.416533 | 0.9977 | 0.0292 | 0.0485 | 0.546807 | 0.9967 | NaN | 0.0157 | 0.0461 | 0.733819 | 0.918 | -0.0339 | 0.0699 | 0.627335 | 0.8191 | 0.0706 | 0.0613 | 0.249404 | 0.7523 |
| AC 18:0 | 427.3648 | 21.812096 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0574 | 0.0735 | 0.43477 | 0.7643 | -0.1133 | 0.0991 | 0.252881 | 0.5561 | 0.0077 | 0.1084 | 0.943515 | 0.9916 | NaN | -0.0364 | 0.0681 | 0.59261 | 0.8776 | -0.0549 | 0.0881 | 0.533603 | 0.7797 | 0.008 | 0.1017 | 0.937592 | 0.9876 | NaN | -0.034 | 0.0517 | 0.510717 | 0.8921 | -0.0107 | 0.0705 | 0.878952 | 0.9513 | -0.0744 | 0.0768 | 0.333098 | 0.7072 | NaN | -0.0495 | 0.0385 | 0.198625 | 0.5115 | -0.0684 | 0.0531 | 0.198024 | 0.4969 | -0.0151 | 0.0557 | 0.785697 | 0.9994 | NaN | -0.0262 | 0.031 | 0.398412 | 0.9708 | 0.0016 | 0.0448 | 0.970735 | 0.9977 | -0.0595 | 0.0435 | 0.171066 | 0.9967 | NaN | -0.0237 | 0.0384 | 0.536025 | 0.8373 | -0.0623 | 0.0528 | 0.238249 | 0.5743 | 0.0301 | 0.0557 | 0.588829 | 0.9367 |
| AC 5:1 | 243.1468 | 4.074276 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1184 | 0.0886 | 0.181678 | 0.5143 | 0.2789 | 0.1339 | 0.037218 | 0.2428 | 0.0218 | 0.1168 | 0.852037 | 0.9565 | NaN | 0.056 | 0.0829 | 0.499212 | 0.7987 | 0.2067 | 0.1191 | 0.082722 | 0.4425 | -0.0381 | 0.1106 | 0.730488 | 0.9342 | NaN | 0.0482 | 0.0627 | 0.44251 | 0.8554 | 0.1507 | 0.0953 | 0.113846 | 0.577 | -0.0201 | 0.0828 | 0.808199 | 0.9477 | NaN | 0.06 | 0.0467 | 0.198424 | 0.5115 | 0.107 | 0.0735 | 0.145349 | 0.4179 | 0.0243 | 0.06 | 0.685021 | 0.9994 | NaN | 0.0857 | 0.0371 | 0.020685 | 0.8627 | 0.0915 | 0.061 | 0.13328 | 0.8645 | 0.0858 | 0.0465 | 0.065057 | 0.9967 | NaN | 0.0614 | 0.0463 | 0.184638 | 0.7516 | 0.0473 | 0.0742 | 0.524257 | 0.7821 | 0.071 | 0.0598 | 0.234859 | 0.7365 |
| AC 7:1 | 271.1774 | 7.654182 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1778 | 0.0885 | 0.044665 | 0.2417 | 0.1701 | 0.1439 | 0.236964 | 0.5379 | 0.1814 | 0.1112 | 0.102783 | 0.4331 | NaN | 0.166 | 0.0819 | 0.042589 | 0.311 | 0.0874 | 0.1278 | 0.494301 | 0.7769 | 0.1885 | 0.104 | 0.070047 | 0.5067 | NaN | 0.1 | 0.0627 | 0.110841 | 0.5674 | 0.1309 | 0.1004 | 0.192222 | 0.652 | 0.0801 | 0.08 | 0.316902 | 0.6914 | NaN | -0.0708 | 0.048 | 0.13993 | 0.4828 | -0.1857 | 0.0788 | 0.01846 | 0.2038 | -0.0057 | 0.0589 | 0.922909 | 0.9994 | NaN | -0.0173 | 0.0382 | 0.651678 | 0.9708 | -0.0344 | 0.0652 | 0.59827 | 0.9977 | -0.0064 | 0.0462 | 0.889479 | 0.9967 | NaN | -0.0809 | 0.0476 | 0.089322 | 0.7516 | -0.1952 | 0.078 | 0.012372 | 0.265 | -0.0156 | 0.0591 | 0.791779 | 0.9748 |
| AC 10:1 | 313.2253 | 13.943843 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0371 | 0.0891 | 0.67716 | 0.8795 | -0.0117 | 0.1346 | 0.930549 | 0.9682 | -0.0668 | 0.1185 | 0.57314 | 0.8352 | NaN | 0.0605 | 0.0839 | 0.471291 | 0.7817 | 0.1551 | 0.1209 | 0.199661 | 0.5489 | 0.0066 | 0.113 | 0.953243 | 0.9893 | NaN | -0.078 | 0.0625 | 0.2118 | 0.7091 | -0.0207 | 0.094 | 0.825959 | 0.9229 | -0.1391 | 0.0833 | 0.094921 | 0.4637 | NaN | -0.0294 | 0.0468 | 0.529821 | 0.7799 | -0.0527 | 0.072 | 0.464657 | 0.7154 | 0.0008 | 0.0611 | 0.98951 | 0.9994 | NaN | -0.005 | 0.0376 | 0.895029 | 0.9722 | 0.0023 | 0.0599 | 0.968866 | 0.9977 | -0.0147 | 0.048 | 0.759393 | 0.9967 | NaN | -0.023 | 0.0465 | 0.620938 | 0.8641 | -0.0676 | 0.0713 | 0.343332 | 0.6499 | 0.0193 | 0.0613 | 0.752844 | 0.9732 |
| AC 11:1 | 327.24 | 15.28524 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0635 | 0.0875 | 0.468392 | 0.7858 | 0.1238 | 0.1235 | 0.316135 | 0.6383 | 0.0122 | 0.1228 | 0.920825 | 0.987 | NaN | 0.1189 | 0.0812 | 0.142944 | 0.4641 | 0.2858 | 0.1086 | 0.008492 | 0.2398 | 0.0359 | 0.1153 | 0.755852 | 0.9436 | NaN | -0.0226 | 0.0619 | 0.715028 | 0.9414 | 0.0328 | 0.0871 | 0.706426 | 0.8816 | -0.069 | 0.0871 | 0.428346 | 0.7865 | NaN | 0.0452 | 0.046 | 0.325231 | 0.6369 | 0.0895 | 0.066 | 0.17505 | 0.457 | -0.0058 | 0.0631 | 0.926236 | 0.9994 | NaN | 0.0077 | 0.037 | 0.834437 | 0.9722 | 0.047 | 0.0552 | 0.394265 | 0.9977 | -0.0281 | 0.0496 | 0.571294 | 0.9967 | NaN | 0.0393 | 0.0457 | 0.38972 | 0.8116 | 0.0899 | 0.0654 | 0.169333 | 0.5381 | -0.0153 | 0.0632 | 0.809223 | 0.9748 |
| AC 12:1 | 341.2561 | 16.741268 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0326 | 0.0889 | 0.71364 | 0.9027 | 0.0767 | 0.1335 | 0.565311 | 0.8174 | 0.0006 | 0.1182 | 0.996217 | 0.997 | NaN | 0.1588 | 0.0841 | 0.058821 | 0.3472 | 0.2804 | 0.1191 | 0.018595 | 0.3208 | 0.1007 | 0.1133 | 0.374273 | 0.7878 | NaN | -0.0042 | 0.0626 | 0.946503 | 0.997 | 0.0427 | 0.0934 | 0.647219 | 0.8476 | -0.0499 | 0.0837 | 0.551204 | 0.8359 | NaN | -0.0353 | 0.0468 | 0.45102 | 0.7308 | -0.062 | 0.072 | 0.388863 | 0.6687 | -0.0074 | 0.0608 | 0.903186 | 0.9994 | NaN | 0.0004 | 0.0375 | 0.99234 | 0.9959 | 0.0281 | 0.0595 | 0.636977 | 0.9977 | -0.0223 | 0.0477 | 0.640293 | 0.9967 | NaN | -0.0311 | 0.0465 | 0.503437 | 0.8283 | -0.0451 | 0.0714 | 0.527883 | 0.7854 | -0.0154 | 0.0609 | 0.799586 | 0.9748 |
| AC 13:1 | 355.2707 | 17.844881 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.002 | 0.0914 | 0.98225 | 0.993 | -0.0583 | 0.1334 | 0.661865 | 0.8782 | 0.0549 | 0.1246 | 0.659357 | 0.8853 | NaN | 0.0616 | 0.0851 | 0.469192 | 0.7817 | 0.0945 | 0.1202 | 0.431607 | 0.7515 | 0.0849 | 0.117 | 0.46808 | 0.8416 | NaN | -0.0272 | 0.0643 | 0.672242 | 0.9288 | -0.0352 | 0.0932 | 0.705729 | 0.8816 | -0.034 | 0.0887 | 0.701715 | 0.9093 | NaN | 0.0535 | 0.048 | 0.264444 | 0.5828 | 0.0326 | 0.0718 | 0.649205 | 0.8257 | 0.0854 | 0.0636 | 0.17946 | 0.9514 | NaN | 0.0071 | 0.0385 | 0.852886 | 0.9722 | 0.016 | 0.0595 | 0.787628 | 0.9977 | -0.0002 | 0.0504 | 0.996702 | 0.9967 | NaN | 0.0508 | 0.0476 | 0.28623 | 0.7695 | 0.0166 | 0.0711 | 0.815187 | 0.9093 | 0.09 | 0.0637 | 0.157627 | 0.7294 |
| AC 14:1 | 369.2874 | 18.959509 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0714 | 0.0875 | 0.414546 | 0.7454 | 0.0167 | 0.1343 | 0.900913 | 0.9573 | -0.1273 | 0.1142 | 0.265264 | 0.6394 | NaN | 0.0454 | 0.0834 | 0.58568 | 0.8776 | 0.2356 | 0.1216 | 0.05273 | 0.4173 | -0.0437 | 0.11 | 0.6914 | 0.9182 | NaN | -0.0878 | 0.0613 | 0.152224 | 0.6546 | -0.0201 | 0.0938 | 0.830375 | 0.9239 | -0.1489 | 0.0801 | 0.063081 | 0.4338 | NaN | -0.0585 | 0.0459 | 0.201959 | 0.5137 | -0.0758 | 0.0718 | 0.291624 | 0.6018 | -0.0364 | 0.0592 | 0.538353 | 0.9885 | NaN | -0.0135 | 0.037 | 0.715953 | 0.971 | 0.0336 | 0.0596 | 0.573177 | 0.9977 | -0.0491 | 0.0463 | 0.288419 | 0.9967 | NaN | -0.0413 | 0.0456 | 0.365049 | 0.7902 | -0.0353 | 0.0714 | 0.621426 | 0.8191 | -0.0395 | 0.0592 | 0.50501 | 0.8935 |
| AC 18:1 | 425.35 | 21.472305 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0649 | 0.0854 | 0.447216 | 0.7691 | 0.0179 | 0.1269 | 0.887685 | 0.9558 | 0.1072 | 0.1148 | 0.350343 | 0.7082 | NaN | 0.136 | 0.0794 | 0.086618 | 0.3825 | 0.1703 | 0.1134 | 0.133163 | 0.4744 | 0.1486 | 0.1077 | 0.167367 | 0.6552 | NaN | 0.0029 | 0.0603 | 0.961933 | 0.9971 | 0.0557 | 0.0886 | 0.529689 | 0.8173 | -0.0552 | 0.083 | 0.506057 | 0.8218 | NaN | -0.0474 | 0.0451 | 0.293377 | 0.6009 | -0.0836 | 0.0678 | 0.217828 | 0.5228 | -0.006 | 0.0596 | 0.92008 | 0.9994 | NaN | 0.0272 | 0.036 | 0.450282 | 0.9708 | 0.0624 | 0.0562 | 0.26614 | 0.9821 | -0.0015 | 0.0468 | 0.973922 | 0.9967 | NaN | 0.0094 | 0.0447 | 0.834186 | 0.9535 | -0.027 | 0.0675 | 0.689567 | 0.8461 | 0.048 | 0.0592 | 0.41786 | 0.8487 |
| AC 8:2 | 283.1773 | 7.484311 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1325 | 0.0885 | 0.134362 | 0.4363 | 0.12 | 0.134 | 0.370452 | 0.6978 | 0.1429 | 0.1178 | 0.224978 | 0.5914 | NaN | 0.1654 | 0.0816 | 0.042823 | 0.311 | 0.1057 | 0.1176 | 0.368683 | 0.7116 | 0.1878 | 0.1103 | 0.088604 | 0.5595 | NaN | 0.0343 | 0.0629 | 0.585655 | 0.9166 | 0.1252 | 0.0931 | 0.178728 | 0.652 | -0.0556 | 0.086 | 0.517802 | 0.826 | NaN | 0.0211 | 0.047 | 0.653984 | 0.846 | -0.0668 | 0.0729 | 0.3595 | 0.659 | 0.1029 | 0.0602 | 0.087352 | 0.8712 | NaN | -0.0041 | 0.0378 | 0.912901 | 0.9722 | -0.01 | 0.0602 | 0.867576 | 0.9977 | -0.0021 | 0.0483 | 0.965587 | 0.9967 | NaN | 0.0068 | 0.0467 | 0.883765 | 0.9712 | -0.0884 | 0.0722 | 0.220958 | 0.5569 | 0.0885 | 0.0605 | 0.143801 | 0.7232 |
| AC 10:2 | 311.2083 | 12.303444 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0603 | 0.089 | 0.49797 | 0.8017 | 0.0237 | 0.1392 | 0.864858 | 0.9547 | -0.1292 | 0.1146 | 0.259622 | 0.6326 | NaN | 0.038 | 0.084 | 0.651066 | 0.9303 | 0.189 | 0.1243 | 0.128312 | 0.4744 | -0.0541 | 0.1099 | 0.622797 | 0.8939 | NaN | -0.0503 | 0.0626 | 0.421261 | 0.8456 | 0.0325 | 0.0972 | 0.73792 | 0.8816 | -0.1153 | 0.0809 | 0.154047 | 0.5522 | NaN | -0.0684 | 0.0466 | 0.141832 | 0.4833 | -0.1117 | 0.0743 | 0.132797 | 0.4016 | -0.0336 | 0.0594 | 0.572439 | 0.9885 | NaN | -0.0165 | 0.0376 | 0.661286 | 0.9708 | 0.0257 | 0.0619 | 0.678284 | 0.9977 | -0.0492 | 0.0465 | 0.289924 | 0.9967 | NaN | -0.0671 | 0.0462 | 0.146513 | 0.7516 | -0.0955 | 0.0738 | 0.195511 | 0.5437 | -0.0452 | 0.0594 | 0.446987 | 0.8627 |
| AC 12:2 | 339.2397 | 15.794398 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1178 | 0.0844 | 0.16276 | 0.4783 | -0.0845 | 0.1294 | 0.513779 | 0.8001 | -0.14 | 0.1102 | 0.203769 | 0.5514 | NaN | 0.0268 | 0.0824 | 0.74487 | 0.964 | 0.0442 | 0.1163 | 0.703747 | 0.8798 | 0.0061 | 0.1117 | 0.956576 | 0.9893 | NaN | -0.0981 | 0.0593 | 0.097735 | 0.5647 | -0.1036 | 0.09 | 0.249777 | 0.6999 | -0.0993 | 0.0781 | 0.203925 | 0.6167 | NaN | 0.0171 | 0.0449 | 0.702834 | 0.8602 | -0.0176 | 0.0696 | 0.800108 | 0.8869 | 0.0491 | 0.0579 | 0.39691 | 0.9735 | NaN | -0.0152 | 0.0359 | 0.672168 | 0.9708 | 0.0298 | 0.0579 | 0.607264 | 0.9977 | -0.0484 | 0.0448 | 0.280007 | 0.9967 | NaN | 0.0016 | 0.0445 | 0.971511 | 0.9949 | -0.0383 | 0.0689 | 0.578814 | 0.8075 | 0.0345 | 0.0579 | 0.552072 | 0.9179 |
| AC 14:2 | 367.2715 | 17.837961 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0399 | 0.0832 | 0.631655 | 0.8777 | 0.037 | 0.121 | 0.759414 | 0.9222 | -0.1009 | 0.1134 | 0.373511 | 0.7082 | NaN | 0.0759 | 0.0792 | 0.338045 | 0.7042 | 0.1945 | 0.108 | 0.071818 | 0.4408 | -0.0002 | 0.1101 | 0.998904 | 0.9993 | NaN | -0.0651 | 0.0584 | 0.26447 | 0.7604 | -0.0418 | 0.0848 | 0.62188 | 0.8438 | -0.0994 | 0.08 | 0.214089 | 0.6205 | NaN | -0.0571 | 0.0436 | 0.190055 | 0.5115 | -0.0528 | 0.0649 | 0.4162 | 0.6838 | -0.051 | 0.0584 | 0.381812 | 0.9735 | NaN | -0.0141 | 0.0351 | 0.686761 | 0.9708 | 0.0205 | 0.0538 | 0.703482 | 0.9977 | -0.0463 | 0.0458 | 0.312193 | 0.9967 | NaN | -0.0369 | 0.0433 | 0.394855 | 0.8117 | -0.0253 | 0.0644 | 0.694626 | 0.8461 | -0.0405 | 0.0585 | 0.489066 | 0.8765 |
| AC 18:2 | 423.3342 | 20.982098 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1058 | 0.087 | 0.223813 | 0.572 | 0.0322 | 0.1323 | 0.807495 | 0.9283 | 0.155 | 0.1158 | 0.180826 | 0.5263 | NaN | 0.1459 | 0.0804 | 0.069423 | 0.3516 | 0.081 | 0.1162 | 0.486024 | 0.7754 | 0.1882 | 0.1083 | 0.082321 | 0.5555 | NaN | 0.0286 | 0.0616 | 0.643051 | 0.9288 | 0.0552 | 0.0923 | 0.550041 | 0.8202 | -0.0102 | 0.0843 | 0.90376 | 0.9707 | NaN | -0.0134 | 0.0462 | 0.772343 | 0.8919 | -0.0667 | 0.0709 | 0.346806 | 0.6506 | 0.0433 | 0.0602 | 0.472436 | 0.9735 | NaN | 0.0476 | 0.0367 | 0.194721 | 0.9708 | 0.0665 | 0.0585 | 0.256114 | 0.9821 | 0.0319 | 0.0474 | 0.500569 | 0.9967 | NaN | 0.0481 | 0.0455 | 0.290582 | 0.7695 | -0.028 | 0.0704 | 0.691036 | 0.8461 | 0.119 | 0.059 | 0.04385 | 0.6979 |
| AC 10:3 | 309.194 | 11.500111 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.096 | 0.0883 | 0.277129 | 0.6386 | 0.1986 | 0.1383 | 0.150936 | 0.4295 | 0.0459 | 0.1146 | 0.688342 | 0.8959 | NaN | 0.0996 | 0.0816 | 0.222234 | 0.5873 | 0.2437 | 0.1204 | 0.042902 | 0.4171 | 0.0323 | 0.1075 | 0.763934 | 0.9436 | NaN | 0.0747 | 0.0621 | 0.228894 | 0.7309 | 0.1541 | 0.0964 | 0.110051 | 0.577 | 0.0076 | 0.0813 | 0.925398 | 0.9766 | NaN | -0.0553 | 0.0469 | 0.237961 | 0.5457 | -0.0535 | 0.0765 | 0.484995 | 0.7322 | -0.0437 | 0.059 | 0.459272 | 0.9735 | NaN | -0.0085 | 0.0375 | 0.820658 | 0.9722 | 0.0256 | 0.0628 | 0.683704 | 0.9977 | -0.0316 | 0.0463 | 0.49503 | 0.9967 | NaN | -0.0566 | 0.0465 | 0.223978 | 0.7516 | -0.0497 | 0.0759 | 0.512468 | 0.7783 | -0.0524 | 0.0591 | 0.374658 | 0.8297 |
| AC 11:3 | 323.2119 | 20.819927 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1168 | 0.0796 | 0.142189 | 0.4418 | -0.1905 | 0.1183 | 0.107314 | 0.3717 | -0.0471 | 0.1065 | 0.658151 | 0.8853 | NaN | -0.0612 | 0.0745 | 0.411571 | 0.7542 | 0.0426 | 0.1148 | 0.710397 | 0.8811 | -0.0477 | 0.0999 | 0.633256 | 0.8939 | NaN | -0.1279 | 0.0556 | 0.021409 | 0.2569 | -0.1056 | 0.0835 | 0.206003 | 0.6538 | -0.1491 | 0.0748 | 0.046157 | 0.3772 | NaN | 0.0295 | 0.0425 | 0.48698 | 0.7545 | -0.006 | 0.0654 | 0.927187 | 0.9554 | 0.0604 | 0.0549 | 0.27066 | 0.9622 | NaN | -0.0455 | 0.0337 | 0.176239 | 0.9708 | -0.0628 | 0.0534 | 0.239274 | 0.9821 | -0.0304 | 0.043 | 0.479724 | 0.9967 | NaN | 0.0582 | 0.0422 | 0.168448 | 0.7516 | 0.0389 | 0.0654 | 0.552004 | 0.7972 | 0.0755 | 0.0549 | 0.168868 | 0.7294 |
| AC 17:3 | 407.3014 | 22.77926 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0057 | 0.0829 | 0.945066 | 0.9733 | -0.0694 | 0.1169 | 0.552849 | 0.8095 | 0.0648 | 0.119 | 0.586116 | 0.8382 | NaN | 0.0025 | 0.0767 | 0.974143 | 0.9933 | -0.081 | 0.1024 | 0.428919 | 0.7515 | 0.0732 | 0.1116 | 0.51174 | 0.8742 | NaN | -0.0662 | 0.0583 | 0.255927 | 0.7568 | -0.1752 | 0.0805 | 0.029481 | 0.3462 | 0.0073 | 0.0846 | 0.931493 | 0.9766 | NaN | 0.052 | 0.0435 | 0.232381 | 0.5455 | 0.1437 | 0.0626 | 0.021653 | 0.2134 | -0.0073 | 0.0614 | 0.905757 | 0.9994 | NaN | 0.0377 | 0.0349 | 0.279985 | 0.9708 | 0.0386 | 0.0522 | 0.460221 | 0.9977 | 0.0368 | 0.048 | 0.444297 | 0.9967 | NaN | 0.0477 | 0.0432 | 0.269413 | 0.7666 | 0.1493 | 0.062 | 0.015928 | 0.2658 | -0.029 | 0.0615 | 0.637042 | 0.9483 |
| AC 19:3 | 435.335 | 23.046375 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0291 | 0.0858 | 0.734055 | 0.916 | 0.0009 | 0.1167 | 0.993755 | 0.9938 | 0.0811 | 0.1253 | 0.517554 | 0.8048 | NaN | 0.0659 | 0.0794 | 0.406676 | 0.7538 | 0.0741 | 0.103 | 0.472158 | 0.7643 | 0.1045 | 0.1174 | 0.373413 | 0.7878 | NaN | -0.0099 | 0.0604 | 0.870395 | 0.9805 | -0.0307 | 0.0815 | 0.706042 | 0.8816 | 0.0136 | 0.0891 | 0.878612 | 0.9674 | NaN | -0.0799 | 0.045 | 0.075995 | 0.3995 | -0.0995 | 0.0621 | 0.10895 | 0.3712 | -0.0581 | 0.0648 | 0.369455 | 0.9622 | NaN | 0.0001 | 0.0362 | 0.998039 | 0.9997 | -0.0157 | 0.0519 | 0.762296 | 0.9977 | 0.0214 | 0.0507 | 0.673413 | 0.9967 | NaN | -0.0555 | 0.0447 | 0.214657 | 0.7516 | -0.0615 | 0.0619 | 0.32041 | 0.6453 | -0.0485 | 0.0649 | 0.45436 | 0.8635 |
| 3-dehydroxycarnitine | 145.1097 | 0.670247 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0109 | 0.0859 | 0.899285 | 0.9586 | 0.0418 | 0.1369 | 0.760215 | 0.9222 | 0.0323 | 0.1129 | 0.774613 | 0.9398 | NaN | 0.0239 | 0.0795 | 0.763889 | 0.9671 | 0.1592 | 0.121 | 0.18837 | 0.5388 | 0.0175 | 0.106 | 0.869256 | 0.9708 | NaN | 0.0106 | 0.0604 | 0.860644 | 0.9805 | -0.0117 | 0.0958 | 0.902586 | 0.9637 | 0.0347 | 0.08 | 0.663889 | 0.8899 | NaN | 0.0848 | 0.0449 | 0.059028 | 0.3995 | 0.0946 | 0.0729 | 0.194411 | 0.49 | 0.0788 | 0.0576 | 0.171855 | 0.9514 | NaN | 0.1103 | 0.0355 | 0.001922 | 0.5305 | 0.1127 | 0.06 | 0.060195 | 0.6733 | 0.1223 | 0.0443 | 0.005742 | 0.4891 | NaN | 0.0885 | 0.0445 | 0.046758 | 0.7271 | 0.0827 | 0.0724 | 0.253282 | 0.5899 | 0.0954 | 0.0576 | 0.097546 | 0.7232 |
| L-carnitine | 161.105 | 0.668089 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.1676 | 0.0855 | 0.050027 | 0.2616 | 0.2407 | 0.1267 | 0.057347 | 0.2819 | 0.089 | 0.1158 | 0.442168 | 0.7487 | NaN | 0.1225 | 0.0797 | 0.124482 | 0.4437 | 0.1823 | 0.1123 | 0.104395 | 0.4511 | 0.0512 | 0.1093 | 0.639499 | 0.8939 | NaN | 0.0289 | 0.0615 | 0.637917 | 0.9288 | 0.1307 | 0.0898 | 0.145776 | 0.5917 | -0.044 | 0.0832 | 0.59668 | 0.8601 | NaN | 0.04 | 0.0456 | 0.381266 | 0.6745 | 0.0002 | 0.071 | 0.99795 | 0.9979 | 0.0597 | 0.0595 | 0.315402 | 0.9622 | NaN | -0.0155 | 0.0369 | 0.674945 | 0.9708 | 0.0093 | 0.0586 | 0.87449 | 0.9977 | -0.037 | 0.0471 | 0.43253 | 0.9967 | NaN | 0.0406 | 0.0453 | 0.370103 | 0.7949 | 0.0043 | 0.0704 | 0.951535 | 0.9788 | 0.061 | 0.0595 | 0.305345 | 0.8042 |
| O-adipoylcarnitine | 289.153 | 2.560197 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0842 | 0.0887 | 0.342805 | 0.6908 | 0.1622 | 0.151 | 0.282843 | 0.5959 | 0.0474 | 0.1088 | 0.663307 | 0.8853 | NaN | 0.125 | 0.0821 | 0.127554 | 0.4437 | 0.1856 | 0.132 | 0.159696 | 0.5063 | 0.0872 | 0.1023 | 0.394121 | 0.8005 | NaN | 0.015 | 0.0627 | 0.810818 | 0.9752 | 0.0081 | 0.1072 | 0.939633 | 0.9762 | 0.0108 | 0.0772 | 0.88828 | 0.9707 | NaN | -0.0277 | 0.047 | 0.554647 | 0.7987 | -0.0431 | 0.0824 | 0.601225 | 0.7883 | -0.0155 | 0.0561 | 0.782039 | 0.9994 | NaN | 0.0524 | 0.0373 | 0.160121 | 0.9708 | 0.1431 | 0.066 | 0.030121 | 0.6225 | 0.0061 | 0.044 | 0.889229 | 0.9967 | NaN | -0.029 | 0.0466 | 0.534431 | 0.8373 | -0.0171 | 0.0816 | 0.834193 | 0.9191 | -0.0317 | 0.0562 | 0.572454 | 0.9321 |
| AC 4:0 (OH) | 247.1422 | 1.145753 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | 0.0015 | 0.0863 | 0.986355 | 0.9936 | 0.1953 | 0.1245 | 0.116865 | 0.3717 | -0.166 | 0.1164 | 0.153918 | 0.5149 | NaN | 0.0663 | 0.0804 | 0.409678 | 0.7538 | 0.1905 | 0.109 | 0.080483 | 0.441 | -0.0808 | 0.1124 | 0.4722 | 0.8435 | NaN | -0.0002 | 0.0607 | 0.997905 | 0.9992 | 0.0593 | 0.089 | 0.505128 | 0.8105 | -0.0654 | 0.0836 | 0.433737 | 0.7865 | NaN | -0.0924 | 0.0451 | 0.040486 | 0.3914 | -0.14 | 0.0696 | 0.044346 | 0.2513 | -0.052 | 0.0606 | 0.390393 | 0.9735 | NaN | -0.034 | 0.0363 | 0.349229 | 0.9708 | 0.0109 | 0.0569 | 0.848102 | 0.9977 | -0.0775 | 0.047 | 0.099626 | 0.9967 | NaN | -0.0926 | 0.0447 | 0.038577 | 0.7271 | -0.1128 | 0.069 | 0.102331 | 0.438 | -0.0767 | 0.0603 | 0.202914 | 0.7294 |
| AC 6:0 (OH) | 275.1739 | 3.553601 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.0039 | 0.0866 | 0.964258 | 0.9784 | 0.1703 | 0.1278 | 0.18262 | 0.4621 | -0.1479 | 0.1156 | 0.200905 | 0.549 | NaN | 0.0865 | 0.0812 | 0.286774 | 0.6553 | 0.2517 | 0.1112 | 0.023567 | 0.3387 | -0.061 | 0.1117 | 0.584854 | 0.8877 | NaN | -0.0146 | 0.0609 | 0.810929 | 0.9752 | 0.0699 | 0.0904 | 0.439437 | 0.7964 | -0.1008 | 0.0821 | 0.219564 | 0.6205 | NaN | -0.0786 | 0.0453 | 0.082819 | 0.407 | -0.1092 | 0.0706 | 0.122161 | 0.3875 | -0.0459 | 0.06 | 0.444348 | 0.9735 | NaN | -0.0084 | 0.0365 | 0.818769 | 0.9722 | 0.0541 | 0.0574 | 0.345627 | 0.9977 | -0.0637 | 0.0468 | 0.173296 | 0.9967 | NaN | -0.0735 | 0.045 | 0.102 | 0.7516 | -0.0803 | 0.07 | 0.251049 | 0.5872 | -0.0635 | 0.0599 | 0.288576 | 0.8005 |
| AC 8:0 (OH) | 303.2045 | 7.959024 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.1393 | 0.0885 | 0.115432 | 0.3958 | -0.0975 | 0.146 | 0.50419 | 0.7975 | -0.1534 | 0.1106 | 0.165468 | 0.5263 | NaN | -0.0082 | 0.0855 | 0.923162 | 0.9933 | 0.141 | 0.135 | 0.296415 | 0.6731 | -0.0574 | 0.1079 | 0.59464 | 0.8877 | NaN | -0.1214 | 0.062 | 0.050363 | 0.4089 | -0.0717 | 0.102 | 0.482199 | 0.8009 | -0.1597 | 0.0776 | 0.039496 | 0.3772 | NaN | -0.0254 | 0.047 | 0.589807 | 0.8139 | -0.0465 | 0.0784 | 0.553183 | 0.772 | -0.003 | 0.058 | 0.959234 | 0.9994 | NaN | -0.009 | 0.0378 | 0.811531 | 0.9722 | 0.0144 | 0.0653 | 0.82516 | 0.9977 | -0.0234 | 0.0454 | 0.605918 | 0.9967 | NaN | -0.0282 | 0.0466 | 0.545354 | 0.8404 | -0.0617 | 0.0776 | 0.426365 | 0.7185 | -0.0023 | 0.0581 | 0.967845 | 0.996 |
| AC 10:0 (OH) | 331.2357 | 12.493725 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.1265 | 0.0903 | 0.16101 | 0.4783 | -0.0708 | 0.1462 | 0.628355 | 0.8607 | -0.1489 | 0.1139 | 0.19117 | 0.5439 | NaN | 0.0059 | 0.0871 | 0.945752 | 0.9933 | 0.1619 | 0.1343 | 0.228094 | 0.5911 | -0.0482 | 0.1111 | 0.664725 | 0.9007 | NaN | -0.1377 | 0.0631 | 0.029006 | 0.2965 | -0.0832 | 0.1019 | 0.414183 | 0.7884 | -0.174 | 0.0796 | 0.028785 | 0.3354 | NaN | -0.0178 | 0.0479 | 0.709761 | 0.8668 | -0.0245 | 0.0785 | 0.755399 | 0.8746 | -0.0099 | 0.0596 | 0.867495 | 0.9994 | NaN | -0.004 | 0.0385 | 0.917133 | 0.9722 | 0.0318 | 0.0652 | 0.625912 | 0.9977 | -0.0254 | 0.0466 | 0.585515 | 0.9967 | NaN | -0.0169 | 0.0475 | 0.722308 | 0.9166 | -0.0379 | 0.0778 | 0.626004 | 0.8191 | -0.0017 | 0.0597 | 0.977067 | 0.996 |
| N-undecanoylglycine | 243.1826 | 15.799677 | Lipid | Fatty Acid, acylglycine | -0.0494 | 0.0811 | 0.542097 | 0.8289 | 0.1055 | 0.1715 | 0.53837 | 0.8052 | -0.0946 | 0.0919 | 0.303187 | 0.6859 | NaN | -0.0509 | 0.075 | 0.497473 | 0.7987 | 0.0548 | 0.151 | 0.716726 | 0.8811 | -0.0941 | 0.0862 | 0.274825 | 0.6833 | NaN | 0.0139 | 0.0573 | 0.808697 | 0.9752 | -0.0587 | 0.121 | 0.627361 | 0.8438 | 0.02 | 0.0663 | 0.763531 | 0.9437 | NaN | -0.0044 | 0.0427 | 0.918121 | 0.969 | 0.1225 | 0.0913 | 0.179785 | 0.463 | -0.0285 | 0.0476 | 0.549578 | 0.9885 | NaN | -0.0291 | 0.0342 | 0.39373 | 0.9708 | 0.0633 | 0.0762 | 0.4063 | 0.9977 | -0.0589 | 0.0369 | 0.110649 | 0.9967 | NaN | -0.0348 | 0.0423 | 0.410281 | 0.8117 | 0.0841 | 0.091 | 0.355655 | 0.6566 | -0.0615 | 0.0472 | 0.193046 | 0.7294 |
| 3-aminoisobutanoate | 103.0638 | 1.812905 | Lipid | Fatty Acid, Amino | -0.0926 | 0.0853 | 0.277669 | 0.6386 | -0.0882 | 0.1186 | 0.45741 | 0.7565 | -0.0925 | 0.1219 | 0.448081 | 0.7518 | NaN | -0.113 | 0.0788 | 0.151544 | 0.4892 | -0.1578 | 0.1039 | 0.128994 | 0.4744 | -0.0987 | 0.1143 | 0.387547 | 0.7982 | NaN | -0.0758 | 0.0599 | 0.20602 | 0.7091 | -0.0651 | 0.0829 | 0.432218 | 0.7964 | -0.1018 | 0.086 | 0.2368 | 0.6205 | NaN | -0.0415 | 0.0449 | 0.355684 | 0.6633 | -0.0478 | 0.0637 | 0.452812 | 0.7061 | -0.0215 | 0.0629 | 0.733005 | 0.9994 | NaN | 0.0445 | 0.0362 | 0.218894 | 0.9708 | 0.0371 | 0.0532 | 0.484987 | 0.9977 | 0.051 | 0.0495 | 0.302722 | 0.9967 | NaN | -0.0118 | 0.0447 | 0.791225 | 0.9482 | -0.0338 | 0.0633 | 0.593522 | 0.8122 | 0.0206 | 0.0632 | 0.744559 | 0.9732 |
| C8 H14 O2 | 142.099 | 8.877983 | Lipid | Fatty acid, branched chain fatty acid | 0.0451 | 0.0808 | 0.576383 | 0.8499 | 0.0922 | 0.1248 | 0.459867 | 0.7578 | 0.021 | 0.1054 | 0.841813 | 0.9565 | NaN | 0.0111 | 0.075 | 0.882641 | 0.9933 | 0.0514 | 0.11 | 0.64025 | 0.8459 | -0.0086 | 0.0991 | 0.930591 | 0.9876 | NaN | -0.0047 | 0.057 | 0.933805 | 0.9968 | 0.1096 | 0.0867 | 0.206102 | 0.6538 | -0.0768 | 0.0749 | 0.305177 | 0.6876 | NaN | -0.0179 | 0.0426 | 0.673613 | 0.846 | -0.1059 | 0.0675 | 0.116588 | 0.3808 | 0.0342 | 0.0541 | 0.527015 | 0.9885 | NaN | 0.0155 | 0.0341 | 0.649036 | 0.9708 | 0.029 | 0.0557 | 0.602167 | 0.9977 | 0.0084 | 0.0426 | 0.842756 | 0.9967 | NaN | -0.0129 | 0.0422 | 0.75995 | 0.924 | -0.093 | 0.0669 | 0.164698 | 0.5362 | 0.0364 | 0.0541 | 0.501367 | 0.8928 |
| C9 H16 O2 | 156.1147 | 11.847941 | Lipid | Fatty acid, branched chain fatty acid | 0.1017 | 0.0861 | 0.237535 | 0.588 | 0.174 | 0.1413 | 0.218186 | 0.506 | 0.0623 | 0.1077 | 0.563134 | 0.8352 | NaN | 0.0821 | 0.0797 | 0.303065 | 0.6692 | 0.1266 | 0.1246 | 0.309919 | 0.6823 | 0.0527 | 0.1011 | 0.601967 | 0.8877 | NaN | -0.0222 | 0.0613 | 0.717983 | 0.9414 | 0.134 | 0.0986 | 0.174133 | 0.6495 | -0.1084 | 0.0774 | 0.161506 | 0.5601 | NaN | 0.0228 | 0.0455 | 0.616596 | 0.8244 | -0.0438 | 0.0776 | 0.571825 | 0.7754 | 0.0537 | 0.0552 | 0.330918 | 0.9622 | NaN | 0.0172 | 0.0365 | 0.637079 | 0.9708 | 0.0192 | 0.0638 | 0.763026 | 0.9977 | 0.0171 | 0.0436 | 0.695281 | 0.9967 | NaN | 0.0317 | 0.0451 | 0.482129 | 0.8239 | -0.0779 | 0.0771 | 0.3121 | 0.6453 | 0.0878 | 0.0549 | 0.10963 | 0.7232 |
| FA 5:0 (DiC) | 132.0424 | 2.036774 | Lipid | Fatty Acid, Dicarboxylate | 0.0975 | 0.0885 | 0.270822 | 0.6373 | 0.2487 | 0.1229 | 0.042969 | 0.2471 | -0.0705 | 0.1248 | 0.572106 | 0.8352 | NaN | 0.0577 | 0.0823 | 0.483377 | 0.7907 | 0.1408 | 0.1113 | 0.206004 | 0.5547 | -0.0846 | 0.117 | 0.469607 | 0.8416 | NaN | -0.0463 | 0.0632 | 0.46341 | 0.8642 | 0.1309 | 0.0875 | 0.134429 | 0.5905 | -0.2335 | 0.087 | 0.007279 | 0.1545 | NaN | 0.0603 | 0.0465 | 0.194901 | 0.5115 | 0.1012 | 0.0672 | 0.132198 | 0.4016 | 0.0282 | 0.0644 | 0.661917 | 0.9994 | NaN | 0.0163 | 0.0375 | 0.664104 | 0.9708 | 0.0395 | 0.0567 | 0.486887 | 0.9977 | -0.0116 | 0.0505 | 0.818986 | 0.9967 | NaN | 0.0482 | 0.0462 | 0.297275 | 0.7695 | 0.0357 | 0.0681 | 0.599717 | 0.8122 | 0.0659 | 0.0645 | 0.306876 | 0.8042 |
| FA 6:0 (DiC) | 146.0586 | 3.541705 | Lipid | Fatty Acid, Dicarboxylate | 0.0841 | 0.0908 | 0.353928 | 0.7019 | 0.2049 | 0.1401 | 0.143664 | 0.415 | -0.0143 | 0.118 | 0.903439 | 0.9854 | NaN | 0.0569 | 0.0841 | 0.498768 | 0.7987 | 0.104 | 0.1254 | 0.406846 | 0.7328 | -0.0196 | 0.1107 | 0.859491 | 0.9708 | NaN | -0.1359 | 0.0651 | 0.036763 | 0.344 | 0 | 0.1011 | 0.99979 | 0.9998 | -0.2418 | 0.0831 | 0.003595 | 0.1228 | NaN | 0.0692 | 0.0476 | 0.14569 | 0.4845 | 0.1106 | 0.0754 | 0.142418 | 0.4129 | 0.0455 | 0.0606 | 0.453262 | 0.9735 | NaN | 0.0334 | 0.0383 | 0.383288 | 0.9708 | 0.0489 | 0.0633 | 0.440019 | 0.9977 | 0.0191 | 0.0477 | 0.687976 | 0.9967 | NaN | 0.0717 | 0.0472 | 0.128625 | 0.7516 | 0.0592 | 0.0757 | 0.434256 | 0.7217 | 0.0841 | 0.0605 | 0.164332 | 0.7294 |
| FA 7:0 (DiC) | 160.074 | 5.69702 | Lipid | Fatty Acid, Dicarboxylate | 0.2096 | 0.0853 | 0.013986 | 0.1287 | 0.2973 | 0.1351 | 0.02774 | 0.2307 | 0.1502 | 0.1092 | 0.168718 | 0.5263 | NaN | 0.1659 | 0.0795 | 0.03699 | 0.2836 | 0.2167 | 0.1205 | 0.072255 | 0.4408 | 0.1159 | 0.1031 | 0.260855 | 0.6818 | NaN | 0.0192 | 0.0624 | 0.757832 | 0.9454 | 0.1101 | 0.098 | 0.261176 | 0.7102 | -0.0501 | 0.0803 | 0.532902 | 0.826 | NaN | 0.0062 | 0.0464 | 0.893678 | 0.9579 | 0.0017 | 0.0768 | 0.982201 | 0.9876 | 0.0142 | 0.0571 | 0.803763 | 0.9994 | NaN | 0.0073 | 0.0371 | 0.843408 | 0.9722 | 0.0178 | 0.0633 | 0.778149 | 0.9977 | -0.001 | 0.045 | 0.981866 | 0.9967 | NaN | 0.0235 | 0.0458 | 0.607739 | 0.8587 | 0.0288 | 0.0757 | 0.704071 | 0.8504 | 0.0243 | 0.0571 | 0.670334 | 0.9564 |
| FA 8:0 (DiC) | 174.0893 | 8.243132 | Lipid | Fatty Acid, Dicarboxylate | 0.1675 | 0.0861 | 0.05172 | 0.2644 | 0.3615 | 0.128 | 0.004731 | 0.1187 | 0.0285 | 0.1135 | 0.801939 | 0.9499 | NaN | 0.0986 | 0.081 | 0.223416 | 0.5873 | 0.1986 | 0.1203 | 0.098793 | 0.4459 | -0.0096 | 0.107 | 0.928784 | 0.9876 | NaN | -0.0582 | 0.0631 | 0.355944 | 0.7983 | 0.095 | 0.0968 | 0.326591 | 0.7705 | -0.1728 | 0.081 | 0.032891 | 0.3426 | NaN | 0.1203 | 0.045 | 0.007463 | 0.3584 | 0.2046 | 0.0691 | 0.003071 | 0.1525 | 0.064 | 0.0581 | 0.27085 | 0.9622 | NaN | 0.0326 | 0.0368 | 0.375697 | 0.9708 | 0.0866 | 0.0604 | 0.151406 | 0.8645 | -0.0054 | 0.0459 | 0.907063 | 0.9967 | NaN | 0.1225 | 0.0446 | 0.005982 | 0.7271 | 0.1803 | 0.0695 | 0.009445 | 0.265 | 0.0852 | 0.058 | 0.141735 | 0.7232 |
| FA 9:0 (DiC) | 188.105 | 10.741281 | Lipid | Fatty Acid, Dicarboxylate | 0.1724 | 0.0819 | 0.035242 | 0.2219 | 0.3184 | 0.1276 | 0.012612 | 0.1655 | 0.0805 | 0.1052 | 0.444534 | 0.7504 | NaN | 0.1234 | 0.0766 | 0.107084 | 0.4163 | 0.21 | 0.1157 | 0.069563 | 0.4408 | 0.0479 | 0.0992 | 0.62901 | 0.8939 | NaN | -0.0037 | 0.0596 | 0.950509 | 0.997 | 0.1064 | 0.094 | 0.258016 | 0.7102 | -0.082 | 0.076 | 0.280272 | 0.6728 | NaN | 0.0308 | 0.0439 | 0.482391 | 0.7522 | 0.0474 | 0.0728 | 0.515322 | 0.7545 | 0.0255 | 0.0543 | 0.638487 | 0.9994 | NaN | 0.0033 | 0.0353 | 0.924681 | 0.9722 | 0.0437 | 0.0602 | 0.467445 | 0.9977 | -0.0225 | 0.0428 | 0.599148 | 0.9967 | NaN | 0.0436 | 0.0434 | 0.315369 | 0.7708 | 0.0791 | 0.0714 | 0.268009 | 0.6088 | 0.0253 | 0.0544 | 0.642273 | 0.9483 |
| FA 10:0 (DiC) | 202.1208 | 13.31509 | Lipid | Fatty Acid, Dicarboxylate | 0.0563 | 0.0858 | 0.5116 | 0.8138 | 0.0902 | 0.1439 | 0.530742 | 0.8052 | 0.0375 | 0.1063 | 0.724065 | 0.9022 | NaN | 0.0608 | 0.0793 | 0.443389 | 0.7757 | 0.0901 | 0.1263 | 0.475604 | 0.7664 | 0.0459 | 0.0997 | 0.645046 | 0.8939 | NaN | 0.011 | 0.0605 | 0.85574 | 0.9805 | 0.1335 | 0.0999 | 0.181429 | 0.652 | -0.0451 | 0.0757 | 0.550911 | 0.8359 | NaN | -0.016 | 0.0453 | 0.7229 | 0.8751 | -0.1602 | 0.0773 | 0.03824 | 0.2454 | 0.05 | 0.0545 | 0.358898 | 0.9622 | NaN | 0.0079 | 0.0362 | 0.827301 | 0.9722 | -0.0258 | 0.0644 | 0.688153 | 0.9977 | 0.0269 | 0.0429 | 0.530511 | 0.9967 | NaN | -0.008 | 0.0449 | 0.85817 | 0.9644 | -0.1745 | 0.0765 | 0.022541 | 0.2725 | 0.0718 | 0.0544 | 0.186924 | 0.7294 |
| FA 11:0 (DiC) | 216.1365 | 14.872025 | Lipid | Fatty Acid, Dicarboxylate | 0.1975 | 0.0827 | 0.016967 | 0.1377 | 0.3282 | 0.1252 | 0.008736 | 0.1461 | 0.1073 | 0.1085 | 0.322613 | 0.6929 | NaN | 0.1494 | 0.0773 | 0.053327 | 0.3365 | 0.2284 | 0.1131 | 0.043528 | 0.4171 | 0.0747 | 0.1023 | 0.465286 | 0.8416 | NaN | 0.0067 | 0.0605 | 0.911869 | 0.9946 | 0.1331 | 0.0918 | 0.147277 | 0.5934 | -0.0897 | 0.079 | 0.256671 | 0.644 | NaN | 0.0358 | 0.0446 | 0.422475 | 0.7088 | 0.0391 | 0.0721 | 0.587913 | 0.7765 | 0.0363 | 0.0561 | 0.517745 | 0.9885 | NaN | 0.0251 | 0.0358 | 0.482966 | 0.9708 | 0.0597 | 0.0591 | 0.31237 | 0.9977 | 0.0012 | 0.0443 | 0.978745 | 0.9967 | NaN | 0.0529 | 0.0441 | 0.230201 | 0.7516 | 0.0615 | 0.0709 | 0.385662 | 0.6823 | 0.0493 | 0.056 | 0.378774 | 0.8297 |
| FA 12:0 (DiC) | 230.1519 | 16.474684 | Lipid | Fatty Acid, Dicarboxylate | 0.0317 | 0.0863 | 0.712914 | 0.9027 | 0.169 | 0.1245 | 0.174449 | 0.45 | -0.0907 | 0.1173 | 0.439204 | 0.7481 | NaN | 0.0311 | 0.0798 | 0.696762 | 0.9341 | 0.0996 | 0.1106 | 0.367692 | 0.7116 | -0.0671 | 0.1103 | 0.542688 | 0.8742 | NaN | -0.1077 | 0.061 | 0.077501 | 0.5033 | 0.0728 | 0.088 | 0.407926 | 0.784 | -0.2792 | 0.0807 | 0.000544 | 0.0522 | NaN | 0.0059 | 0.0454 | 0.897151 | 0.9579 | 0.0229 | 0.068 | 0.736568 | 0.8684 | -0.0026 | 0.0607 | 0.965677 | 0.9994 | NaN | 0.0208 | 0.0364 | 0.566487 | 0.9708 | 0.0516 | 0.056 | 0.356777 | 0.9977 | -0.0087 | 0.0476 | 0.855514 | 0.9967 | NaN | 0.038 | 0.045 | 0.398155 | 0.8117 | 0.0064 | 0.0677 | 0.924937 | 0.9688 | 0.0707 | 0.0609 | 0.245097 | 0.7434 |
| FA 13:0 (DiC) | 244.1675 | 17.88523 | Lipid | Fatty Acid, Dicarboxylate | 0.1034 | 0.0886 | 0.243357 | 0.5944 | 0.1698 | 0.1243 | 0.17181 | 0.4474 | 0.032 | 0.1248 | 0.797838 | 0.948 | NaN | 0.0685 | 0.0823 | 0.40558 | 0.7538 | 0.0699 | 0.1116 | 0.530917 | 0.7797 | 0.0198 | 0.1171 | 0.865816 | 0.9708 | NaN | -0.0771 | 0.0636 | 0.225155 | 0.7309 | 0.0458 | 0.0884 | 0.604643 | 0.8395 | -0.2161 | 0.089 | 0.015202 | 0.2543 | NaN | 0.0693 | 0.0465 | 0.13613 | 0.4828 | 0.0985 | 0.0667 | 0.139522 | 0.4097 | 0.0475 | 0.064 | 0.457624 | 0.9735 | NaN | 0.0365 | 0.0375 | 0.330416 | 0.9708 | 0.0608 | 0.0558 | 0.275605 | 0.9834 | 0.0102 | 0.0504 | 0.83978 | 0.9967 | NaN | 0.0891 | 0.046 | 0.05266 | 0.7271 | 0.0674 | 0.0667 | 0.312591 | 0.6453 | 0.1161 | 0.0634 | 0.067266 | 0.7232 |
| FA 14:0 (DiC) | 258.1833 | 19.113493 | Lipid | Fatty Acid, Dicarboxylate | -0.0642 | 0.0852 | 0.450625 | 0.7691 | 0.0857 | 0.1258 | 0.495756 | 0.7932 | -0.2119 | 0.1139 | 0.062859 | 0.3614 | NaN | -0.0009 | 0.0796 | 0.991453 | 0.9933 | 0.1093 | 0.1102 | 0.321356 | 0.6906 | -0.1376 | 0.1098 | 0.210016 | 0.6714 | NaN | -0.0766 | 0.0598 | 0.20009 | 0.7091 | 0.087 | 0.0876 | 0.3208 | 0.7699 | -0.2243 | 0.0791 | 0.004574 | 0.1228 | NaN | -0.0731 | 0.0445 | 0.100637 | 0.4561 | -0.1273 | 0.0678 | 0.060301 | 0.2766 | -0.0261 | 0.0604 | 0.665841 | 0.9994 | NaN | -0.0073 | 0.036 | 0.838514 | 0.9722 | -0.0136 | 0.0563 | 0.808802 | 0.9977 | -0.0099 | 0.0476 | 0.834526 | 0.9967 | NaN | -0.052 | 0.0443 | 0.240998 | 0.7516 | -0.1449 | 0.0671 | 0.030667 | 0.2981 | 0.0246 | 0.0611 | 0.687866 | 0.9564 |
| FA 16:0 (DiC) | 286.2147 | 21.107553 | Lipid | Fatty Acid, Dicarboxylate | -0.0521 | 0.0853 | 0.541255 | 0.8289 | 0.1251 | 0.1274 | 0.325933 | 0.6472 | -0.2168 | 0.1126 | 0.054264 | 0.3614 | NaN | 0.0246 | 0.08 | 0.758781 | 0.9671 | 0.1304 | 0.1116 | 0.242279 | 0.6051 | -0.1222 | 0.1103 | 0.267777 | 0.6818 | NaN | -0.0664 | 0.0599 | 0.267448 | 0.7604 | 0.0957 | 0.0889 | 0.281673 | 0.7284 | -0.2045 | 0.0787 | 0.009382 | 0.1838 | NaN | -0.0849 | 0.0445 | 0.05636 | 0.3989 | -0.1371 | 0.0693 | 0.04793 | 0.2516 | -0.0465 | 0.0596 | 0.434689 | 0.9735 | NaN | -0.0198 | 0.036 | 0.581925 | 0.9708 | -0.031 | 0.0574 | 0.588772 | 0.9977 | -0.02 | 0.047 | 0.671163 | 0.9967 | NaN | -0.0747 | 0.0442 | 0.091147 | 0.7516 | -0.1464 | 0.0686 | 0.032918 | 0.2981 | -0.0245 | 0.06 | 0.682663 | 0.9564 |
| FA 18:0 (DiC) | 314.2461 | 22.242228 | Lipid | Fatty Acid, Dicarboxylate | 0.1253 | 0.0888 | 0.15818 | 0.4783 | 0.1196 | 0.1367 | 0.381769 | 0.698 | 0.1786 | 0.118 | 0.130107 | 0.4747 | NaN | 0.0617 | 0.0831 | 0.457775 | 0.7771 | 0.0143 | 0.1221 | 0.90674 | 0.9654 | 0.1213 | 0.1123 | 0.280323 | 0.6877 | NaN | 0.0039 | 0.0633 | 0.950671 | 0.997 | 0.0225 | 0.0963 | 0.815547 | 0.9217 | -0.0212 | 0.0867 | 0.806703 | 0.9477 | NaN | 0.0172 | 0.0471 | 0.714935 | 0.8693 | 0.0258 | 0.0738 | 0.726452 | 0.8643 | 0.0218 | 0.062 | 0.724816 | 0.9994 | NaN | 0.007 | 0.0378 | 0.852126 | 0.9722 | 0.0396 | 0.0611 | 0.51615 | 0.9977 | -0.0115 | 0.0489 | 0.813267 | 0.9967 | NaN | 0.0445 | 0.0466 | 0.339795 | 0.7759 | 0.0386 | 0.0731 | 0.59694 | 0.8122 | 0.0595 | 0.0615 | 0.333193 | 0.8205 |
| FA 19:0 (DiC) | 328.2614 | 22.461948 | Lipid | Fatty Acid, Dicarboxylate | -0.1133 | 0.0816 | 0.16513 | 0.4815 | -0.1153 | 0.1337 | 0.388832 | 0.7038 | -0.0976 | 0.1027 | 0.341643 | 0.7068 | NaN | -0.0623 | 0.0762 | 0.413815 | 0.7542 | -0.0606 | 0.1181 | 0.607758 | 0.8385 | -0.0503 | 0.0974 | 0.605572 | 0.889 | NaN | -0.087 | 0.0574 | 0.12959 | 0.6167 | -0.2007 | 0.0919 | 0.029019 | 0.3462 | -0.0232 | 0.0734 | 0.75132 | 0.9374 | NaN | 0.0351 | 0.0435 | 0.419847 | 0.7088 | 0.1241 | 0.0725 | 0.087063 | 0.3183 | -0.0137 | 0.0532 | 0.79652 | 0.9994 | NaN | -0.0249 | 0.0346 | 0.472589 | 0.9708 | -0.0842 | 0.0591 | 0.154335 | 0.8645 | 0.0112 | 0.0419 | 0.789528 | 0.9967 | NaN | 0.0543 | 0.0432 | 0.208621 | 0.7516 | 0.1487 | 0.0718 | 0.038314 | 0.3022 | 0.0027 | 0.0534 | 0.959601 | 0.996 |
| FA 20:0 (DiC) | 342.2767 | 22.332983 | Lipid | Fatty Acid, Dicarboxylate | -0.1398 | 0.0837 | 0.094929 | 0.3614 | -0.3067 | 0.1197 | 0.010392 | 0.1606 | 0.02 | 0.1146 | 0.86149 | 0.9597 | NaN | -0.1584 | 0.0772 | 0.04019 | 0.3024 | -0.2819 | 0.1048 | 0.007148 | 0.2321 | -0.0184 | 0.1079 | 0.864477 | 0.9708 | NaN | -0.0807 | 0.0592 | 0.172732 | 0.6546 | -0.1081 | 0.0882 | 0.220572 | 0.6655 | -0.0637 | 0.0813 | 0.433231 | 0.7865 | NaN | -0.0851 | 0.044 | 0.05292 | 0.3914 | -0.1484 | 0.0654 | 0.023358 | 0.2149 | -0.0289 | 0.0589 | 0.623863 | 0.9994 | NaN | -0.0394 | 0.0356 | 0.267522 | 0.9708 | -0.0612 | 0.0562 | 0.275968 | 0.9834 | -0.0193 | 0.0463 | 0.677456 | 0.9967 | NaN | -0.0803 | 0.0437 | 0.066088 | 0.7496 | -0.1489 | 0.0649 | 0.02174 | 0.2725 | -0.0206 | 0.059 | 0.726966 | 0.968 |
| FA 24:0 (DiC) | 398.3392 | 23.17186 | Lipid | Fatty Acid, Dicarboxylate | -0.0488 | 0.0852 | 0.566746 | 0.8447 | -0.3028 | 0.1205 | 0.011943 | 0.1645 | 0.2216 | 0.1171 | 0.058425 | 0.3614 | NaN | -0.0759 | 0.0788 | 0.335401 | 0.704 | -0.2405 | 0.1071 | 0.024649 | 0.3387 | 0.1534 | 0.1123 | 0.171919 | 0.6598 | NaN | -0.0045 | 0.06 | 0.940237 | 0.9968 | -0.0863 | 0.0894 | 0.334297 | 0.7705 | 0.0588 | 0.0857 | 0.492563 | 0.8203 | NaN | -0.0908 | 0.0444 | 0.040751 | 0.3914 | -0.1637 | 0.0652 | 0.012105 | 0.1777 | -0.0193 | 0.0628 | 0.758546 | 0.9994 | NaN | -0.0048 | 0.036 | 0.893795 | 0.9722 | -0.0372 | 0.057 | 0.513915 | 0.9977 | 0.0312 | 0.0487 | 0.521216 | 0.9967 | NaN | -0.0438 | 0.0444 | 0.323076 | 0.7727 | -0.1344 | 0.0657 | 0.040726 | 0.3085 | 0.0454 | 0.062 | 0.463562 | 0.8635 |
| FA 7:1 (DiC) | 158.0578 | 2.836201 | Lipid | Fatty Acid, Dicarboxylate | 0.0602 | 0.0862 | 0.48463 | 0.7986 | 0.2081 | 0.1156 | 0.071796 | 0.3049 | -0.0951 | 0.1273 | 0.454953 | 0.755 | NaN | 0.0403 | 0.0798 | 0.614045 | 0.9015 | 0.1215 | 0.1038 | 0.241639 | 0.6051 | -0.078 | 0.1195 | 0.513963 | 0.8742 | NaN | -0.0104 | 0.0609 | 0.864989 | 0.9805 | 0.0769 | 0.0828 | 0.353065 | 0.7705 | -0.0943 | 0.0899 | 0.294555 | 0.6783 | NaN | 0.0415 | 0.0453 | 0.359948 | 0.6667 | 0.0864 | 0.0629 | 0.169801 | 0.4506 | -0.0248 | 0.0657 | 0.706303 | 0.9994 | NaN | 0.044 | 0.0363 | 0.224741 | 0.9708 | 0.0573 | 0.0525 | 0.27525 | 0.9834 | 0.0339 | 0.0517 | 0.512609 | 0.9967 | NaN | 0.026 | 0.045 | 0.563013 | 0.8527 | 0.0313 | 0.0635 | 0.622008 | 0.8191 | 0.0104 | 0.066 | 0.875105 | 0.993 |
| FA 10:1 (DiC) | 200.1056 | 10.504287 | Lipid | Fatty Acid, Dicarboxylate | -0.1252 | 0.0843 | 0.137309 | 0.4388 | -0.1589 | 0.1212 | 0.189831 | 0.4657 | -0.0704 | 0.1206 | 0.55954 | 0.8352 | NaN | -0.1072 | 0.078 | 0.169434 | 0.5196 | 0.0056 | 0.112 | 0.960399 | 0.9835 | -0.1047 | 0.1132 | 0.35498 | 0.7684 | NaN | -0.0359 | 0.0599 | 0.548857 | 0.9017 | -0.0167 | 0.0866 | 0.847006 | 0.9285 | -0.0272 | 0.0856 | 0.750411 | 0.9374 | NaN | -0.006 | 0.0448 | 0.894338 | 0.9579 | -0.0699 | 0.0654 | 0.285457 | 0.5969 | 0.0359 | 0.0623 | 0.564468 | 0.9885 | NaN | 0.0146 | 0.036 | 0.685234 | 0.9708 | 0.036 | 0.0552 | 0.513993 | 0.9977 | 0.0051 | 0.0489 | 0.916673 | 0.9967 | NaN | -0.018 | 0.0444 | 0.684589 | 0.8913 | -0.11 | 0.0641 | 0.086375 | 0.3973 | 0.0573 | 0.0624 | 0.358239 | 0.8297 |
| FA 14:1 (DiC) | 256.1678 | 18.092892 | Lipid | Fatty Acid, Dicarboxylate | -0.1177 | 0.0843 | 0.162892 | 0.4783 | -0.0336 | 0.1338 | 0.801808 | 0.9244 | -0.1661 | 0.1091 | 0.128003 | 0.4742 | NaN | -0.0722 | 0.0786 | 0.358122 | 0.7295 | 0.0785 | 0.1191 | 0.509737 | 0.7797 | -0.1337 | 0.103 | 0.194323 | 0.6714 | NaN | -0.0472 | 0.0597 | 0.428987 | 0.8487 | 0.0416 | 0.0937 | 0.657306 | 0.8517 | -0.0888 | 0.078 | 0.25498 | 0.644 | NaN | 0.0345 | 0.045 | 0.44314 | 0.728 | -0.0345 | 0.0717 | 0.630259 | 0.8091 | 0.0712 | 0.0579 | 0.218996 | 0.9519 | NaN | 0.021 | 0.036 | 0.559787 | 0.9708 | -0.0366 | 0.0595 | 0.538503 | 0.9977 | 0.065 | 0.0452 | 0.150538 | 0.9967 | NaN | 0.0308 | 0.0446 | 0.489834 | 0.8283 | -0.0712 | 0.0709 | 0.315166 | 0.6453 | 0.0957 | 0.0581 | 0.099199 | 0.7232 |
| FA 18:1 (DiC) | 312.2305 | 21.571661 | Lipid | Fatty Acid, Dicarboxylate | -0.1682 | 0.091 | 0.064731 | 0.3054 | -0.0865 | 0.1341 | 0.519027 | 0.8001 | -0.2579 | 0.1223 | 0.034998 | 0.3207 | NaN | -0.1394 | 0.0845 | 0.098948 | 0.4077 | -0.0738 | 0.1178 | 0.530829 | 0.7797 | -0.2211 | 0.1156 | 0.055734 | 0.4962 | NaN | -0.1622 | 0.0636 | 0.01076 | 0.1776 | -0.0474 | 0.0939 | 0.613413 | 0.8437 | -0.2588 | 0.0848 | 0.002279 | 0.111 | NaN | -0.0577 | 0.0483 | 0.233026 | 0.5455 | -0.1027 | 0.0713 | 0.149785 | 0.4218 | -0.0208 | 0.0657 | 0.751656 | 0.9994 | NaN | -0.0333 | 0.0389 | 0.391571 | 0.9708 | -0.0661 | 0.0594 | 0.266079 | 0.9821 | -0.0099 | 0.0516 | 0.848049 | 0.9967 | NaN | -0.0414 | 0.0481 | 0.389395 | 0.8116 | -0.1087 | 0.0706 | 0.124008 | 0.4644 | 0.0154 | 0.0663 | 0.815843 | 0.9748 |
| FA 20:1 (DiC) | 340.2575 | 22.070116 | Lipid | Fatty Acid, Dicarboxylate | -0.1734 | 0.0842 | 0.039527 | 0.2321 | -0.2517 | 0.122 | 0.039081 | 0.2428 | -0.1034 | 0.115 | 0.368427 | 0.7082 | NaN | -0.2085 | 0.0776 | 0.007179 | 0.1043 | -0.3167 | 0.1052 | 0.002598 | 0.1769 | -0.1318 | 0.1077 | 0.221234 | 0.6714 | NaN | -0.0983 | 0.0597 | 0.099619 | 0.5669 | -0.0928 | 0.0881 | 0.292521 | 0.7407 | -0.1075 | 0.0811 | 0.184977 | 0.5977 | NaN | -0.1102 | 0.0442 | 0.012625 | 0.3584 | -0.1105 | 0.0666 | 0.096918 | 0.3408 | -0.105 | 0.0584 | 0.072437 | 0.8712 | NaN | -0.028 | 0.0361 | 0.438418 | 0.9708 | -0.0528 | 0.0562 | 0.347552 | 0.9977 | -0.0076 | 0.0468 | 0.871671 | 0.9967 | NaN | -0.0887 | 0.0441 | 0.044323 | 0.7271 | -0.1282 | 0.0655 | 0.050317 | 0.3429 | -0.0515 | 0.0593 | 0.385277 | 0.8324 |
| FA 21:1 (DiC) | 354.2763 | 22.34594 | Lipid | Fatty Acid, Dicarboxylate | -0.0549 | 0.0858 | 0.522719 | 0.8174 | -0.0719 | 0.1252 | 0.565678 | 0.8174 | -0.0254 | 0.1173 | 0.828617 | 0.9565 | NaN | -0.093 | 0.0795 | 0.241674 | 0.6038 | -0.1026 | 0.1097 | 0.34971 | 0.702 | -0.0671 | 0.1104 | 0.543184 | 0.8742 | NaN | -0.0661 | 0.0603 | 0.273064 | 0.7604 | 0.0031 | 0.0879 | 0.971701 | 0.9915 | -0.1196 | 0.0828 | 0.148686 | 0.5464 | NaN | 0.0408 | 0.0453 | 0.367998 | 0.6693 | -0.0662 | 0.0669 | 0.322699 | 0.6384 | 0.1331 | 0.0596 | 0.025597 | 0.8712 | NaN | 0.0372 | 0.0363 | 0.304779 | 0.9708 | 0.0465 | 0.0559 | 0.405745 | 0.9977 | 0.0331 | 0.0474 | 0.484448 | 0.9967 | NaN | 0.0597 | 0.0449 | 0.183831 | 0.7516 | -0.0366 | 0.0666 | 0.583136 | 0.8108 | 0.1435 | 0.0596 | 0.016032 | 0.6979 |
| FA 24:1 (DiC) | 396.3218 | 22.667086 | Lipid | Fatty Acid, Dicarboxylate | -0.1079 | 0.09 | 0.230487 | 0.581 | -0.1273 | 0.1078 | 0.237764 | 0.5379 | -0.0166 | 0.1623 | 0.918496 | 0.9864 | NaN | -0.118 | 0.0831 | 0.155684 | 0.4921 | -0.1228 | 0.0945 | 0.193821 | 0.5416 | -0.0517 | 0.1524 | 0.73448 | 0.9342 | NaN | -0.039 | 0.0636 | 0.539975 | 0.9005 | 0.0156 | 0.0772 | 0.840192 | 0.9257 | -0.1603 | 0.1148 | 0.162468 | 0.5601 | NaN | -0.0841 | 0.0471 | 0.074214 | 0.3995 | -0.0803 | 0.0577 | 0.16433 | 0.4447 | -0.0859 | 0.0831 | 0.301245 | 0.9622 | NaN | -0.009 | 0.0382 | 0.813945 | 0.9722 | 0.0033 | 0.0488 | 0.945815 | 0.9977 | -0.0275 | 0.0655 | 0.67526 | 0.9967 | NaN | -0.0476 | 0.0471 | 0.311739 | 0.7708 | -0.0707 | 0.0574 | 0.218453 | 0.5557 | 0.0101 | 0.0836 | 0.904136 | 0.9953 |
| FA 26:1 (DiC) | 424.355 | 22.844032 | Lipid | Fatty Acid, Dicarboxylate | -0.1295 | 0.0856 | 0.130321 | 0.4282 | -0.1747 | 0.1203 | 0.146314 | 0.4185 | -0.0532 | 0.1236 | 0.666818 | 0.8854 | NaN | -0.1065 | 0.0794 | 0.179661 | 0.5419 | -0.1199 | 0.1065 | 0.260543 | 0.6226 | -0.039 | 0.116 | 0.73693 | 0.9351 | NaN | -0.0517 | 0.0607 | 0.39449 | 0.8313 | 0.0062 | 0.0869 | 0.943585 | 0.9762 | -0.0934 | 0.0872 | 0.284104 | 0.6732 | NaN | -0.0717 | 0.0451 | 0.111641 | 0.4618 | -0.0589 | 0.0654 | 0.367714 | 0.659 | -0.0991 | 0.0629 | 0.11511 | 0.9077 | NaN | 0.0106 | 0.0366 | 0.77279 | 0.9722 | 0.0003 | 0.0548 | 0.995721 | 0.9977 | 0.0295 | 0.05 | 0.555317 | 0.9967 | NaN | -0.0322 | 0.0451 | 0.474546 | 0.8239 | -0.0315 | 0.0653 | 0.628884 | 0.8191 | -0.0404 | 0.0636 | 0.524522 | 0.8961 |
| FA 27:1 (DiC) | 438.3719 | 23.034887 | Lipid | Fatty Acid, Dicarboxylate | -0.0516 | 0.086 | 0.548284 | 0.8315 | -0.0405 | 0.1152 | 0.725243 | 0.9045 | -0.0353 | 0.1291 | 0.784424 | 0.9451 | NaN | -0.0858 | 0.0795 | 0.280512 | 0.6479 | -0.0357 | 0.1011 | 0.724127 | 0.8829 | -0.103 | 0.1219 | 0.398282 | 0.8005 | NaN | -0.0359 | 0.0605 | 0.552317 | 0.902 | 0.0478 | 0.0809 | 0.554082 | 0.8202 | -0.1483 | 0.091 | 0.103028 | 0.4845 | NaN | -0.0679 | 0.045 | 0.131372 | 0.4825 | -0.0953 | 0.0611 | 0.119135 | 0.3845 | -0.0248 | 0.0663 | 0.708197 | 0.9994 | NaN | 0.0402 | 0.0363 | 0.268194 | 0.9708 | 0.0464 | 0.0513 | 0.365565 | 0.9977 | 0.0365 | 0.0521 | 0.483762 | 0.9967 | NaN | -0.0045 | 0.0449 | 0.919347 | 0.9724 | -0.0531 | 0.0611 | 0.38491 | 0.6823 | 0.0641 | 0.0664 | 0.334313 | 0.8205 |
| FA 28:1 (DiC) | 452.3876 | 23.075253 | Lipid | Fatty Acid, Dicarboxylate | -0.1264 | 0.0855 | 0.139373 | 0.4388 | -0.2741 | 0.12 | 0.022416 | 0.2091 | 0.0445 | 0.1205 | 0.712071 | 0.9015 | NaN | -0.1296 | 0.079 | 0.100931 | 0.4077 | -0.1835 | 0.1081 | 0.089455 | 0.4459 | -0.0015 | 0.1137 | 0.989347 | 0.9993 | NaN | -0.0442 | 0.0607 | 0.466533 | 0.8642 | -0.0405 | 0.0894 | 0.650331 | 0.8476 | -0.0454 | 0.0857 | 0.596805 | 0.8601 | NaN | -0.1233 | 0.0444 | 0.005455 | 0.34 | -0.1711 | 0.0641 | 0.0076 | 0.1672 | -0.0827 | 0.0619 | 0.181701 | 0.9514 | NaN | -0.0113 | 0.0364 | 0.75633 | 0.9722 | -0.0393 | 0.0561 | 0.483023 | 0.9977 | 0.0205 | 0.0487 | 0.673485 | 0.9967 | NaN | -0.066 | 0.0447 | 0.140013 | 0.7516 | -0.1204 | 0.0652 | 0.064694 | 0.3895 | -0.0159 | 0.0622 | 0.798434 | 0.9748 |
| FA 17:2 (DiC) | 296.1984 | 22.410254 | Lipid | Fatty Acid, Dicarboxylate | 0.0643 | 0.0818 | 0.431588 | 0.7611 | -0.0409 | 0.1265 | 0.746641 | 0.92 | 0.1368 | 0.1056 | 0.195469 | 0.5449 | NaN | 0.0854 | 0.0756 | 0.258507 | 0.6275 | 0.0962 | 0.1135 | 0.396603 | 0.7241 | 0.1225 | 0.0992 | 0.217093 | 0.6714 | NaN | 0.035 | 0.0576 | 0.543659 | 0.9012 | 0.1276 | 0.089 | 0.151662 | 0.6041 | -0.0301 | 0.0771 | 0.696543 | 0.909 | NaN | -0.0554 | 0.0432 | 0.199819 | 0.5115 | -0.1348 | 0.0667 | 0.043375 | 0.2513 | 0.0048 | 0.0553 | 0.930371 | 0.9994 | NaN | 0.0288 | 0.0345 | 0.404296 | 0.9708 | 0.0168 | 0.0564 | 0.765306 | 0.9977 | 0.038 | 0.0431 | 0.377597 | 0.9967 | NaN | -0.01 | 0.0428 | 0.814515 | 0.9499 | -0.0988 | 0.0667 | 0.138234 | 0.4987 | 0.0557 | 0.0547 | 0.308861 | 0.8042 |
| FA 18:2 (DiC) | 310.2144 | 21.042389 | Lipid | Fatty Acid, Dicarboxylate | -0.1495 | 0.0889 | 0.092698 | 0.3578 | -0.0592 | 0.1406 | 0.673667 | 0.8854 | -0.2188 | 0.1142 | 0.055254 | 0.3614 | NaN | -0.1255 | 0.0825 | 0.127858 | 0.4437 | -0.0218 | 0.1237 | 0.859886 | 0.9418 | -0.2034 | 0.1072 | 0.057719 | 0.4962 | NaN | -0.1471 | 0.0622 | 0.017919 | 0.2387 | -0.0333 | 0.0983 | 0.734843 | 0.8816 | -0.2424 | 0.0789 | 0.002117 | 0.111 | NaN | -0.0323 | 0.0473 | 0.494751 | 0.7563 | -0.0904 | 0.0749 | 0.227703 | 0.5371 | 0.0239 | 0.0613 | 0.696341 | 0.9994 | NaN | -0.0316 | 0.0379 | 0.404054 | 0.9708 | -0.0717 | 0.0622 | 0.249129 | 0.9821 | -0.0105 | 0.0477 | 0.825188 | 0.9967 | NaN | -0.0254 | 0.047 | 0.58854 | 0.8527 | -0.101 | 0.0742 | 0.173267 | 0.5384 | 0.0374 | 0.0615 | 0.543826 | 0.9124 |
| FA 22:2 (DiC) | 366.2777 | 22.203842 | Lipid | Fatty Acid, Dicarboxylate | -0.1821 | 0.0858 | 0.033861 | 0.2202 | -0.1789 | 0.1273 | 0.160131 | 0.4348 | -0.1898 | 0.1149 | 0.098551 | 0.4331 | NaN | -0.1448 | 0.0798 | 0.069761 | 0.3516 | -0.1747 | 0.1115 | 0.117175 | 0.4674 | -0.139 | 0.1092 | 0.203132 | 0.6714 | NaN | -0.1256 | 0.0605 | 0.037905 | 0.3464 | -0.0708 | 0.0902 | 0.432451 | 0.7964 | -0.1626 | 0.0809 | 0.044583 | 0.3772 | NaN | -0.0235 | 0.0461 | 0.610908 | 0.8244 | -0.0617 | 0.0691 | 0.371868 | 0.6609 | 0.0045 | 0.0609 | 0.941711 | 0.9994 | NaN | -0.0121 | 0.037 | 0.743645 | 0.9722 | -0.0103 | 0.0579 | 0.859099 | 0.9977 | -0.014 | 0.0476 | 0.768665 | 0.9967 | NaN | -0.0211 | 0.0458 | 0.644244 | 0.8687 | -0.0673 | 0.0685 | 0.325796 | 0.6453 | 0.0139 | 0.0611 | 0.820316 | 0.9774 |
| FA 26:2 (DiC) | 422.3414 | 22.776163 | Lipid | Fatty Acid, Dicarboxylate | -0.1733 | 0.0895 | 0.052687 | 0.2644 | -0.192 | 0.1298 | 0.139097 | 0.4106 | -0.1293 | 0.1241 | 0.297313 | 0.6793 | NaN | -0.1693 | 0.0827 | 0.040534 | 0.3024 | -0.153 | 0.1144 | 0.181085 | 0.5289 | -0.1431 | 0.1162 | 0.218137 | 0.6714 | NaN | -0.066 | 0.0638 | 0.301273 | 0.782 | 0.0239 | 0.0943 | 0.799982 | 0.9217 | -0.1472 | 0.0872 | 0.091462 | 0.4613 | NaN | -0.1153 | 0.0468 | 0.013844 | 0.3584 | -0.064 | 0.0706 | 0.364866 | 0.659 | -0.1558 | 0.0623 | 0.012451 | 0.8712 | NaN | -0.0418 | 0.0382 | 0.274347 | 0.9708 | -0.0704 | 0.0583 | 0.227301 | 0.96 | -0.0141 | 0.0506 | 0.779751 | 0.9967 | NaN | -0.0633 | 0.0471 | 0.17913 | 0.7516 | -0.0746 | 0.0698 | 0.285244 | 0.6248 | -0.0478 | 0.0642 | 0.456461 | 0.8635 |
| FA 27:2 (DiC) | 436.3568 | 22.928392 | Lipid | Fatty Acid, Dicarboxylate | -0.0771 | 0.0854 | 0.366599 | 0.7078 | -0.2471 | 0.1202 | 0.03971 | 0.2428 | 0.091 | 0.1179 | 0.440435 | 0.7481 | NaN | -0.0323 | 0.0795 | 0.684876 | 0.9339 | -0.187 | 0.1067 | 0.079595 | 0.441 | 0.1331 | 0.1107 | 0.229384 | 0.6771 | NaN | -0.0188 | 0.0603 | 0.755347 | 0.9454 | -0.0326 | 0.0885 | 0.71257 | 0.8816 | -0.0011 | 0.0842 | 0.989369 | 0.9973 | NaN | -0.0945 | 0.0445 | 0.03376 | 0.3584 | -0.1383 | 0.0647 | 0.032593 | 0.2309 | -0.0581 | 0.0611 | 0.34242 | 0.9622 | NaN | -0.0465 | 0.036 | 0.195603 | 0.9708 | -0.0572 | 0.0552 | 0.300465 | 0.9835 | -0.0341 | 0.048 | 0.47694 | 0.9967 | NaN | -0.0783 | 0.0443 | 0.07722 | 0.7496 | -0.1186 | 0.0647 | 0.066803 | 0.3895 | -0.0435 | 0.0612 | 0.477143 | 0.8651 |
| Methyl 8-2-2-formyl-vinyl-3-hydroxy-5-oxo-cyclopentyl]-octanoate | 310.1761 | 17.698135 | Lipid | Fatty Acid, Dicarboxylate | 0.014 | 0.0832 | 0.866682 | 0.9457 | 0.0654 | 0.1314 | 0.618896 | 0.8589 | -0.019 | 0.1088 | 0.86147 | 0.9597 | NaN | 0.0369 | 0.077 | 0.632163 | 0.9159 | 0.0647 | 0.1153 | 0.574421 | 0.8172 | 0.0189 | 0.1025 | 0.854119 | 0.9708 | NaN | 0.0283 | 0.0585 | 0.628195 | 0.9288 | 0.1 | 0.0914 | 0.273773 | 0.7263 | 0.0061 | 0.0771 | 0.937328 | 0.9766 | NaN | 0.0183 | 0.0437 | 0.676087 | 0.846 | -0.0815 | 0.0707 | 0.249359 | 0.5603 | 0.0656 | 0.0558 | 0.239446 | 0.9622 | NaN | 0.0174 | 0.0351 | 0.619396 | 0.9708 | -0.0146 | 0.0587 | 0.803563 | 0.9977 | 0.0428 | 0.0439 | 0.329059 | 0.9967 | NaN | -0.0005 | 0.0434 | 0.99141 | 0.9972 | -0.115 | 0.0699 | 0.100049 | 0.438 | 0.061 | 0.0559 | 0.275106 | 0.7921 |
| FA 11:3 (DiC, diOH) | 242.077 | 2.402914 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | 0.0433 | 0.0857 | 0.613439 | 0.8736 | 0.0174 | 0.1401 | 0.901317 | 0.9573 | 0.0296 | 0.1093 | 0.786305 | 0.9451 | NaN | 0.0801 | 0.0793 | 0.312353 | 0.6816 | 0.0508 | 0.123 | 0.679264 | 0.8726 | 0.0677 | 0.1028 | 0.509768 | 0.8742 | NaN | -0.0586 | 0.0606 | 0.333155 | 0.7904 | 0.1061 | 0.0976 | 0.277162 | 0.7263 | -0.1688 | 0.078 | 0.030409 | 0.3354 | NaN | -0.0313 | 0.0451 | 0.487983 | 0.7545 | -0.1658 | 0.0741 | 0.025244 | 0.2177 | 0.0473 | 0.056 | 0.398573 | 0.9735 | NaN | -0.0097 | 0.0362 | 0.788583 | 0.9722 | -0.0062 | 0.0623 | 0.920553 | 0.9977 | -0.0164 | 0.0442 | 0.711203 | 0.9967 | NaN | -0.0001 | 0.0448 | 0.998856 | 0.9989 | -0.157 | 0.0736 | 0.032891 | 0.2981 | 0.0928 | 0.0557 | 0.095582 | 0.7232 |
| FA 13:3 (DiC, diOH) | 270.1081 | 7.462934 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0578 | 0.0846 | 0.494095 | 0.8017 | 0.027 | 0.1343 | 0.840877 | 0.9453 | -0.1162 | 0.1076 | 0.280124 | 0.6622 | NaN | -0.1048 | 0.0783 | 0.181055 | 0.5432 | -0.1068 | 0.12 | 0.373428 | 0.7136 | -0.1361 | 0.1007 | 0.176621 | 0.6632 | NaN | -0.1238 | 0.0591 | 0.036153 | 0.344 | -0.0696 | 0.0941 | 0.459143 | 0.7964 | -0.1545 | 0.0752 | 0.040016 | 0.3772 | NaN | 0.0559 | 0.0446 | 0.210213 | 0.5203 | 0.017 | 0.072 | 0.813433 | 0.8934 | 0.079 | 0.0562 | 0.159785 | 0.9514 | NaN | -0.0091 | 0.0357 | 0.798765 | 0.9722 | 0.0528 | 0.0595 | 0.375351 | 0.9977 | -0.0492 | 0.0435 | 0.257882 | 0.9967 | NaN | 0.0446 | 0.0443 | 0.31372 | 0.7708 | 0.0165 | 0.0714 | 0.816984 | 0.9093 | 0.0603 | 0.0563 | 0.284013 | 0.7999 |
| FA 14:3 (DiC, diOH) | 284.1241 | 8.084486 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.091 | 0.0835 | 0.275813 | 0.6386 | -0.0045 | 0.1362 | 0.973652 | 0.9839 | -0.1288 | 0.1078 | 0.232125 | 0.596 | NaN | -0.0872 | 0.0772 | 0.25855 | 0.6275 | -0.0057 | 0.1196 | 0.962211 | 0.9835 | -0.118 | 0.1012 | 0.243276 | 0.6818 | NaN | -0.045 | 0.0589 | 0.445159 | 0.8554 | 0.0668 | 0.0952 | 0.482553 | 0.8009 | -0.0945 | 0.0764 | 0.215955 | 0.6205 | NaN | 0.0485 | 0.0443 | 0.273879 | 0.5828 | 0.006 | 0.0731 | 0.934614 | 0.9554 | 0.0628 | 0.0565 | 0.266769 | 0.9622 | NaN | 0.0126 | 0.0355 | 0.722435 | 0.971 | 0.0206 | 0.0606 | 0.733506 | 0.9977 | 0.0134 | 0.0442 | 0.761202 | 0.9967 | NaN | 0.0315 | 0.044 | 0.4734 | 0.8239 | -0.0574 | 0.0723 | 0.427121 | 0.7185 | 0.0806 | 0.0566 | 0.154601 | 0.7294 |
| FA 16:3 (DiC, diOH) | 312.1554 | 12.519212 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | 0.1009 | 0.0807 | 0.210999 | 0.5594 | 0.071 | 0.1146 | 0.535766 | 0.8052 | 0.1071 | 0.1136 | 0.345738 | 0.7068 | NaN | 0.1506 | 0.0746 | 0.043491 | 0.3118 | 0.0908 | 0.1004 | 0.366 | 0.7116 | 0.1779 | 0.107 | 0.096399 | 0.5686 | NaN | 0.0577 | 0.0569 | 0.310494 | 0.782 | 0.03 | 0.0802 | 0.708506 | 0.8816 | 0.0855 | 0.0804 | 0.287245 | 0.6745 | NaN | 0.0588 | 0.0424 | 0.165528 | 0.5067 | 0.0925 | 0.0609 | 0.128298 | 0.4016 | 0.0234 | 0.0588 | 0.690098 | 0.9994 | NaN | 0.063 | 0.0339 | 0.062973 | 0.9656 | 0.0119 | 0.0512 | 0.815888 | 0.9977 | 0.1104 | 0.0448 | 0.01384 | 0.6366 | NaN | 0.0756 | 0.0419 | 0.071639 | 0.7496 | 0.1206 | 0.0599 | 0.044004 | 0.3175 | 0.031 | 0.0588 | 0.597917 | 0.9367 |
| FA 17:3 (DiC, diOH) | 326.1711 | 14.668848 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.1554 | 0.083 | 0.061117 | 0.2974 | -0.241 | 0.1262 | 0.056117 | 0.2819 | -0.0854 | 0.1103 | 0.439013 | 0.7481 | NaN | -0.095 | 0.0779 | 0.22267 | 0.5873 | -0.1114 | 0.1152 | 0.333529 | 0.6989 | -0.0409 | 0.1043 | 0.694987 | 0.9182 | NaN | -0.0642 | 0.0591 | 0.276886 | 0.7604 | -0.0307 | 0.0923 | 0.739552 | 0.8816 | -0.0698 | 0.0781 | 0.371519 | 0.7398 | NaN | -0.0179 | 0.0444 | 0.686483 | 0.8515 | -0.1255 | 0.0682 | 0.065477 | 0.2844 | 0.0487 | 0.0572 | 0.394623 | 0.9735 | NaN | 0.0262 | 0.0357 | 0.463436 | 0.9708 | -0.0263 | 0.0582 | 0.65167 | 0.9977 | 0.0689 | 0.0447 | 0.123155 | 0.9967 | NaN | -0.0112 | 0.0441 | 0.79903 | 0.9482 | -0.1573 | 0.0667 | 0.018307 | 0.2716 | 0.0896 | 0.0572 | 0.1172 | 0.7232 |
| FA 18:3 (DiC, diOH) | 340.186 | 14.15057 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.1032 | 0.0821 | 0.208962 | 0.5594 | -0.0662 | 0.132 | 0.616197 | 0.8589 | -0.1166 | 0.1065 | 0.273423 | 0.6562 | NaN | -0.1012 | 0.0759 | 0.182596 | 0.5448 | -0.0406 | 0.1161 | 0.726185 | 0.8829 | -0.1155 | 0.0998 | 0.247248 | 0.6818 | NaN | -0.033 | 0.0582 | 0.57105 | 0.9163 | 0.0807 | 0.0931 | 0.38644 | 0.7775 | -0.0832 | 0.0755 | 0.270031 | 0.6654 | NaN | 0.0428 | 0.0437 | 0.327675 | 0.6369 | -0.054 | 0.0707 | 0.44482 | 0.7003 | 0.0952 | 0.0556 | 0.087142 | 0.8712 | NaN | 0.004 | 0.0349 | 0.908204 | 0.9722 | -0.0266 | 0.0588 | 0.650388 | 0.9977 | 0.0287 | 0.0436 | 0.510072 | 0.9967 | NaN | 0.0206 | 0.0433 | 0.634255 | 0.8685 | -0.1221 | 0.0693 | 0.078142 | 0.3895 | 0.1081 | 0.0557 | 0.052203 | 0.702 |
| FA 19:3 (DiC, diOH) | 354.2024 | 16.772755 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0826 | 0.0838 | 0.324032 | 0.6827 | -0.0944 | 0.1367 | 0.490154 | 0.7888 | -0.0694 | 0.1065 | 0.514454 | 0.8041 | NaN | -0.0345 | 0.0781 | 0.658348 | 0.9303 | -0.0126 | 0.1213 | 0.917351 | 0.9682 | -0.0264 | 0.1007 | 0.793509 | 0.9535 | NaN | 0.0038 | 0.0594 | 0.948492 | 0.997 | 0.0644 | 0.0968 | 0.505796 | 0.8105 | -0.0126 | 0.0758 | 0.868359 | 0.9625 | NaN | 0.0063 | 0.0443 | 0.886341 | 0.9579 | -0.1324 | 0.0723 | 0.066989 | 0.2844 | 0.0791 | 0.055 | 0.150192 | 0.9514 | NaN | 0.0176 | 0.0355 | 0.620809 | 0.9708 | -0.0177 | 0.0611 | 0.771846 | 0.9977 | 0.0424 | 0.0432 | 0.326223 | 0.9967 | NaN | -0.0195 | 0.0439 | 0.657136 | 0.8716 | -0.1795 | 0.0708 | 0.011213 | 0.265 | 0.068 | 0.0551 | 0.217204 | 0.7294 |
| FA 20:3 (DiC, diOH) | 368.2165 | 17.202263 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0091 | 0.0831 | 0.913199 | 0.9586 | 0.1466 | 0.1304 | 0.261168 | 0.5698 | -0.0963 | 0.1072 | 0.369285 | 0.7082 | NaN | -0.0545 | 0.0771 | 0.479578 | 0.7902 | 0.0465 | 0.1167 | 0.690306 | 0.8728 | -0.1225 | 0.1005 | 0.222615 | 0.6714 | NaN | -0.0569 | 0.0584 | 0.32991 | 0.7884 | 0.0642 | 0.0918 | 0.484591 | 0.8009 | -0.1277 | 0.0753 | 0.089799 | 0.4613 | NaN | 0.0249 | 0.0437 | 0.56783 | 0.8059 | -0.0296 | 0.0713 | 0.67833 | 0.8471 | 0.0542 | 0.0558 | 0.330784 | 0.9622 | NaN | -0.0095 | 0.035 | 0.785474 | 0.9722 | -0.0136 | 0.059 | 0.817277 | 0.9977 | -0.0052 | 0.0436 | 0.906043 | 0.9967 | NaN | 0.01 | 0.0433 | 0.816777 | 0.9499 | -0.0699 | 0.0708 | 0.323523 | 0.6453 | 0.0568 | 0.0558 | 0.30878 | 0.8042 |
| FA 21:3 (DiC, diOH) | 382.2322 | 19.090963 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0558 | 0.0722 | 0.439474 | 0.7653 | -0.1108 | 0.1085 | 0.307176 | 0.6351 | -0.0063 | 0.0967 | 0.947666 | 0.9916 | NaN | -0.0309 | 0.067 | 0.644287 | 0.9286 | -0.0878 | 0.0954 | 0.357598 | 0.7021 | 0.0244 | 0.091 | 0.788268 | 0.9535 | NaN | -0.0241 | 0.0509 | 0.635089 | 0.9288 | 0.0585 | 0.0779 | 0.452182 | 0.7964 | -0.069 | 0.0684 | 0.313256 | 0.6892 | NaN | -0.0191 | 0.038 | 0.615532 | 0.8244 | -0.1678 | 0.0561 | 0.002763 | 0.1525 | 0.0856 | 0.0493 | 0.082714 | 0.8712 | NaN | -0.005 | 0.0305 | 0.86891 | 0.9722 | -0.0689 | 0.0481 | 0.151776 | 0.8645 | 0.0478 | 0.0389 | 0.218639 | 0.9967 | NaN | -0.0062 | 0.0378 | 0.868718 | 0.9644 | -0.1609 | 0.0557 | 0.003909 | 0.2424 | 0.1076 | 0.0491 | 0.028524 | 0.6979 |
| FA 8:0 (Dic, OH) | 190.0842 | 3.548903 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0174 | 0.0923 | 0.850684 | 0.9457 | 0.0248 | 0.1319 | 0.850952 | 0.9493 | -0.0503 | 0.1277 | 0.693428 | 0.8959 | NaN | -0.042 | 0.0854 | 0.622906 | 0.9049 | -0.0313 | 0.1162 | 0.787767 | 0.9213 | -0.0637 | 0.1197 | 0.594776 | 0.8877 | NaN | -0.0956 | 0.0648 | 0.140293 | 0.6296 | -0.0477 | 0.0923 | 0.605173 | 0.8395 | -0.1401 | 0.0899 | 0.119131 | 0.5098 | NaN | 0.0835 | 0.0484 | 0.084059 | 0.407 | 0.0963 | 0.0702 | 0.169801 | 0.4506 | 0.0709 | 0.0657 | 0.280551 | 0.9622 | NaN | 0.0119 | 0.0389 | 0.75977 | 0.9722 | -0.0114 | 0.0587 | 0.845443 | 0.9977 | 0.0337 | 0.0516 | 0.513391 | 0.9967 | NaN | 0.0635 | 0.0481 | 0.186673 | 0.7516 | 0.0152 | 0.0701 | 0.828397 | 0.9165 | 0.1091 | 0.0656 | 0.095982 | 0.7232 |
| FA 9:0 (DiC,OH) | 204.1001 | 5.214559 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0436 | 0.0844 | 0.605389 | 0.8708 | 0.0997 | 0.1359 | 0.463483 | 0.7592 | 0.0066 | 0.1066 | 0.950949 | 0.9916 | NaN | 0.0145 | 0.0782 | 0.853294 | 0.9933 | 0.0549 | 0.1198 | 0.646537 | 0.8459 | -0.0165 | 0.1001 | 0.868916 | 0.9708 | NaN | -0.0306 | 0.0596 | 0.608034 | 0.9199 | 0.0703 | 0.095 | 0.459147 | 0.7964 | -0.091 | 0.0756 | 0.228479 | 0.6205 | NaN | -0.0035 | 0.0444 | 0.937232 | 0.9731 | -0.0667 | 0.0736 | 0.364461 | 0.659 | 0.0323 | 0.0547 | 0.555397 | 0.9885 | NaN | -0.0124 | 0.0356 | 0.728379 | 0.971 | -0.0166 | 0.0609 | 0.784936 | 0.9977 | -0.0105 | 0.0431 | 0.808189 | 0.9967 | NaN | 0.0098 | 0.0441 | 0.823748 | 0.9529 | -0.0535 | 0.073 | 0.463696 | 0.7446 | 0.0462 | 0.0547 | 0.398998 | 0.8439 |
| FA 10:0 (DiC,OH) | 218.1156 | 9.113856 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1673 | 0.0826 | 0.04288 | 0.2367 | 0.3576 | 0.1317 | 0.006609 | 0.1275 | 0.0636 | 0.1047 | 0.543358 | 0.8195 | NaN | 0.1194 | 0.0772 | 0.122068 | 0.4437 | 0.2567 | 0.1188 | 0.030684 | 0.3624 | 0.0335 | 0.0987 | 0.734393 | 0.9342 | NaN | 0.0013 | 0.0599 | 0.983213 | 0.9992 | 0.1817 | 0.0954 | 0.056891 | 0.499 | -0.0998 | 0.0753 | 0.185384 | 0.5977 | NaN | 0.0483 | 0.0441 | 0.272646 | 0.5828 | 0.0462 | 0.0761 | 0.544303 | 0.7679 | 0.0445 | 0.0538 | 0.407565 | 0.9735 | NaN | 0.0217 | 0.0355 | 0.540013 | 0.9708 | 0.0448 | 0.0628 | 0.47569 | 0.9977 | 0.0104 | 0.0424 | 0.806178 | 0.9967 | NaN | 0.0537 | 0.0437 | 0.219111 | 0.7516 | 0.0239 | 0.076 | 0.75334 | 0.884 | 0.0671 | 0.0536 | 0.210997 | 0.7294 |
| FA 11:0 (DiC,OH) | 232.131 | 10.740578 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1034 | 0.0828 | 0.211807 | 0.5594 | 0.2695 | 0.1492 | 0.070866 | 0.3039 | 0.0391 | 0.0991 | 0.693507 | 0.8959 | NaN | 0.0753 | 0.0768 | 0.326635 | 0.6998 | 0.2209 | 0.1316 | 0.093134 | 0.4459 | 0.0205 | 0.0932 | 0.825729 | 0.9616 | NaN | -0.0107 | 0.059 | 0.855817 | 0.9805 | 0.1846 | 0.1046 | 0.077785 | 0.549 | -0.0852 | 0.0708 | 0.228939 | 0.6205 | NaN | 0.0382 | 0.0437 | 0.382426 | 0.6745 | -0.0223 | 0.0836 | 0.789438 | 0.8867 | 0.0545 | 0.0507 | 0.282792 | 0.9622 | NaN | 0.0199 | 0.0351 | 0.570846 | 0.9708 | 0.021 | 0.0687 | 0.759797 | 0.9977 | 0.0213 | 0.04 | 0.594098 | 0.9967 | NaN | 0.041 | 0.0433 | 0.343816 | 0.7759 | -0.0748 | 0.0834 | 0.370028 | 0.6653 | 0.082 | 0.0505 | 0.104655 | 0.7232 |
| FA 12:0 (DiC,OH) | 246.1469 | 12.772049 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0147 | 0.085 | 0.862782 | 0.9457 | 0.0842 | 0.1395 | 0.546153 | 0.8065 | -0.0613 | 0.109 | 0.57424 | 0.8352 | NaN | -0.0129 | 0.0786 | 0.869884 | 0.9933 | 0.096 | 0.1223 | 0.432611 | 0.7515 | -0.0552 | 0.1023 | 0.589375 | 0.8877 | NaN | -0.0082 | 0.0598 | 0.89139 | 0.9865 | 0.1485 | 0.0967 | 0.124379 | 0.577 | -0.0778 | 0.077 | 0.312145 | 0.6892 | NaN | 0.0265 | 0.0447 | 0.552785 | 0.7987 | -0.0588 | 0.0753 | 0.434695 | 0.6955 | 0.0608 | 0.0563 | 0.279699 | 0.9622 | NaN | 0.0272 | 0.0358 | 0.447402 | 0.9708 | 0.0049 | 0.0623 | 0.937346 | 0.9977 | 0.0467 | 0.0441 | 0.289443 | 0.9967 | NaN | 0.0139 | 0.0444 | 0.753734 | 0.9221 | -0.1305 | 0.0744 | 0.079377 | 0.3895 | 0.088 | 0.0562 | 0.117543 | 0.7232 |
| FA 13:0 (DiC,OH) | 260.1627 | 14.14954 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0144 | 0.0841 | 0.863743 | 0.9457 | 0.1057 | 0.1359 | 0.436624 | 0.7348 | -0.0752 | 0.1095 | 0.492491 | 0.788 | NaN | -0.0149 | 0.0778 | 0.847684 | 0.9933 | 0.1163 | 0.119 | 0.328513 | 0.6975 | -0.0712 | 0.1027 | 0.488018 | 0.8579 | NaN | 0.0034 | 0.0592 | 0.953667 | 0.997 | 0.148 | 0.0941 | 0.115792 | 0.577 | -0.0613 | 0.0775 | 0.429 | 0.7865 | NaN | 0.0481 | 0.0442 | 0.275881 | 0.5835 | -0.0173 | 0.0735 | 0.814093 | 0.8934 | 0.0737 | 0.0566 | 0.193293 | 0.9514 | NaN | 0.0372 | 0.0354 | 0.293564 | 0.9708 | 0.0247 | 0.0607 | 0.684273 | 0.9977 | 0.0533 | 0.0444 | 0.229382 | 0.9967 | NaN | 0.0321 | 0.0439 | 0.463865 | 0.8239 | -0.0783 | 0.073 | 0.283555 | 0.6236 | 0.0917 | 0.0566 | 0.105535 | 0.7232 |
| FA 14:0 (DiC,OH) | 274.1783 | 15.688103 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0985 | 0.0806 | 0.221339 | 0.5715 | 0.0376 | 0.1456 | 0.796179 | 0.9222 | -0.139 | 0.0978 | 0.155252 | 0.5163 | NaN | -0.1127 | 0.0744 | 0.130019 | 0.4437 | 0.0371 | 0.1277 | 0.771769 | 0.9103 | -0.1531 | 0.0915 | 0.094112 | 0.5647 | NaN | -0.0168 | 0.0572 | 0.76862 | 0.9513 | 0.0795 | 0.1015 | 0.433502 | 0.7964 | -0.0505 | 0.0703 | 0.472731 | 0.8005 | NaN | -0.0054 | 0.0427 | 0.899303 | 0.9579 | -0.0285 | 0.0781 | 0.715736 | 0.8608 | -0.0018 | 0.0514 | 0.972768 | 0.9994 | NaN | -0.0128 | 0.0342 | 0.708112 | 0.971 | -0.019 | 0.0648 | 0.769012 | 0.9977 | -0.0071 | 0.0403 | 0.860509 | 0.9967 | NaN | -0.0324 | 0.0422 | 0.44356 | 0.8178 | -0.0706 | 0.0774 | 0.36179 | 0.6653 | -0.0217 | 0.0512 | 0.672115 | 0.9564 |
| FA 15:0 (Dic, OH) | 288.1942 | 17.041286 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0867 | 0.0834 | 0.298506 | 0.6636 | 0.0418 | 0.1284 | 0.744701 | 0.9196 | -0.1762 | 0.1132 | 0.11972 | 0.4621 | NaN | -0.0667 | 0.0773 | 0.388482 | 0.7434 | 0.0253 | 0.1128 | 0.822418 | 0.9389 | -0.1338 | 0.1072 | 0.212152 | 0.6714 | NaN | -0.0122 | 0.0591 | 0.836104 | 0.9805 | 0.0515 | 0.0896 | 0.565074 | 0.8252 | -0.0311 | 0.0823 | 0.705252 | 0.9096 | NaN | 0.0248 | 0.0442 | 0.57457 | 0.8059 | 0.0176 | 0.0689 | 0.798159 | 0.8869 | 0.0061 | 0.0598 | 0.91921 | 0.9994 | NaN | 0.0204 | 0.0354 | 0.564299 | 0.9708 | 0.0006 | 0.0572 | 0.991456 | 0.9977 | 0.0448 | 0.047 | 0.341254 | 0.9967 | NaN | 0.0041 | 0.0438 | 0.925246 | 0.9724 | -0.0447 | 0.0684 | 0.513292 | 0.7783 | 0.025 | 0.0601 | 0.676779 | 0.9564 |
| FA 16:0 (DiC,OH) | 302.2097 | 18.320814 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0088 | 0.0825 | 0.91523 | 0.9586 | 0.1855 | 0.127 | 0.144335 | 0.415 | -0.0991 | 0.1105 | 0.369762 | 0.7082 | NaN | -0.0085 | 0.0763 | 0.911485 | 0.9933 | 0.1291 | 0.1125 | 0.251044 | 0.6132 | -0.0973 | 0.1036 | 0.347812 | 0.7619 | NaN | -0.0172 | 0.0581 | 0.766388 | 0.9507 | 0.144 | 0.0886 | 0.104065 | 0.577 | -0.1111 | 0.0778 | 0.153644 | 0.5522 | NaN | 0.0683 | 0.0432 | 0.113875 | 0.4618 | 0.0153 | 0.0698 | 0.825989 | 0.9029 | 0.0954 | 0.0574 | 0.096279 | 0.8712 | NaN | 0.0301 | 0.0347 | 0.385685 | 0.9708 | 0.0406 | 0.0575 | 0.480116 | 0.9977 | 0.0306 | 0.0451 | 0.497697 | 0.9967 | NaN | 0.0522 | 0.0429 | 0.224319 | 0.7516 | -0.0337 | 0.0697 | 0.629137 | 0.8191 | 0.1082 | 0.0574 | 0.059473 | 0.702 |
| FA 17:0 (DiC,OH) | 316.2246 | 19.429361 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.111 | 0.0837 | 0.184744 | 0.5203 | 0.3009 | 0.1349 | 0.02571 | 0.2208 | 0.014 | 0.1059 | 0.894742 | 0.98 | NaN | 0.0637 | 0.078 | 0.413969 | 0.7542 | 0.2045 | 0.1211 | 0.091355 | 0.4459 | -0.0156 | 0.0996 | 0.875669 | 0.9745 | NaN | -0.034 | 0.0599 | 0.570924 | 0.9163 | 0.1556 | 0.0965 | 0.106891 | 0.577 | -0.1352 | 0.0753 | 0.072321 | 0.4537 | NaN | 0.0669 | 0.044 | 0.127903 | 0.4803 | 0.0147 | 0.0766 | 0.847383 | 0.919 | 0.0897 | 0.0539 | 0.096298 | 0.8712 | NaN | 0.0319 | 0.0354 | 0.367638 | 0.9708 | 0.0591 | 0.0625 | 0.344985 | 0.9977 | 0.02 | 0.0428 | 0.640446 | 0.9967 | NaN | 0.0705 | 0.0436 | 0.106051 | 0.7516 | -0.0103 | 0.0764 | 0.892556 | 0.9587 | 0.1123 | 0.0538 | 0.036675 | 0.6979 |
| FA 18:0 (DiC,OH) | 330.2409 | 20.418041 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0949 | 0.0832 | 0.254352 | 0.6104 | 0.2793 | 0.1349 | 0.038443 | 0.2428 | 0.0004 | 0.1046 | 0.997045 | 0.997 | NaN | 0.049 | 0.0776 | 0.527677 | 0.8346 | 0.1715 | 0.1217 | 0.158795 | 0.5063 | -0.0256 | 0.0983 | 0.794571 | 0.9535 | NaN | -0.0575 | 0.0596 | 0.334706 | 0.7904 | 0.1419 | 0.0963 | 0.140479 | 0.5905 | -0.1683 | 0.074 | 0.022972 | 0.3251 | NaN | 0.0597 | 0.0437 | 0.172066 | 0.5115 | 0.0184 | 0.076 | 0.808559 | 0.8909 | 0.0789 | 0.0534 | 0.139528 | 0.9514 | NaN | 0.0341 | 0.0352 | 0.331986 | 0.9708 | 0.069 | 0.0619 | 0.265305 | 0.9821 | 0.0169 | 0.0422 | 0.689294 | 0.9967 | NaN | 0.0693 | 0.0433 | 0.10964 | 0.7516 | -0.0019 | 0.0757 | 0.980396 | 0.9974 | 0.1074 | 0.0532 | 0.043599 | 0.6979 |
| FA 10:1 (DiC, OH) | 216.1 | 4.325327 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1118 | 0.0851 | 0.188964 | 0.5295 | 0.3628 | 0.1534 | 0.018039 | 0.1879 | 0.0091 | 0.1015 | 0.928545 | 0.9914 | NaN | 0.0697 | 0.0792 | 0.37913 | 0.7403 | 0.2766 | 0.1367 | 0.043042 | 0.4171 | -0.0174 | 0.0954 | 0.855309 | 0.9708 | NaN | -0.0214 | 0.0608 | 0.725206 | 0.9415 | 0.2145 | 0.1091 | 0.049336 | 0.4695 | -0.1087 | 0.072 | 0.131225 | 0.5272 | NaN | 0.0724 | 0.0447 | 0.105144 | 0.4581 | 0.0365 | 0.0874 | 0.675743 | 0.8471 | 0.0795 | 0.0518 | 0.12443 | 0.9514 | NaN | 0.031 | 0.0361 | 0.390033 | 0.9708 | 0.1148 | 0.0705 | 0.103325 | 0.7937 | -0.001 | 0.041 | 0.981469 | 0.9967 | NaN | 0.0788 | 0.0443 | 0.074944 | 0.7496 | -0.012 | 0.0876 | 0.891281 | 0.9587 | 0.1107 | 0.0515 | 0.031493 | 0.6979 |
| FA 11:1 (DiC, OH) | 230.1147 | 5.828099 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0625 | 0.0863 | 0.46926 | 0.7858 | 0.2712 | 0.1468 | 0.064605 | 0.2923 | -0.0324 | 0.1053 | 0.757964 | 0.9339 | NaN | 0.0258 | 0.0802 | 0.747449 | 0.964 | 0.1797 | 0.131 | 0.170048 | 0.5189 | -0.0541 | 0.0988 | 0.583718 | 0.8877 | NaN | -0.0337 | 0.0611 | 0.581193 | 0.9166 | 0.1783 | 0.1032 | 0.083861 | 0.549 | -0.1387 | 0.0741 | 0.061182 | 0.4338 | NaN | 0.0153 | 0.0455 | 0.736349 | 0.8848 | -0.0609 | 0.0828 | 0.461903 | 0.7154 | 0.0508 | 0.0541 | 0.347735 | 0.9622 | NaN | 0.0268 | 0.0364 | 0.461795 | 0.9708 | 0.0593 | 0.0671 | 0.376854 | 0.9977 | 0.0114 | 0.0426 | 0.787962 | 0.9967 | NaN | 0.0276 | 0.0451 | 0.54095 | 0.8373 | -0.0799 | 0.0823 | 0.331804 | 0.6453 | 0.0778 | 0.0541 | 0.150173 | 0.7294 |
| FA 11:1 (DiC,OH) | 244.1289 | 6.840248 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0855 | 0.0824 | 0.299175 | 0.6636 | 0.0806 | 0.1332 | 0.545021 | 0.8065 | 0.0871 | 0.1044 | 0.403915 | 0.7334 | NaN | 0.0617 | 0.0764 | 0.419302 | 0.7614 | 0.1169 | 0.1167 | 0.316549 | 0.6852 | 0.0522 | 0.0985 | 0.59619 | 0.8877 | NaN | -0.0082 | 0.0585 | 0.888166 | 0.9865 | 0.1312 | 0.0924 | 0.155634 | 0.6093 | -0.0851 | 0.0756 | 0.260126 | 0.6468 | NaN | -0.0132 | 0.0436 | 0.762156 | 0.8918 | -0.1598 | 0.0714 | 0.02514 | 0.2177 | 0.0624 | 0.0535 | 0.243673 | 0.9622 | NaN | 0.005 | 0.0349 | 0.886189 | 0.9722 | -0.0092 | 0.0595 | 0.876955 | 0.9977 | 0.0154 | 0.0424 | 0.716939 | 0.9967 | NaN | -0.0037 | 0.0433 | 0.931724 | 0.9741 | -0.2002 | 0.0702 | 0.004384 | 0.2424 | 0.1024 | 0.053 | 0.053349 | 0.702 |
| FA 14:1 (DiC, OH) | 272.1624 | 12.077606 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0645 | 0.0838 | 0.442032 | 0.7673 | -0.0205 | 0.1419 | 0.884998 | 0.9558 | -0.0793 | 0.105 | 0.450206 | 0.7531 | NaN | -0.0574 | 0.0776 | 0.458959 | 0.7771 | -0.0184 | 0.1245 | 0.882336 | 0.9494 | -0.066 | 0.0986 | 0.503416 | 0.8742 | NaN | -0.0198 | 0.0591 | 0.738268 | 0.9415 | 0.0704 | 0.0993 | 0.477937 | 0.8009 | -0.0488 | 0.0745 | 0.512631 | 0.826 | NaN | 0.0387 | 0.0443 | 0.382469 | 0.6745 | -0.0362 | 0.076 | 0.633735 | 0.8117 | 0.0671 | 0.0544 | 0.217557 | 0.9519 | NaN | 0.0138 | 0.0355 | 0.69757 | 0.971 | 0.0163 | 0.0631 | 0.796593 | 0.9977 | 0.0167 | 0.0427 | 0.695058 | 0.9967 | NaN | 0.0143 | 0.0439 | 0.744642 | 0.9216 | -0.1122 | 0.0748 | 0.133567 | 0.4915 | 0.0748 | 0.0545 | 0.169793 | 0.7294 |
| 3-methyladipic acid | 160.0736 | 5.688393 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.1902 | 0.087 | 0.028785 | 0.207 | 0.3214 | 0.133 | 0.015634 | 0.1765 | 0.0924 | 0.1138 | 0.416836 | 0.7446 | NaN | 0.1226 | 0.0818 | 0.134157 | 0.4462 | 0.1673 | 0.1232 | 0.174335 | 0.523 | 0.0498 | 0.1075 | 0.643128 | 0.8939 | NaN | -0.0611 | 0.0643 | 0.341893 | 0.793 | 0.0652 | 0.0992 | 0.510796 | 0.8105 | -0.1622 | 0.0829 | 0.050499 | 0.3872 | NaN | 0.1092 | 0.0458 | 0.017012 | 0.3584 | 0.1778 | 0.0718 | 0.013272 | 0.1826 | 0.0686 | 0.0583 | 0.239448 | 0.9622 | NaN | 0.0267 | 0.0375 | 0.476464 | 0.9708 | 0.0625 | 0.0621 | 0.314079 | 0.9977 | 0.0003 | 0.0463 | 0.99568 | 0.9967 | NaN | 0.1122 | 0.0454 | 0.013369 | 0.7271 | 0.1438 | 0.0723 | 0.046764 | 0.3227 | 0.0958 | 0.058 | 0.098538 | 0.7232 |
| LL-2,6-diaminoheptanedioate | 190.0948 | 0.684274 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.0472 | 0.0914 | 0.605784 | 0.8708 | 0.0958 | 0.1342 | 0.475246 | 0.7739 | -0.0057 | 0.1236 | 0.962934 | 0.9916 | NaN | 0.0196 | 0.0847 | 0.817274 | 0.9803 | -0.028 | 0.1204 | 0.816151 | 0.9349 | 0.0022 | 0.116 | 0.984797 | 0.9993 | NaN | 0.0425 | 0.0643 | 0.50794 | 0.8921 | 0.081 | 0.0936 | 0.38716 | 0.7775 | 0.0158 | 0.0876 | 0.856375 | 0.9569 | NaN | 0.074 | 0.0478 | 0.121468 | 0.4656 | 0.0741 | 0.0718 | 0.301889 | 0.6082 | 0.0692 | 0.0633 | 0.27437 | 0.9622 | NaN | -0.0075 | 0.0386 | 0.845196 | 0.9722 | -0.0772 | 0.06 | 0.198429 | 0.9357 | 0.0467 | 0.0498 | 0.348081 | 0.9967 | NaN | 0.0345 | 0.0477 | 0.4685 | 0.8239 | 0.0326 | 0.0716 | 0.649216 | 0.8334 | 0.0322 | 0.0636 | 0.612557 | 0.9393 |
| 2-methylmaleate | 130.0277 | 1.828859 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.0709 | 0.0854 | 0.406499 | 0.7391 | 0.0798 | 0.1222 | 0.513621 | 0.8001 | 0.0745 | 0.1183 | 0.528682 | 0.8099 | NaN | 0.0553 | 0.0791 | 0.48416 | 0.7907 | 0.0736 | 0.1072 | 0.492478 | 0.7769 | 0.0539 | 0.1112 | 0.627675 | 0.8939 | NaN | 0.0004 | 0.0604 | 0.995324 | 0.9992 | 0.0281 | 0.0856 | 0.742831 | 0.8816 | -0.0257 | 0.0845 | 0.761355 | 0.9437 | NaN | 0.0846 | 0.0446 | 0.057776 | 0.3995 | 0.0598 | 0.0654 | 0.360536 | 0.659 | 0.1083 | 0.0601 | 0.071432 | 0.8712 | NaN | 0.0345 | 0.036 | 0.338124 | 0.9708 | 0.0438 | 0.0543 | 0.420569 | 0.9977 | 0.028 | 0.0479 | 0.558632 | 0.9967 | NaN | 0.0948 | 0.0442 | 0.031877 | 0.7271 | 0.0554 | 0.0649 | 0.393363 | 0.687 | 0.1322 | 0.0598 | 0.026978 | 0.6979 |
| Keto 14:0 | 242.1884 | 20.796713 | Lipid | Fatty Acid, Keto | -0.0903 | 0.0871 | 0.300022 | 0.6636 | -0.0208 | 0.1278 | 0.870464 | 0.9553 | -0.133 | 0.1181 | 0.259997 | 0.6326 | NaN | 0.0153 | 0.0828 | 0.853112 | 0.9933 | 0.1054 | 0.1141 | 0.355284 | 0.7021 | -0.0341 | 0.1146 | 0.766079 | 0.9436 | NaN | -0.0914 | 0.0611 | 0.134535 | 0.6294 | 0.0433 | 0.0894 | 0.628353 | 0.8438 | -0.2133 | 0.082 | 0.009246 | 0.1838 | NaN | -0.0811 | 0.0456 | 0.075167 | 0.3995 | -0.1209 | 0.0677 | 0.074307 | 0.2979 | -0.0415 | 0.0612 | 0.497505 | 0.988 | NaN | -0.0187 | 0.0369 | 0.612195 | 0.9708 | -0.0012 | 0.0569 | 0.982563 | 0.9977 | -0.0334 | 0.0481 | 0.486915 | 0.9967 | NaN | -0.0714 | 0.0453 | 0.114737 | 0.7516 | -0.1366 | 0.0669 | 0.04135 | 0.3085 | -0.013 | 0.0615 | 0.832336 | 0.9809 |
| Keto 18:0 | 298.2504 | 21.835537 | Lipid | Fatty Acid, Keto | 0.095 | 0.0852 | 0.264819 | 0.6274 | 0.1075 | 0.1287 | 0.403449 | 0.7124 | 0.0845 | 0.1127 | 0.452997 | 0.755 | NaN | 0.1582 | 0.0789 | 0.045029 | 0.3187 | 0.1461 | 0.1126 | 0.194267 | 0.5416 | 0.1556 | 0.1063 | 0.143411 | 0.6249 | NaN | 0.026 | 0.0603 | 0.665844 | 0.9288 | 0.1786 | 0.0886 | 0.043922 | 0.4408 | -0.0972 | 0.0814 | 0.232339 | 0.6205 | NaN | -0.0767 | 0.0452 | 0.089801 | 0.4273 | -0.1588 | 0.0695 | 0.022254 | 0.2149 | -0.0138 | 0.0583 | 0.813558 | 0.9994 | NaN | -0.0093 | 0.0362 | 0.797853 | 0.9722 | -0.0171 | 0.0578 | 0.767145 | 0.9977 | -0.0044 | 0.0458 | 0.923975 | 0.9967 | NaN | -0.0528 | 0.0449 | 0.239476 | 0.7516 | -0.1563 | 0.0689 | 0.023275 | 0.2725 | 0.0239 | 0.0582 | 0.681116 | 0.9564 |
| 5-oxo-7-octenoic acid | 156.0766 | 3.918678 | Lipid | Fatty Acid, Keto | -0.053 | 0.0858 | 0.536578 | 0.8273 | 0.0277 | 0.1272 | 0.82775 | 0.9363 | -0.1362 | 0.1158 | 0.239859 | 0.6101 | NaN | -0.0205 | 0.0796 | 0.797095 | 0.976 | 0.0441 | 0.1116 | 0.692802 | 0.8728 | -0.0907 | 0.1097 | 0.408466 | 0.8024 | NaN | -0.0277 | 0.0604 | 0.647144 | 0.9288 | 0.066 | 0.0887 | 0.457208 | 0.7964 | -0.088 | 0.0823 | 0.284589 | 0.6732 | NaN | 0.0384 | 0.0453 | 0.395848 | 0.685 | 0.0479 | 0.0681 | 0.481382 | 0.732 | 0.0156 | 0.0606 | 0.796583 | 0.9994 | NaN | -0.0149 | 0.0362 | 0.680741 | 0.9708 | 0.0005 | 0.0566 | 0.993353 | 0.9977 | -0.0289 | 0.0472 | 0.540006 | 0.9967 | NaN | 0.0338 | 0.0449 | 0.452338 | 0.8178 | 0.0292 | 0.0676 | 0.665942 | 0.8393 | 0.0271 | 0.0607 | 0.655089 | 0.9541 |
| traumatin | 212.1393 | 14.682874 | Lipid | Fatty Acid, Keto | -0.0098 | 0.09 | 0.913097 | 0.9586 | 0.1549 | 0.1348 | 0.250519 | 0.5535 | -0.1332 | 0.1183 | 0.260137 | 0.6326 | NaN | -0.0318 | 0.0833 | 0.702242 | 0.9341 | 0.0745 | 0.1199 | 0.534435 | 0.7797 | -0.1363 | 0.1108 | 0.218627 | 0.6714 | NaN | -0.0523 | 0.0633 | 0.408705 | 0.8406 | 0.0488 | 0.0953 | 0.608323 | 0.8395 | -0.1323 | 0.0833 | 0.112293 | 0.4999 | NaN | 0.0429 | 0.0473 | 0.364654 | 0.6693 | 0.0605 | 0.0728 | 0.406309 | 0.6798 | 0.033 | 0.0618 | 0.593764 | 0.9994 | NaN | 0.056 | 0.0378 | 0.138189 | 0.9708 | 0.1124 | 0.0593 | 0.058323 | 0.6733 | 0.0113 | 0.0485 | 0.815562 | 0.9967 | NaN | 0.0564 | 0.0469 | 0.229356 | 0.7516 | 0.0617 | 0.0722 | 0.392945 | 0.687 | 0.0549 | 0.062 | 0.376076 | 0.8297 |
| 7-oxo-11E-tetradecenoic acid | 240.1727 | 19.634645 | Lipid | Fatty Acid, Keto | -0.0768 | 0.0877 | 0.380919 | 0.7152 | 0.0041 | 0.1297 | 0.975023 | 0.9839 | -0.1411 | 0.1179 | 0.231488 | 0.596 | NaN | 0.0023 | 0.0824 | 0.97815 | 0.9933 | 0.0712 | 0.1143 | 0.533036 | 0.7797 | -0.0605 | 0.1133 | 0.593061 | 0.8877 | NaN | -0.0927 | 0.0615 | 0.131442 | 0.6201 | 0.0578 | 0.0906 | 0.523265 | 0.8173 | -0.231 | 0.0815 | 0.004599 | 0.1228 | NaN | -0.0681 | 0.0459 | 0.138343 | 0.4828 | -0.141 | 0.0687 | 0.040033 | 0.2511 | 0.002 | 0.0616 | 0.974544 | 0.9994 | NaN | -0.0216 | 0.0371 | 0.560107 | 0.9708 | -0.0191 | 0.0577 | 0.74073 | 0.9977 | -0.0268 | 0.0481 | 0.577145 | 0.9967 | NaN | -0.0631 | 0.0456 | 0.166412 | 0.7516 | -0.1682 | 0.0677 | 0.012963 | 0.265 | 0.0283 | 0.0618 | 0.646744 | 0.9483 |
| 7-oxo-11-hexadecenoic acid | 268.2032 | 21.295565 | Lipid | Fatty Acid, Keto | -0.0187 | 0.0856 | 0.827231 | 0.9415 | -0.0133 | 0.1287 | 0.917996 | 0.967 | -0.0247 | 0.1138 | 0.828334 | 0.9565 | NaN | 0.0614 | 0.0802 | 0.444087 | 0.7757 | 0.0731 | 0.1139 | 0.520633 | 0.7797 | 0.0519 | 0.1084 | 0.632412 | 0.8939 | NaN | -0.0562 | 0.0602 | 0.350414 | 0.793 | 0.0709 | 0.09 | 0.430657 | 0.7964 | -0.166 | 0.0801 | 0.038281 | 0.3772 | NaN | -0.1022 | 0.0446 | 0.021924 | 0.3584 | -0.1894 | 0.0672 | 0.004825 | 0.161 | -0.0294 | 0.0584 | 0.614456 | 0.9994 | NaN | -0.0198 | 0.0361 | 0.583757 | 0.9708 | -0.0246 | 0.0572 | 0.667227 | 0.9977 | -0.018 | 0.0459 | 0.695899 | 0.9967 | NaN | -0.0854 | 0.0444 | 0.054226 | 0.7271 | -0.1982 | 0.0664 | 0.002849 | 0.2424 | 0.0033 | 0.0586 | 0.954605 | 0.996 |
| 7-oxo-11-octadecenoic acid | 296.2354 | 22.077984 | Lipid | Fatty Acid, Keto | 0.015 | 0.085 | 0.859726 | 0.9457 | -0.011 | 0.1314 | 0.933249 | 0.9682 | 0.0496 | 0.1108 | 0.654765 | 0.885 | NaN | 0.0419 | 0.0787 | 0.594629 | 0.8776 | 0.0733 | 0.1161 | 0.527724 | 0.7797 | 0.0564 | 0.1039 | 0.587531 | 0.8877 | NaN | -0.0086 | 0.0598 | 0.885374 | 0.9865 | 0.081 | 0.0919 | 0.377696 | 0.775 | -0.0771 | 0.0792 | 0.329843 | 0.703 | NaN | -0.083 | 0.0445 | 0.062257 | 0.3995 | -0.1445 | 0.0694 | 0.037416 | 0.243 | -0.0347 | 0.0571 | 0.543381 | 0.9885 | NaN | -0.0068 | 0.0358 | 0.84868 | 0.9722 | -0.0131 | 0.0584 | 0.822094 | 0.9977 | -0.0007 | 0.0449 | 0.987598 | 0.9967 | NaN | -0.0497 | 0.0443 | 0.262133 | 0.7516 | -0.1247 | 0.0691 | 0.070988 | 0.3895 | 0.007 | 0.0571 | 0.903127 | 0.9953 |
| C8 H12 N6 O2 | 224.1031 | 13.587468 | Lipid | Fatty Acid, Keto | 0.0543 | 0.0859 | 0.527418 | 0.8201 | 0.0878 | 0.1438 | 0.54119 | 0.8052 | 0.0351 | 0.1065 | 0.741751 | 0.9222 | NaN | 0.0612 | 0.0794 | 0.441016 | 0.7757 | 0.0885 | 0.1261 | 0.482702 | 0.7746 | 0.046 | 0.0999 | 0.64492 | 0.8939 | NaN | 0.007 | 0.0606 | 0.907354 | 0.9918 | 0.124 | 0.0999 | 0.214314 | 0.6538 | -0.0471 | 0.0758 | 0.534183 | 0.826 | NaN | -0.0132 | 0.0453 | 0.770982 | 0.8919 | -0.1516 | 0.0772 | 0.049703 | 0.2517 | 0.051 | 0.0546 | 0.349751 | 0.9622 | NaN | 0.0097 | 0.0363 | 0.789471 | 0.9722 | -0.0175 | 0.0643 | 0.78581 | 0.9977 | 0.0252 | 0.043 | 0.557974 | 0.9967 | NaN | -0.0052 | 0.0449 | 0.907778 | 0.9724 | -0.1638 | 0.0765 | 0.032176 | 0.2981 | 0.0717 | 0.0545 | 0.188088 | 0.7294 |
| 7-oxo-13-tetradecadienoic acid | 238.1186 | 15.035772 | Lipid | Fatty Acid, Keto | -0.1819 | 0.0818 | 0.026224 | 0.193 | -0.1568 | 0.1133 | 0.166448 | 0.4386 | -0.1885 | 0.118 | 0.110168 | 0.4472 | NaN | -0.1286 | 0.0766 | 0.093212 | 0.3985 | -0.0531 | 0.1023 | 0.604096 | 0.8357 | -0.1539 | 0.1114 | 0.167145 | 0.6552 | NaN | -0.0468 | 0.059 | 0.426838 | 0.8487 | -0.1287 | 0.0789 | 0.102951 | 0.577 | 0.0413 | 0.0875 | 0.636867 | 0.8767 | NaN | -0.0391 | 0.0439 | 0.373479 | 0.6715 | -0.0352 | 0.0618 | 0.568945 | 0.7754 | -0.036 | 0.0619 | 0.560565 | 0.9885 | NaN | -0.0587 | 0.0349 | 0.092395 | 0.9708 | -0.0811 | 0.0504 | 0.107674 | 0.7937 | -0.0336 | 0.0486 | 0.488922 | 0.9967 | NaN | -0.0764 | 0.0431 | 0.07628 | 0.7496 | -0.0306 | 0.0613 | 0.617443 | 0.8191 | -0.1215 | 0.0605 | 0.044469 | 0.6979 |
| FA 5:0 (OH) | 118.0634 | 3.490162 | Lipid | Fatty acid,hydroxy | 0.0825 | 0.0872 | 0.343862 | 0.6908 | 0.1703 | 0.1121 | 0.128677 | 0.3869 | 0.0041 | 0.1398 | 0.976352 | 0.994 | NaN | 0.059 | 0.0808 | 0.465115 | 0.7817 | 0.0848 | 0.1005 | 0.398972 | 0.7244 | 0.0173 | 0.1311 | 0.894845 | 0.9798 | NaN | 0.006 | 0.0617 | 0.922234 | 0.9965 | -0.0004 | 0.0811 | 0.995724 | 0.9998 | 0.0258 | 0.099 | 0.794125 | 0.9477 | NaN | 0.0126 | 0.046 | 0.783949 | 0.8997 | 0.0519 | 0.0611 | 0.395281 | 0.6734 | -0.0568 | 0.0717 | 0.428155 | 0.9735 | NaN | 0.0179 | 0.0369 | 0.626903 | 0.9708 | 0.0146 | 0.0511 | 0.774981 | 0.9977 | 0.0311 | 0.0564 | 0.581645 | 0.9967 | NaN | 0.0187 | 0.0457 | 0.682344 | 0.8913 | 0.0589 | 0.0605 | 0.329801 | 0.6453 | -0.0472 | 0.0719 | 0.511157 | 0.8952 |
| FA 9:0 (OH) | 174.1256 | 11.971786 | Lipid | Fatty acid,hydroxy | 0.0101 | 0.0869 | 0.907362 | 0.9586 | 0.081 | 0.1312 | 0.537111 | 0.8052 | -0.0407 | 0.1149 | 0.723054 | 0.9022 | NaN | -0.0088 | 0.0805 | 0.913117 | 0.9933 | 0.004 | 0.1163 | 0.97282 | 0.9835 | -0.0388 | 0.1077 | 0.719054 | 0.9342 | NaN | -0.0701 | 0.0612 | 0.252563 | 0.7568 | 0.0064 | 0.0922 | 0.94424 | 0.9762 | -0.1228 | 0.0809 | 0.129258 | 0.5265 | NaN | 0.0017 | 0.0457 | 0.97075 | 0.9898 | 0.0179 | 0.0706 | 0.799394 | 0.8869 | -0.0166 | 0.0591 | 0.778666 | 0.9994 | NaN | 0.0218 | 0.0366 | 0.552576 | 0.9708 | 0.0125 | 0.0586 | 0.831282 | 0.9977 | 0.0292 | 0.0464 | 0.528939 | 0.9967 | NaN | 0.0095 | 0.0454 | 0.834302 | 0.9535 | -0.0331 | 0.0702 | 0.637693 | 0.8224 | 0.0376 | 0.0592 | 0.525982 | 0.8961 |
| FA 10:0 (OH) | 188.1411 | 16.303364 | Lipid | Fatty acid,hydroxy | -0.0699 | 0.0875 | 0.424176 | 0.7578 | 0.0496 | 0.1289 | 0.700483 | 0.8949 | -0.1633 | 0.1173 | 0.163692 | 0.5263 | NaN | 0.0041 | 0.082 | 0.959714 | 0.9933 | 0.1017 | 0.1131 | 0.368567 | 0.7116 | -0.0841 | 0.1128 | 0.45585 | 0.8391 | NaN | -0.0861 | 0.0614 | 0.160808 | 0.6546 | 0.0639 | 0.0899 | 0.477049 | 0.8009 | -0.2184 | 0.0813 | 0.007222 | 0.1545 | NaN | -0.0653 | 0.0458 | 0.154159 | 0.4947 | -0.1202 | 0.0689 | 0.081351 | 0.3118 | -0.0148 | 0.0614 | 0.809943 | 0.9994 | NaN | -0.0174 | 0.037 | 0.637775 | 0.9708 | -0.0071 | 0.0575 | 0.90225 | 0.9977 | -0.0286 | 0.0481 | 0.552524 | 0.9967 | NaN | -0.0699 | 0.0455 | 0.123904 | 0.7516 | -0.1488 | 0.0681 | 0.028815 | 0.2981 | -0.0041 | 0.0616 | 0.947331 | 0.996 |
| FA 12:0 (OH) | 216.1724 | 19.386652 | Lipid | Fatty acid,hydroxy | -0.0763 | 0.0855 | 0.372576 | 0.7078 | 0.0202 | 0.1271 | 0.873978 | 0.9553 | -0.1454 | 0.1142 | 0.202739 | 0.5513 | NaN | 0.0072 | 0.0805 | 0.929021 | 0.9933 | 0.0973 | 0.112 | 0.385054 | 0.7136 | -0.0617 | 0.1101 | 0.575121 | 0.8877 | NaN | -0.0975 | 0.0599 | 0.103874 | 0.5671 | 0.0519 | 0.0887 | 0.557984 | 0.8202 | -0.2246 | 0.0789 | 0.004416 | 0.1228 | NaN | -0.0782 | 0.0447 | 0.080397 | 0.4034 | -0.1287 | 0.0676 | 0.056826 | 0.2719 | -0.034 | 0.0594 | 0.56728 | 0.9885 | NaN | -0.0189 | 0.0362 | 0.601907 | 0.9708 | -0.0175 | 0.0565 | 0.756649 | 0.9977 | -0.0213 | 0.0467 | 0.648052 | 0.9967 | NaN | -0.0724 | 0.0444 | 0.103316 | 0.7516 | -0.1446 | 0.0668 | 0.030371 | 0.2981 | -0.0135 | 0.0597 | 0.821597 | 0.9774 |
| FA 14:0 (OH) | 244.2039 | 20.779514 | Lipid | Fatty acid,hydroxy | 0.0093 | 0.0826 | 0.910812 | 0.9586 | 0.1052 | 0.1256 | 0.402038 | 0.7124 | -0.0422 | 0.1093 | 0.699562 | 0.8959 | NaN | 0.0179 | 0.0764 | 0.814662 | 0.9803 | 0.0398 | 0.1112 | 0.720329 | 0.8829 | -0.0086 | 0.1029 | 0.933409 | 0.9876 | NaN | -0.0638 | 0.0582 | 0.272481 | 0.7604 | 0.0431 | 0.0881 | 0.624799 | 0.8438 | -0.1406 | 0.0768 | 0.06718 | 0.4364 | NaN | -0.0204 | 0.0434 | 0.639061 | 0.846 | 0.011 | 0.0678 | 0.870715 | 0.9311 | -0.0484 | 0.056 | 0.387369 | 0.9735 | NaN | -0.0078 | 0.0348 | 0.822124 | 0.9722 | 0.0158 | 0.0562 | 0.778442 | 0.9977 | -0.0228 | 0.0441 | 0.605832 | 0.9967 | NaN | -0.0054 | 0.0431 | 0.900834 | 0.9724 | -0.0136 | 0.0674 | 0.840017 | 0.9237 | -0.0021 | 0.0563 | 0.969685 | 0.996 |
| FA 16:0 (OH) | 272.2351 | 22.279013 | Lipid | Fatty acid,hydroxy | -0.0719 | 0.084 | 0.392024 | 0.7224 | -0.3008 | 0.1213 | 0.013097 | 0.1655 | 0.1368 | 0.1127 | 0.224738 | 0.5914 | NaN | -0.0728 | 0.0776 | 0.348657 | 0.7175 | -0.1637 | 0.1122 | 0.144476 | 0.4923 | 0.0841 | 0.107 | 0.432016 | 0.8249 | NaN | 0.0001 | 0.0594 | 0.99804 | 0.9992 | -0.0496 | 0.0912 | 0.586568 | 0.8374 | 0.0446 | 0.0807 | 0.580546 | 0.8571 | NaN | -0.0875 | 0.0438 | 0.045784 | 0.3914 | -0.153 | 0.066 | 0.020355 | 0.2134 | -0.0392 | 0.0591 | 0.506958 | 0.9885 | NaN | -0.0268 | 0.0355 | 0.449562 | 0.9708 | -0.0927 | 0.0559 | 0.097359 | 0.7937 | 0.0302 | 0.046 | 0.511645 | 0.9967 | NaN | -0.0462 | 0.0438 | 0.291041 | 0.7695 | -0.1224 | 0.0664 | 0.065331 | 0.3895 | 0.0138 | 0.0588 | 0.814148 | 0.9748 |
| FA 18:0 (OH) | 300.2659 | 22.115673 | Lipid | Fatty acid,hydroxy | 0.0152 | 0.0852 | 0.858858 | 0.9457 | 0.0806 | 0.1345 | 0.54909 | 0.8065 | -0.0071 | 0.1097 | 0.948396 | 0.9916 | NaN | 0.0348 | 0.0788 | 0.659028 | 0.9303 | 0.0879 | 0.118 | 0.456378 | 0.7611 | 0.0132 | 0.103 | 0.898108 | 0.9798 | NaN | -0.0642 | 0.06 | 0.284759 | 0.7662 | 0.0916 | 0.0937 | 0.32801 | 0.7705 | -0.1778 | 0.0775 | 0.021823 | 0.3181 | NaN | -0.0585 | 0.0447 | 0.191177 | 0.5115 | -0.1106 | 0.0724 | 0.126874 | 0.4002 | -0.0212 | 0.0564 | 0.70746 | 0.9994 | NaN | 0.0206 | 0.0359 | 0.566765 | 0.9708 | 0.0458 | 0.0598 | 0.443667 | 0.9977 | 0.006 | 0.0443 | 0.892446 | 0.9967 | NaN | -0.0337 | 0.0444 | 0.447717 | 0.8178 | -0.0954 | 0.0719 | 0.184788 | 0.5427 | 0.0088 | 0.0565 | 0.876647 | 0.993 |
| FA 24:0 (OH) | 384.3594 | 22.877468 | Lipid | Fatty acid,hydroxy | -0.0418 | 0.0921 | 0.650201 | 0.8782 | -0.2764 | 0.1273 | 0.029892 | 0.2362 | 0.1958 | 0.1277 | 0.125296 | 0.4673 | NaN | -0.0257 | 0.0853 | 0.763089 | 0.9671 | -0.2089 | 0.1132 | 0.064992 | 0.4408 | 0.1877 | 0.1198 | 0.117134 | 0.6043 | NaN | 0.0098 | 0.065 | 0.879828 | 0.9865 | -0.1461 | 0.0908 | 0.107634 | 0.577 | 0.1552 | 0.0903 | 0.085734 | 0.4613 | NaN | -0.0474 | 0.0484 | 0.327414 | 0.6369 | -0.0728 | 0.0708 | 0.303888 | 0.61 | -0.0204 | 0.0675 | 0.762272 | 0.9994 | NaN | -0.011 | 0.0389 | 0.777712 | 0.9722 | -0.063 | 0.0587 | 0.283121 | 0.9834 | 0.042 | 0.0524 | 0.422517 | 0.9967 | NaN | -0.05 | 0.048 | 0.297297 | 0.7695 | -0.0949 | 0.0697 | 0.173442 | 0.5384 | -0.004 | 0.0675 | 0.953025 | 0.996 |
| FA 25:0 (OH) | 398.3769 | 23.011435 | Lipid | Fatty acid,hydroxy | -0.0952 | 0.0913 | 0.296897 | 0.6636 | -0.2375 | 0.1228 | 0.053031 | 0.2788 | 0.1082 | 0.1347 | 0.421808 | 0.7447 | NaN | -0.1015 | 0.0844 | 0.228776 | 0.5924 | -0.1634 | 0.1095 | 0.13566 | 0.4744 | 0.0555 | 0.1274 | 0.663266 | 0.9007 | NaN | 0.0057 | 0.0648 | 0.929527 | 0.9968 | 0.0395 | 0.0919 | 0.667381 | 0.8587 | -0.0265 | 0.0966 | 0.784009 | 0.9449 | NaN | -0.113 | 0.0475 | 0.017324 | 0.3584 | -0.1631 | 0.0652 | 0.012358 | 0.1777 | -0.0532 | 0.0699 | 0.447044 | 0.9735 | NaN | -0.0278 | 0.0386 | 0.472019 | 0.9708 | -0.064 | 0.056 | 0.253116 | 0.9821 | 0.0191 | 0.0547 | 0.726335 | 0.9967 | NaN | -0.0842 | 0.0474 | 0.075684 | 0.7496 | -0.1362 | 0.0654 | 0.037407 | 0.3022 | -0.022 | 0.0699 | 0.752821 | 0.9732 |
| FA 26:0 (OH) | 412.3936 | 23.14789 | Lipid | Fatty acid,hydroxy | -0.0814 | 0.0869 | 0.348924 | 0.6978 | -0.3211 | 0.1371 | 0.019138 | 0.1918 | 0.1084 | 0.1123 | 0.334355 | 0.7038 | NaN | -0.0818 | 0.0803 | 0.308653 | 0.6788 | -0.2179 | 0.1234 | 0.077459 | 0.4408 | 0.0745 | 0.1059 | 0.481421 | 0.849 | NaN | -0.0008 | 0.0615 | 0.989765 | 0.9992 | -0.0191 | 0.1034 | 0.853383 | 0.9316 | 0.0108 | 0.0804 | 0.893495 | 0.9707 | NaN | -0.0993 | 0.0452 | 0.028125 | 0.3584 | -0.2023 | 0.0731 | 0.00566 | 0.1623 | -0.0348 | 0.0585 | 0.55136 | 0.9885 | NaN | -0.0157 | 0.0368 | 0.668805 | 0.9708 | -0.0583 | 0.0639 | 0.361986 | 0.9977 | 0.0165 | 0.0457 | 0.71822 | 0.9967 | NaN | -0.0665 | 0.0452 | 0.140922 | 0.7516 | -0.1666 | 0.0737 | 0.023801 | 0.2725 | -0.0026 | 0.0584 | 0.964211 | 0.996 |
| FA 27:0 (OH) | 426.4057 | 23.29134 | Lipid | Fatty acid,hydroxy | -0.0854 | 0.0861 | 0.32107 | 0.6817 | -0.304 | 0.1231 | 0.01349 | 0.1655 | 0.1473 | 0.1191 | 0.216184 | 0.5793 | NaN | -0.12 | 0.0796 | 0.131766 | 0.4462 | -0.2336 | 0.1097 | 0.033184 | 0.3816 | 0.0705 | 0.1142 | 0.536843 | 0.8742 | NaN | -0.0132 | 0.0609 | 0.827903 | 0.9805 | -0.0465 | 0.0926 | 0.615449 | 0.8437 | 0.0254 | 0.0858 | 0.767458 | 0.9437 | NaN | -0.0813 | 0.045 | 0.070862 | 0.3995 | -0.1509 | 0.0671 | 0.024437 | 0.2177 | -0.0314 | 0.0625 | 0.615517 | 0.9994 | NaN | -0.0261 | 0.0364 | 0.47323 | 0.9708 | -0.0749 | 0.0572 | 0.190464 | 0.9357 | 0.0234 | 0.0487 | 0.631555 | 0.9967 | NaN | -0.0372 | 0.045 | 0.408671 | 0.8117 | -0.107 | 0.0679 | 0.114966 | 0.4593 | 0.0192 | 0.0622 | 0.757461 | 0.9745 |
| PA 17:3 | 418.2211 | 16.179428 | Lipid | Phosphatidic Acid | -0.0416 | 0.0832 | 0.617448 | 0.8762 | 0.1093 | 0.1126 | 0.33166 | 0.6562 | -0.199 | 0.1258 | 0.113605 | 0.4498 | NaN | -0.0579 | 0.0769 | 0.451563 | 0.7771 | 0.0216 | 0.1007 | 0.830203 | 0.9389 | -0.1734 | 0.1184 | 0.142834 | 0.6249 | NaN | -0.02 | 0.0586 | 0.733113 | 0.9415 | 0.0673 | 0.0789 | 0.393516 | 0.7775 | -0.103 | 0.0901 | 0.253009 | 0.644 | NaN | 0.0194 | 0.0438 | 0.657223 | 0.846 | 0.0338 | 0.0608 | 0.578312 | 0.7754 | -0.0203 | 0.0662 | 0.759524 | 0.9994 | NaN | 0.0048 | 0.0351 | 0.891119 | 0.9722 | 0.0217 | 0.0505 | 0.666981 | 0.9977 | -0.0095 | 0.052 | 0.854588 | 0.9967 | NaN | -0.002 | 0.0435 | 0.963825 | 0.9907 | -0.0264 | 0.0608 | 0.663536 | 0.8393 | 0.0119 | 0.0667 | 0.858294 | 0.985 |
| PA 18:3 | 432.237 | 16.17762 | Lipid | Phosphatidic Acid | 0.0776 | 0.0865 | 0.369258 | 0.7078 | 0.2389 | 0.1221 | 0.050361 | 0.2757 | -0.0526 | 0.1211 | 0.66398 | 0.8853 | NaN | 0.0674 | 0.08 | 0.399305 | 0.7523 | 0.1578 | 0.1092 | 0.148546 | 0.4937 | -0.0298 | 0.1138 | 0.793395 | 0.9535 | NaN | 0.0115 | 0.0611 | 0.850955 | 0.9805 | 0.1242 | 0.0868 | 0.152645 | 0.6041 | -0.0788 | 0.0855 | 0.356693 | 0.7319 | NaN | 0.0602 | 0.0454 | 0.184315 | 0.5115 | 0.1047 | 0.0665 | 0.115173 | 0.3784 | 0.0093 | 0.0624 | 0.88162 | 0.9994 | NaN | 0.0196 | 0.0366 | 0.59109 | 0.9708 | 0.0117 | 0.0566 | 0.836814 | 0.9977 | 0.0303 | 0.049 | 0.53592 | 0.9967 | NaN | 0.0583 | 0.045 | 0.195558 | 0.7516 | 0.0649 | 0.0669 | 0.331982 | 0.6453 | 0.0472 | 0.0625 | 0.450016 | 0.8635 |
| PA 19.3 | 446.2526 | 18.066814 | Lipid | Phosphatidic Acid | -0.0417 | 0.0826 | 0.613751 | 0.8736 | 0.068 | 0.1356 | 0.616197 | 0.8589 | -0.1011 | 0.1058 | 0.33933 | 0.7068 | NaN | 0.0044 | 0.0769 | 0.954765 | 0.9933 | 0.1114 | 0.1189 | 0.348665 | 0.702 | -0.0478 | 0.1006 | 0.634354 | 0.8939 | NaN | 0.0244 | 0.0583 | 0.676206 | 0.9288 | 0.0714 | 0.0945 | 0.450291 | 0.7964 | 0.0221 | 0.0762 | 0.771909 | 0.9437 | NaN | 0.0098 | 0.0435 | 0.821689 | 0.9314 | -0.019 | 0.073 | 0.79482 | 0.8869 | 0.0076 | 0.055 | 0.890736 | 0.9994 | NaN | 0.0302 | 0.0349 | 0.386051 | 0.9708 | 0.0054 | 0.0605 | 0.928628 | 0.9977 | 0.0511 | 0.0431 | 0.236342 | 0.9967 | NaN | -0.0132 | 0.0432 | 0.758809 | 0.924 | -0.0784 | 0.0724 | 0.278501 | 0.6224 | 0.0107 | 0.0551 | 0.845836 | 0.9809 |
| PA 20:3 | 460.2681 | 17.864069 | Lipid | Phosphatidic Acid | 0.0041 | 0.0881 | 0.963101 | 0.9784 | 0.1568 | 0.1247 | 0.208504 | 0.4927 | -0.1184 | 0.1255 | 0.345637 | 0.7068 | NaN | -0.0162 | 0.0815 | 0.842383 | 0.9933 | 0.0804 | 0.111 | 0.468647 | 0.7643 | -0.1109 | 0.1177 | 0.346207 | 0.7614 | NaN | -0.0385 | 0.062 | 0.534796 | 0.9005 | 0.0857 | 0.0877 | 0.328151 | 0.7705 | -0.1421 | 0.0882 | 0.107274 | 0.4894 | NaN | 0.0669 | 0.0462 | 0.147533 | 0.4862 | 0.0984 | 0.0668 | 0.140558 | 0.4105 | 0.0219 | 0.0653 | 0.737308 | 0.9994 | NaN | -0.0015 | 0.0371 | 0.966995 | 0.9912 | 0.0249 | 0.0563 | 0.658243 | 0.9977 | -0.0225 | 0.051 | 0.659712 | 0.9967 | NaN | 0.0615 | 0.0458 | 0.179529 | 0.7516 | 0.0382 | 0.0672 | 0.569341 | 0.8038 | 0.0787 | 0.0654 | 0.22916 | 0.7294 |
| PA 21:3 | 474.2836 | 19.388664 | Lipid | Phosphatidic Acid | -0.0755 | 0.0816 | 0.354759 | 0.7019 | -0.0346 | 0.1281 | 0.787011 | 0.9222 | -0.0961 | 0.1087 | 0.37661 | 0.7082 | NaN | -0.0308 | 0.076 | 0.685194 | 0.9339 | 0.0127 | 0.1128 | 0.910389 | 0.9659 | -0.0419 | 0.1033 | 0.684604 | 0.9172 | NaN | -0.04 | 0.0575 | 0.486635 | 0.8893 | -0.0127 | 0.0896 | 0.886822 | 0.9527 | -0.0337 | 0.0774 | 0.663075 | 0.8899 | NaN | -0.0134 | 0.0431 | 0.755903 | 0.8904 | -0.0804 | 0.0683 | 0.23915 | 0.5547 | 0.0105 | 0.0564 | 0.852753 | 0.9994 | NaN | -0.0013 | 0.0346 | 0.969667 | 0.9912 | -0.008 | 0.057 | 0.888831 | 0.9977 | 0.0089 | 0.0443 | 0.840414 | 0.9967 | NaN | -0.0278 | 0.0427 | 0.514437 | 0.8328 | -0.1179 | 0.0673 | 0.0799 | 0.3895 | 0.0184 | 0.0565 | 0.744896 | 0.9732 |
| PA 22:3 | 488.2996 | 19.989008 | Lipid | Phosphatidic Acid | -0.0553 | 0.0827 | 0.50361 | 0.8075 | -0.0555 | 0.1345 | 0.679817 | 0.8879 | -0.042 | 0.1069 | 0.694063 | 0.8959 | NaN | 0.0312 | 0.0779 | 0.689209 | 0.9341 | 0.0542 | 0.1197 | 0.650554 | 0.8469 | 0.0466 | 0.1028 | 0.650375 | 0.8939 | NaN | 0.048 | 0.0586 | 0.412294 | 0.8406 | 0.0804 | 0.0946 | 0.395618 | 0.7775 | 0.0566 | 0.0762 | 0.457452 | 0.7916 | NaN | -0.0131 | 0.0435 | 0.763032 | 0.8918 | -0.0676 | 0.0718 | 0.346447 | 0.6506 | 0.0015 | 0.055 | 0.977615 | 0.9994 | NaN | 0.0305 | 0.0349 | 0.382114 | 0.9708 | -0.0168 | 0.0599 | 0.778875 | 0.9977 | 0.0672 | 0.043 | 0.117675 | 0.9967 | NaN | -0.0216 | 0.0432 | 0.617285 | 0.8626 | -0.0932 | 0.071 | 0.189271 | 0.5437 | 0.0093 | 0.0551 | 0.865793 | 0.9885 |
| PA 23:3 | 502.3153 | 20.654627 | Lipid | Phosphatidic Acid | -0.1014 | 0.0829 | 0.221227 | 0.5715 | -0.0226 | 0.1315 | 0.863225 | 0.9547 | -0.1474 | 0.109 | 0.176262 | 0.5263 | NaN | -0.0497 | 0.0774 | 0.520711 | 0.8283 | 0.0189 | 0.1156 | 0.870334 | 0.942 | -0.0847 | 0.1042 | 0.416579 | 0.8154 | NaN | -0.0079 | 0.0589 | 0.892755 | 0.9865 | 0.0424 | 0.092 | 0.64454 | 0.8476 | -0.0161 | 0.0789 | 0.838366 | 0.9506 | NaN | -0.0196 | 0.0439 | 0.654528 | 0.846 | -0.0576 | 0.0703 | 0.412562 | 0.6798 | -0.0158 | 0.057 | 0.782148 | 0.9994 | NaN | 0.0014 | 0.0352 | 0.96936 | 0.9912 | -0.0191 | 0.0585 | 0.743833 | 0.9977 | 0.0205 | 0.045 | 0.648615 | 0.9967 | NaN | -0.0358 | 0.0434 | 0.41025 | 0.8117 | -0.1086 | 0.0693 | 0.116971 | 0.4593 | -0.0026 | 0.0572 | 0.963118 | 0.996 |
| PA 24:3 | 516.3306 | 21.119514 | Lipid | Phosphatidic Acid | -0.0865 | 0.0831 | 0.297672 | 0.6636 | 0.0382 | 0.133 | 0.774031 | 0.9222 | -0.1566 | 0.1093 | 0.151794 | 0.5142 | NaN | -0.0471 | 0.0773 | 0.542496 | 0.8388 | 0.0644 | 0.1167 | 0.581437 | 0.8209 | -0.1051 | 0.1039 | 0.311906 | 0.7142 | NaN | -0.0137 | 0.0588 | 0.816402 | 0.9797 | 0.0601 | 0.0928 | 0.516865 | 0.8105 | -0.0373 | 0.0789 | 0.636137 | 0.8767 | NaN | 0.0003 | 0.044 | 0.994528 | 0.9999 | -0.0198 | 0.0714 | 0.781878 | 0.8826 | -0.0083 | 0.0574 | 0.885551 | 0.9994 | NaN | 0.0199 | 0.0353 | 0.573131 | 0.9708 | 0.0079 | 0.0592 | 0.894025 | 0.9977 | 0.0357 | 0.0452 | 0.429792 | 0.9967 | NaN | -0.0117 | 0.0436 | 0.788435 | 0.9482 | -0.0731 | 0.0708 | 0.301595 | 0.6411 | 0.0137 | 0.0576 | 0.811483 | 0.9748 |
| PA 25:3 | 530.3468 | 21.493023 | Lipid | Phosphatidic Acid | -0.0861 | 0.0832 | 0.300561 | 0.6636 | 0.0349 | 0.1256 | 0.781112 | 0.9222 | -0.1696 | 0.116 | 0.14377 | 0.4991 | NaN | -0.0714 | 0.077 | 0.353954 | 0.7236 | 0.0239 | 0.1103 | 0.828424 | 0.9389 | -0.135 | 0.1095 | 0.217896 | 0.6714 | NaN | -0.0216 | 0.0588 | 0.713061 | 0.9414 | 0.0614 | 0.0876 | 0.483479 | 0.8009 | -0.0612 | 0.0835 | 0.463335 | 0.7968 | NaN | 0.0055 | 0.044 | 0.901138 | 0.9579 | -0.0049 | 0.0674 | 0.942595 | 0.9603 | -0.0126 | 0.0609 | 0.836015 | 0.9994 | NaN | 0.0142 | 0.0353 | 0.688307 | 0.9708 | 0.0022 | 0.0559 | 0.968711 | 0.9977 | 0.0344 | 0.048 | 0.473921 | 0.9967 | NaN | -0.0028 | 0.0437 | 0.948025 | 0.9786 | -0.0506 | 0.0669 | 0.4493 | 0.7348 | 0.0195 | 0.0613 | 0.750701 | 0.9732 |
| PA 26:3 | 544.3617 | 21.772911 | Lipid | Phosphatidic Acid | -0.1183 | 0.0831 | 0.15447 | 0.4711 | -0.0748 | 0.1156 | 0.517577 | 0.8001 | -0.1522 | 0.1269 | 0.230544 | 0.596 | NaN | -0.1217 | 0.0767 | 0.112915 | 0.422 | -0.0709 | 0.1014 | 0.484868 | 0.7754 | -0.1489 | 0.119 | 0.210704 | 0.6714 | NaN | -0.0528 | 0.0588 | 0.369185 | 0.8094 | 0.0017 | 0.0813 | 0.983411 | 0.9998 | -0.0811 | 0.0904 | 0.370007 | 0.7398 | NaN | -0.0203 | 0.0441 | 0.645137 | 0.846 | -0.0407 | 0.062 | 0.511727 | 0.7513 | -0.033 | 0.066 | 0.61724 | 0.9994 | NaN | 0.0034 | 0.0354 | 0.924347 | 0.9722 | -0.0102 | 0.0517 | 0.843707 | 0.9977 | 0.0312 | 0.0521 | 0.550022 | 0.9967 | NaN | -0.0113 | 0.0438 | 0.795953 | 0.9482 | -0.0581 | 0.0613 | 0.343222 | 0.6499 | 0.0211 | 0.0665 | 0.751599 | 0.9732 |
| PC 20:0 | 565.3707 | 22.624731 | Lipid | Phosphatidylcholine | 0.0533 | 0.0819 | 0.515091 | 0.817 | 0.0543 | 0.1106 | 0.623285 | 0.8596 | 0.0592 | 0.1201 | 0.622098 | 0.8585 | NaN | 0.1019 | 0.0759 | 0.179136 | 0.5419 | 0.1649 | 0.0978 | 0.091695 | 0.4459 | 0.0845 | 0.1127 | 0.45308 | 0.8391 | NaN | 0.042 | 0.0576 | 0.465959 | 0.8642 | 0.0959 | 0.0769 | 0.211992 | 0.6538 | -0.0213 | 0.0855 | 0.803382 | 0.9477 | NaN | -0.0098 | 0.0432 | 0.820271 | 0.9314 | -0.0234 | 0.0596 | 0.694014 | 0.8567 | 0.0081 | 0.0619 | 0.895897 | 0.9994 | NaN | -0.0232 | 0.0346 | 0.501785 | 0.9708 | -0.0163 | 0.0494 | 0.7407 | 0.9977 | -0.0306 | 0.0486 | 0.529245 | 0.9967 | NaN | 0.0028 | 0.0428 | 0.948117 | 0.9786 | -0.0319 | 0.0591 | 0.589053 | 0.8122 | 0.0446 | 0.0617 | 0.469717 | 0.8648 |
| PC 34:0 | 761.5932 | 25.417608 | Lipid | Phosphatidylcholine | -0.0342 | 0.0828 | 0.67987 | 0.8796 | -0.1701 | 0.1191 | 0.153435 | 0.4298 | 0.1107 | 0.1149 | 0.335317 | 0.7038 | NaN | -0.024 | 0.0766 | 0.754186 | 0.9649 | -0.0902 | 0.1064 | 0.396808 | 0.7241 | 0.0856 | 0.1081 | 0.42842 | 0.8249 | NaN | 0.0004 | 0.0583 | 0.994864 | 0.9992 | 0.0031 | 0.0859 | 0.971147 | 0.9915 | -0.0202 | 0.0827 | 0.807396 | 0.9477 | NaN | -0.089 | 0.0432 | 0.039411 | 0.3914 | -0.1427 | 0.0629 | 0.023311 | 0.2149 | -0.0228 | 0.0598 | 0.702461 | 0.9994 | NaN | -0.0309 | 0.0349 | 0.375042 | 0.9708 | -0.0627 | 0.0535 | 0.241163 | 0.9821 | -0.0023 | 0.0469 | 0.9616 | 0.9967 | NaN | -0.0528 | 0.0431 | 0.220553 | 0.7516 | -0.1223 | 0.0629 | 0.051838 | 0.349 | 0.0235 | 0.0596 | 0.693123 | 0.9612 |
| PC 32:0/PE 35:0 | 733.5648 | 24.662941 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1398 | 0.0896 | 0.118826 | 0.4014 | -0.2276 | 0.1394 | 0.102514 | 0.3627 | -0.0666 | 0.1174 | 0.570317 | 0.8352 | NaN | -0.1259 | 0.0829 | 0.129046 | 0.4437 | -0.1947 | 0.1226 | 0.112326 | 0.4674 | -0.0652 | 0.1101 | 0.55358 | 0.8762 | NaN | -0.0202 | 0.064 | 0.752586 | 0.9454 | -0.037 | 0.1006 | 0.712811 | 0.8816 | -0.0244 | 0.0833 | 0.769824 | 0.9437 | NaN | -0.0311 | 0.0476 | 0.513163 | 0.774 | -0.039 | 0.0767 | 0.611294 | 0.7932 | -0.0085 | 0.0605 | 0.888784 | 0.9994 | NaN | -0.0374 | 0.0381 | 0.32631 | 0.9708 | -0.0486 | 0.0634 | 0.443364 | 0.9977 | -0.0308 | 0.0474 | 0.516486 | 0.9967 | NaN | -0.0394 | 0.0472 | 0.402992 | 0.8117 | -0.044 | 0.076 | 0.562676 | 0.8024 | -0.025 | 0.0605 | 0.679799 | 0.9564 |
| PC 32:1/PE 35:1 | 731.5476 | 24.215395 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2037 | 0.0843 | 0.015681 | 0.1374 | 0.1831 | 0.1154 | 0.112725 | 0.3717 | 0.2283 | 0.1217 | 0.060783 | 0.3614 | NaN | 0.1344 | 0.0795 | 0.090831 | 0.3948 | 0.1569 | 0.1015 | 0.122171 | 0.4674 | 0.131 | 0.1187 | 0.269504 | 0.6818 | NaN | 0.1705 | 0.059 | 0.003855 | 0.0925 | 0.2349 | 0.0783 | 0.00269 | 0.173 | 0.1011 | 0.088 | 0.2504 | 0.6429 | NaN | 0.0333 | 0.0455 | 0.465069 | 0.7407 | -0.0113 | 0.064 | 0.859516 | 0.9253 | 0.0833 | 0.0636 | 0.190468 | 0.9514 | NaN | -0.0025 | 0.0367 | 0.946336 | 0.9801 | -0.0432 | 0.0531 | 0.416278 | 0.9977 | 0.0411 | 0.0505 | 0.415798 | 0.9967 | NaN | 0.0058 | 0.0454 | 0.8981 | 0.9724 | -0.0391 | 0.0637 | 0.539952 | 0.7906 | 0.0556 | 0.0643 | 0.386672 | 0.8324 |
| PC 34:1/PE 37:1 | 759.5781 | 24.803432 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.013 | 0.0832 | 0.876112 | 0.9457 | -0.0321 | 0.109 | 0.768245 | 0.9222 | 0.0029 | 0.1279 | 0.981845 | 0.9945 | NaN | -0.0222 | 0.077 | 0.773466 | 0.9675 | 0.0175 | 0.0961 | 0.855444 | 0.9418 | -0.047 | 0.1206 | 0.696943 | 0.9182 | NaN | 0.018 | 0.0586 | 0.758709 | 0.9454 | 0.0467 | 0.0764 | 0.541169 | 0.8173 | -0.0309 | 0.0906 | 0.733285 | 0.9305 | NaN | -0.0448 | 0.0437 | 0.305223 | 0.6127 | -0.0234 | 0.0584 | 0.688525 | 0.8532 | -0.0638 | 0.0656 | 0.330494 | 0.9622 | NaN | 0.0152 | 0.0351 | 0.66433 | 0.9708 | 0.022 | 0.0485 | 0.650219 | 0.9977 | 0.0035 | 0.0517 | 0.945763 | 0.9967 | NaN | -0.041 | 0.0434 | 0.343778 | 0.7759 | -0.0293 | 0.0579 | 0.612875 | 0.8191 | -0.0501 | 0.0657 | 0.445971 | 0.8627 |
| PC 36:1/PE 39:1 | 787.6113 | 25.608099 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0538 | 0.0849 | 0.526821 | 0.8201 | 0.0169 | 0.1283 | 0.89511 | 0.9568 | 0.1014 | 0.1126 | 0.367782 | 0.7082 | NaN | 0.059 | 0.0785 | 0.452182 | 0.7771 | 0.0534 | 0.1127 | 0.635515 | 0.8459 | 0.0943 | 0.1056 | 0.371836 | 0.7878 | NaN | 0.0253 | 0.0598 | 0.67237 | 0.9288 | 0.1168 | 0.0894 | 0.191335 | 0.652 | -0.0463 | 0.0812 | 0.568678 | 0.8507 | NaN | -0.0293 | 0.0448 | 0.512947 | 0.774 | -0.093 | 0.0685 | 0.174462 | 0.457 | 0.0234 | 0.0582 | 0.688103 | 0.9994 | NaN | -0.0413 | 0.0359 | 0.249634 | 0.9708 | -0.0489 | 0.057 | 0.390154 | 0.9977 | -0.0331 | 0.0459 | 0.471309 | 0.9967 | NaN | -0.0153 | 0.0444 | 0.730983 | 0.918 | -0.0843 | 0.068 | 0.214753 | 0.5528 | 0.0408 | 0.0581 | 0.483062 | 0.8686 |
| PC 32:2/PE 35:2 | 729.5338 | 23.893877 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0258 | 0.0814 | 0.751667 | 0.9192 | -0.1074 | 0.1306 | 0.410892 | 0.7178 | 0.1382 | 0.1038 | 0.182995 | 0.5263 | NaN | 0.0013 | 0.0754 | 0.986593 | 0.9933 | -0.1079 | 0.1145 | 0.345659 | 0.702 | 0.1085 | 0.0979 | 0.268097 | 0.6818 | NaN | 0.011 | 0.0573 | 0.847158 | 0.9805 | 0.0199 | 0.0924 | 0.829091 | 0.9239 | 0.0153 | 0.0751 | 0.838689 | 0.9506 | NaN | -0.0133 | 0.0428 | 0.756489 | 0.8904 | -0.0882 | 0.0697 | 0.205521 | 0.5052 | 0.03 | 0.0541 | 0.579559 | 0.9905 | NaN | 0.0146 | 0.0343 | 0.669679 | 0.9708 | -0.055 | 0.0581 | 0.343703 | 0.9977 | 0.0653 | 0.0419 | 0.119427 | 0.9967 | NaN | -0.0093 | 0.0425 | 0.82761 | 0.9529 | -0.107 | 0.0688 | 0.119804 | 0.4625 | 0.0509 | 0.0539 | 0.34471 | 0.8286 |
| PC 34:2/PE 37:2 | 757.5632 | 24.41449 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.04 | 0.089 | 0.653272 | 0.8782 | -0.0105 | 0.1399 | 0.939978 | 0.9682 | 0.0661 | 0.1148 | 0.564889 | 0.8352 | NaN | 0.0442 | 0.0823 | 0.591114 | 0.8776 | -0.1652 | 0.1248 | 0.185812 | 0.537 | 0.1118 | 0.1079 | 0.30024 | 0.7079 | NaN | 0.0747 | 0.0625 | 0.231708 | 0.7309 | -0.0518 | 0.0977 | 0.596214 | 0.8374 | 0.1494 | 0.0806 | 0.06363 | 0.4338 | NaN | -0.0129 | 0.0469 | 0.783062 | 0.8997 | 0.0439 | 0.075 | 0.557847 | 0.7737 | -0.0432 | 0.0593 | 0.466243 | 0.9735 | NaN | 0.0497 | 0.0374 | 0.183591 | 0.9708 | 0.0211 | 0.0622 | 0.73492 | 0.9977 | 0.0669 | 0.046 | 0.146034 | 0.9967 | NaN | -0.0425 | 0.0465 | 0.360335 | 0.7862 | 0.0124 | 0.0744 | 0.867835 | 0.9449 | -0.0748 | 0.0593 | 0.207554 | 0.7294 |
| PC 36:2/PE 39:2 | 785.5938 | 25.064062 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.034 | 0.0897 | 0.704404 | 0.9008 | -0.1842 | 0.1492 | 0.216733 | 0.5048 | 0.1822 | 0.1117 | 0.102774 | 0.4331 | NaN | -0.0052 | 0.0832 | 0.950121 | 0.9933 | -0.2019 | 0.1304 | 0.121454 | 0.4674 | 0.1333 | 0.1061 | 0.208979 | 0.6714 | NaN | 0.0248 | 0.0631 | 0.694302 | 0.9393 | -0.035 | 0.106 | 0.741675 | 0.8816 | 0.0436 | 0.0811 | 0.591295 | 0.8601 | NaN | -0.0358 | 0.0472 | 0.448207 | 0.7298 | -0.1005 | 0.0801 | 0.210016 | 0.5107 | 0.0174 | 0.0589 | 0.767882 | 0.9994 | NaN | 0.0068 | 0.0378 | 0.858159 | 0.9722 | -0.0214 | 0.0674 | 0.750797 | 0.9977 | 0.0261 | 0.0461 | 0.571377 | 0.9967 | NaN | -0.0249 | 0.0468 | 0.594619 | 0.8527 | -0.1055 | 0.0794 | 0.183793 | 0.5427 | 0.0333 | 0.0587 | 0.571228 | 0.9321 |
| PC 33:3/PE 36:3 | 741.568 | 25.137949 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1664 | 0.0801 | 0.037676 | 0.2244 | -0.2686 | 0.1253 | 0.032117 | 0.2396 | -0.0936 | 0.1044 | 0.370224 | 0.7082 | NaN | -0.0574 | 0.0773 | 0.457761 | 0.7771 | -0.1897 | 0.112 | 0.090376 | 0.4459 | 0.0235 | 0.1032 | 0.819514 | 0.9616 | NaN | -0.0117 | 0.058 | 0.840317 | 0.9805 | -0.0986 | 0.0908 | 0.277642 | 0.7263 | 0.0294 | 0.0751 | 0.695115 | 0.909 | NaN | -0.0664 | 0.0425 | 0.118373 | 0.4618 | -0.0777 | 0.0695 | 0.263677 | 0.5776 | -0.0441 | 0.0538 | 0.412135 | 0.9735 | NaN | -0.0313 | 0.0343 | 0.362164 | 0.9708 | -0.0841 | 0.0572 | 0.141757 | 0.8645 | 0.0009 | 0.0425 | 0.983767 | 0.9967 | NaN | -0.0806 | 0.042 | 0.055145 | 0.7271 | -0.0622 | 0.0693 | 0.369496 | 0.6653 | -0.0837 | 0.0533 | 0.116752 | 0.7232 |
| PC 33:3/PE 36:3 | 741.5698 | 24.691595 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0486 | 0.0829 | 0.558026 | 0.8393 | -0.1201 | 0.126 | 0.340469 | 0.6665 | 0.1666 | 0.108 | 0.122824 | 0.4648 | NaN | 0.0347 | 0.0767 | 0.650705 | 0.9303 | -0.051 | 0.1118 | 0.648226 | 0.8459 | 0.1307 | 0.1021 | 0.200544 | 0.6714 | NaN | 0.0443 | 0.0583 | 0.446929 | 0.8554 | -0.0289 | 0.0889 | 0.744801 | 0.8816 | 0.1105 | 0.0768 | 0.150282 | 0.5464 | NaN | -0.0061 | 0.0437 | 0.88896 | 0.9579 | -0.0391 | 0.068 | 0.564812 | 0.7754 | 0.0082 | 0.0569 | 0.885622 | 0.9994 | NaN | 0.0484 | 0.0348 | 0.164882 | 0.9708 | 0.037 | 0.0568 | 0.514195 | 0.9977 | 0.0611 | 0.0439 | 0.164141 | 0.9967 | NaN | 0.0239 | 0.0433 | 0.581188 | 0.8527 | -0.0003 | 0.0678 | 0.99603 | 0.9991 | 0.0365 | 0.0566 | 0.519475 | 0.8961 |
| PC 34:3/PE 37:3 | 755.5473 | 24.082075 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1093 | 0.0862 | 0.204506 | 0.5561 | 0.02 | 0.1197 | 0.867134 | 0.9547 | 0.2037 | 0.1228 | 0.097096 | 0.4331 | NaN | 0.0849 | 0.0799 | 0.287735 | 0.6553 | 0.0482 | 0.1051 | 0.646392 | 0.8459 | 0.1498 | 0.1166 | 0.198965 | 0.6714 | NaN | 0.1269 | 0.0602 | 0.035014 | 0.344 | 0.1446 | 0.0832 | 0.082364 | 0.549 | 0.1039 | 0.088 | 0.237738 | 0.6205 | NaN | -0.061 | 0.0459 | 0.183751 | 0.5115 | -0.1253 | 0.0636 | 0.048767 | 0.2516 | 0.0195 | 0.0648 | 0.763174 | 0.9994 | NaN | 0.0131 | 0.0366 | 0.721226 | 0.971 | -0.0215 | 0.0533 | 0.686811 | 0.9977 | 0.0495 | 0.0504 | 0.326549 | 0.9967 | NaN | -0.0617 | 0.0455 | 0.175193 | 0.7516 | -0.114 | 0.0632 | 0.071125 | 0.3895 | 0.003 | 0.0651 | 0.963365 | 0.996 |
| PC 35:3/PE 38:3 | 769.5958 | 24.92041 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1413 | 0.0858 | 0.099524 | 0.3712 | -0.0701 | 0.1297 | 0.588999 | 0.8358 | -0.1765 | 0.1151 | 0.124981 | 0.4673 | NaN | -0.0944 | 0.08 | 0.237797 | 0.6038 | -0.0728 | 0.1138 | 0.522434 | 0.7797 | -0.1186 | 0.1096 | 0.279441 | 0.6877 | NaN | -0.0584 | 0.0609 | 0.337602 | 0.792 | -0.0466 | 0.0907 | 0.606937 | 0.8395 | -0.0863 | 0.0824 | 0.294932 | 0.6783 | NaN | -0.0703 | 0.0452 | 0.120004 | 0.4632 | -0.0261 | 0.0697 | 0.707649 | 0.8608 | -0.0901 | 0.0594 | 0.128909 | 0.9514 | NaN | 0.0006 | 0.0367 | 0.986799 | 0.9922 | 0.0385 | 0.0579 | 0.505987 | 0.9977 | -0.0297 | 0.0473 | 0.530484 | 0.9967 | NaN | -0.0577 | 0.045 | 0.199778 | 0.7516 | -0.0237 | 0.0691 | 0.731608 | 0.8666 | -0.0747 | 0.0597 | 0.211276 | 0.7294 |
| PC 35:3/PE 38:3 | 769.5964 | 26.10005 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1364 | 0.0855 | 0.110743 | 0.3866 | -0.1916 | 0.1366 | 0.160683 | 0.4348 | -0.1107 | 0.1107 | 0.317233 | 0.6905 | NaN | -0.073 | 0.0802 | 0.362746 | 0.7308 | -0.122 | 0.1212 | 0.313976 | 0.6823 | -0.0553 | 0.1052 | 0.59911 | 0.8877 | NaN | -0.1002 | 0.0602 | 0.096185 | 0.5647 | -0.0638 | 0.097 | 0.51103 | 0.8105 | -0.1474 | 0.0775 | 0.05733 | 0.4204 | NaN | -0.0237 | 0.0455 | 0.603137 | 0.818 | 0.0392 | 0.0754 | 0.60343 | 0.7893 | -0.0444 | 0.0571 | 0.4368 | 0.9735 | NaN | -0.0216 | 0.0365 | 0.553557 | 0.9708 | 0.0152 | 0.0623 | 0.807659 | 0.9977 | -0.0489 | 0.0447 | 0.273957 | 0.9967 | NaN | 0.0202 | 0.0454 | 0.655786 | 0.8716 | 0.077 | 0.075 | 0.304672 | 0.6419 | -0.0006 | 0.0576 | 0.992078 | 0.996 |
| PC 36:3/PE 39:3 | 783.5786 | 24.554457 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0696 | 0.085 | 0.412626 | 0.7443 | -0.0526 | 0.1278 | 0.680665 | 0.8879 | 0.1783 | 0.1131 | 0.11482 | 0.4498 | NaN | 0.0392 | 0.0789 | 0.619456 | 0.9037 | -0.0071 | 0.1126 | 0.949952 | 0.9801 | 0.1166 | 0.108 | 0.280129 | 0.6877 | NaN | 0.0561 | 0.0598 | 0.348336 | 0.793 | 0.1196 | 0.0901 | 0.1846 | 0.652 | -0.0046 | 0.083 | 0.955751 | 0.9766 | NaN | -0.0691 | 0.0449 | 0.123801 | 0.4681 | -0.1329 | 0.0674 | 0.048705 | 0.2516 | -0.0022 | 0.0597 | 0.971245 | 0.9994 | NaN | -0.0075 | 0.036 | 0.834729 | 0.9722 | -0.055 | 0.0566 | 0.331207 | 0.9977 | 0.0306 | 0.0465 | 0.511085 | 0.9967 | NaN | -0.035 | 0.0446 | 0.432584 | 0.8178 | -0.1357 | 0.0668 | 0.042173 | 0.3104 | 0.057 | 0.059 | 0.334009 | 0.8205 |
| PC 32:4/PE 35:4 | 725.5072 | 23.725977 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0376 | 0.0877 | 0.668575 | 0.8782 | 0.1052 | 0.1196 | 0.378856 | 0.6978 | -0.0137 | 0.1281 | 0.914711 | 0.9854 | NaN | -0.0068 | 0.0815 | 0.933194 | 0.9933 | 0.0789 | 0.1052 | 0.453396 | 0.7607 | -0.0742 | 0.121 | 0.539673 | 0.8742 | NaN | 0.1364 | 0.0614 | 0.026336 | 0.28 | 0.2043 | 0.0818 | 0.012531 | 0.2845 | 0.0705 | 0.0909 | 0.437581 | 0.7876 | NaN | -0.0635 | 0.0461 | 0.168718 | 0.5068 | -0.0672 | 0.065 | 0.300904 | 0.6082 | -0.0643 | 0.0656 | 0.327053 | 0.9622 | NaN | -0.0181 | 0.037 | 0.625541 | 0.9708 | -0.0556 | 0.0537 | 0.301098 | 0.9835 | 0.0245 | 0.0517 | 0.635796 | 0.9967 | NaN | -0.0699 | 0.0458 | 0.126666 | 0.7516 | -0.0899 | 0.0644 | 0.163089 | 0.5359 | -0.0526 | 0.0658 | 0.423998 | 0.8529 |
| PC 33:4/PE 36:4 | 739.5503 | 24.66426 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1 | 0.0957 | 0.29635 | 0.6636 | -0.0418 | 0.1475 | 0.776593 | 0.9222 | -0.1259 | 0.1267 | 0.320244 | 0.6905 | NaN | -0.0514 | 0.0891 | 0.564266 | 0.8617 | 0.0615 | 0.1307 | 0.638218 | 0.8459 | -0.1008 | 0.1191 | 0.397606 | 0.8005 | NaN | -0.0178 | 0.0678 | 0.792701 | 0.9638 | 0.1136 | 0.1035 | 0.272489 | 0.7263 | -0.1322 | 0.0892 | 0.138519 | 0.5347 | NaN | -0.011 | 0.0506 | 0.828523 | 0.9372 | -0.0509 | 0.0789 | 0.519009 | 0.7556 | 0.042 | 0.066 | 0.524706 | 0.9885 | NaN | -0.0171 | 0.0405 | 0.673173 | 0.9708 | -0.0018 | 0.0657 | 0.977614 | 0.9977 | -0.0305 | 0.0515 | 0.553706 | 0.9967 | NaN | -0.01 | 0.0502 | 0.842139 | 0.9563 | -0.0403 | 0.0783 | 0.606607 | 0.8167 | 0.0277 | 0.066 | 0.675267 | 0.9564 |
| PC 35:4/PE 38:4 | 767.5821 | 24.73068 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0274 | 0.0855 | 0.748361 | 0.9192 | -0.007 | 0.1273 | 0.956257 | 0.974 | -0.0222 | 0.1159 | 0.847736 | 0.9565 | NaN | -0.0083 | 0.0792 | 0.916356 | 0.9933 | -0.0341 | 0.1118 | 0.760167 | 0.8985 | 0.008 | 0.109 | 0.941583 | 0.9876 | NaN | 0.0103 | 0.0602 | 0.863694 | 0.9805 | -0.0472 | 0.0889 | 0.595111 | 0.8374 | 0.0416 | 0.0822 | 0.612586 | 0.8637 | NaN | -0.0534 | 0.0448 | 0.23369 | 0.5455 | 0.0246 | 0.0682 | 0.718575 | 0.8623 | -0.1048 | 0.0589 | 0.075115 | 0.8712 | NaN | 0.0036 | 0.0361 | 0.920857 | 0.9722 | -0.0022 | 0.0566 | 0.969028 | 0.9977 | 0.0088 | 0.0468 | 0.851043 | 0.9967 | NaN | -0.0541 | 0.0445 | 0.224027 | 0.7516 | -0.0002 | 0.0677 | 0.997937 | 0.9991 | -0.0895 | 0.0592 | 0.130446 | 0.7232 |
| PC 36:4/PE 39:4 | 781.5616 | 24.310883 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0365 | 0.0846 | 0.665745 | 0.8782 | 0.0827 | 0.1186 | 0.48585 | 0.7842 | -0.0066 | 0.1201 | 0.956092 | 0.9916 | NaN | 0.0302 | 0.0782 | 0.6995 | 0.9341 | 0.0777 | 0.1041 | 0.455501 | 0.7611 | -0.0088 | 0.1127 | 0.937804 | 0.9876 | NaN | -0.008 | 0.0596 | 0.893611 | 0.9865 | -0.0699 | 0.0841 | 0.405829 | 0.784 | 0.0658 | 0.0852 | 0.439758 | 0.7876 | NaN | -0.0056 | 0.0445 | 0.899515 | 0.9579 | 0.0537 | 0.0636 | 0.398046 | 0.6761 | -0.0823 | 0.0614 | 0.179893 | 0.9514 | NaN | 0.0143 | 0.0357 | 0.689362 | 0.9708 | 0.023 | 0.0529 | 0.663695 | 0.9977 | 0.0081 | 0.0485 | 0.867736 | 0.9967 | NaN | -0.0154 | 0.0442 | 0.726714 | 0.918 | 0.0615 | 0.0629 | 0.328556 | 0.6453 | -0.1052 | 0.0613 | 0.086097 | 0.7232 |
| PC 37:4/PE 40:4 | 795.6124 | 25.543018 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1886 | 0.0882 | 0.032483 | 0.2187 | -0.2194 | 0.1384 | 0.113039 | 0.3717 | -0.1462 | 0.1176 | 0.213808 | 0.5757 | NaN | -0.1084 | 0.0834 | 0.193582 | 0.548 | -0.0868 | 0.1255 | 0.489178 | 0.7759 | -0.0874 | 0.1119 | 0.434882 | 0.8249 | NaN | -0.0789 | 0.063 | 0.210496 | 0.7091 | -0.0642 | 0.099 | 0.516657 | 0.8105 | -0.1178 | 0.0832 | 0.156565 | 0.5549 | NaN | -0.0902 | 0.0467 | 0.053177 | 0.3914 | -0.0716 | 0.0755 | 0.342657 | 0.6506 | -0.0823 | 0.0605 | 0.173676 | 0.9514 | NaN | -0.0177 | 0.038 | 0.640922 | 0.9708 | 0.003 | 0.0634 | 0.962139 | 0.9977 | -0.0326 | 0.048 | 0.497379 | 0.9967 | NaN | -0.0772 | 0.0465 | 0.096685 | 0.7516 | -0.0629 | 0.075 | 0.401512 | 0.6948 | -0.0735 | 0.0607 | 0.225886 | 0.7294 |
| PC 32:5/PE 35:5 | 723.5265 | 24.594513 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1591 | 0.084 | 0.058302 | 0.2873 | 0.1197 | 0.1186 | 0.313086 | 0.6377 | 0.2217 | 0.1194 | 0.063423 | 0.3614 | NaN | 0.1037 | 0.0786 | 0.187093 | 0.5455 | 0.0401 | 0.1057 | 0.704628 | 0.8798 | 0.1624 | 0.1139 | 0.1538 | 0.6481 | NaN | 0.0936 | 0.0594 | 0.115119 | 0.5674 | 0.0214 | 0.0839 | 0.798406 | 0.9217 | 0.1443 | 0.0851 | 0.090105 | 0.4613 | NaN | 0.0847 | 0.0443 | 0.055806 | 0.3989 | 0.1194 | 0.0628 | 0.057119 | 0.2719 | 0.0748 | 0.0625 | 0.231356 | 0.9622 | NaN | 0.0492 | 0.0357 | 0.168912 | 0.9708 | 0.0035 | 0.0534 | 0.947504 | 0.9977 | 0.0967 | 0.0484 | 0.045896 | 0.9967 | NaN | 0.0792 | 0.044 | 0.071697 | 0.7496 | 0.0981 | 0.0627 | 0.117334 | 0.4593 | 0.0793 | 0.0625 | 0.20459 | 0.7294 |
| PC 34:5/PE 37:5 | 751.5536 | 25.308743 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0589 | 0.0859 | 0.492628 | 0.8017 | 0.0095 | 0.1388 | 0.945379 | 0.9718 | 0.1243 | 0.1099 | 0.258149 | 0.6326 | NaN | 0.004 | 0.0801 | 0.960199 | 0.9933 | -0.0239 | 0.122 | 0.844695 | 0.9389 | 0.0603 | 0.105 | 0.565847 | 0.8848 | NaN | 0.0399 | 0.0605 | 0.509577 | 0.8921 | 0.0206 | 0.097 | 0.831879 | 0.9239 | 0.0443 | 0.0786 | 0.573362 | 0.8532 | NaN | 0.046 | 0.0451 | 0.30799 | 0.616 | 0.0692 | 0.0742 | 0.351349 | 0.6511 | 0.0443 | 0.0569 | 0.435926 | 0.9735 | NaN | -0.0049 | 0.0363 | 0.892864 | 0.9722 | -0.0244 | 0.0618 | 0.692434 | 0.9977 | 0.0111 | 0.0449 | 0.804604 | 0.9967 | NaN | 0.0424 | 0.0448 | 0.34321 | 0.7759 | 0.032 | 0.0738 | 0.664122 | 0.8393 | 0.0591 | 0.0568 | 0.298038 | 0.8042 |
| PC 35:5/PE 38:5 | 765.5646 | 24.605843 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2 | 0.088 | 0.022981 | 0.1738 | -0.2279 | 0.1241 | 0.066224 | 0.2948 | -0.1519 | 0.1244 | 0.222085 | 0.5894 | NaN | -0.1824 | 0.0814 | 0.025139 | 0.2243 | -0.171 | 0.11 | 0.119845 | 0.4674 | -0.1497 | 0.1166 | 0.199308 | 0.6714 | NaN | -0.0728 | 0.0631 | 0.248664 | 0.7568 | -0.1055 | 0.0884 | 0.232699 | 0.6761 | -0.0346 | 0.0894 | 0.698428 | 0.9093 | NaN | 0.0139 | 0.0478 | 0.770287 | 0.8919 | 0.0095 | 0.0695 | 0.891183 | 0.9424 | 0.0181 | 0.0651 | 0.781177 | 0.9994 | NaN | -0.0016 | 0.0381 | 0.965796 | 0.9912 | -0.0059 | 0.0573 | 0.918251 | 0.9977 | 0.0068 | 0.0511 | 0.894721 | 0.9967 | NaN | -0.0097 | 0.0472 | 0.836396 | 0.9539 | -0.015 | 0.0686 | 0.82737 | 0.9165 | -0.0051 | 0.0651 | 0.937211 | 0.996 |
| PC 36:5/PE 39:5 | 779.5674 | 24.645178 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1059 | 0.0846 | 0.210586 | 0.5594 | -0.2949 | 0.1171 | 0.011762 | 0.1645 | 0.0742 | 0.119 | 0.533088 | 0.8099 | NaN | -0.0766 | 0.0785 | 0.329108 | 0.701 | -0.2273 | 0.1044 | 0.029473 | 0.3624 | 0.0834 | 0.1116 | 0.454892 | 0.8391 | NaN | -0.0402 | 0.0598 | 0.501772 | 0.8921 | -0.1367 | 0.0849 | 0.107388 | 0.577 | 0.0336 | 0.0845 | 0.690649 | 0.9056 | NaN | -0.058 | 0.0445 | 0.192504 | 0.5115 | -0.0703 | 0.0662 | 0.287878 | 0.599 | -0.0354 | 0.0615 | 0.564975 | 0.9885 | NaN | -0.0508 | 0.0357 | 0.154029 | 0.9708 | -0.1101 | 0.0535 | 0.039547 | 0.6733 | 0.0018 | 0.0483 | 0.969643 | 0.9967 | NaN | -0.0343 | 0.0443 | 0.43984 | 0.8178 | -0.0678 | 0.0657 | 0.301982 | 0.6411 | 0.0059 | 0.0615 | 0.923683 | 0.996 |
| PC 36:5/PE 39:5 | 779.5741 | 27.296911 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0004 | 0.0841 | 0.996369 | 0.9964 | -0.273 | 0.1202 | 0.023105 | 0.2091 | 0.2287 | 0.1118 | 0.040737 | 0.3497 | NaN | 0.0073 | 0.0778 | 0.925115 | 0.9933 | -0.1642 | 0.1092 | 0.132824 | 0.4744 | 0.1973 | 0.1055 | 0.061505 | 0.4962 | NaN | 0.031 | 0.0592 | 0.600917 | 0.9166 | -0.0949 | 0.0876 | 0.279026 | 0.7265 | 0.1351 | 0.0802 | 0.091928 | 0.4613 | NaN | -0.0657 | 0.0441 | 0.135966 | 0.4828 | -0.1306 | 0.0655 | 0.04619 | 0.2513 | -0.0107 | 0.0602 | 0.858417 | 0.9994 | NaN | -0.0185 | 0.0355 | 0.60207 | 0.9708 | -0.1019 | 0.0546 | 0.062208 | 0.6733 | 0.0537 | 0.0464 | 0.247014 | 0.9967 | NaN | -0.0347 | 0.0439 | 0.428676 | 0.8178 | -0.1111 | 0.0655 | 0.089784 | 0.4046 | 0.0319 | 0.0597 | 0.5934 | 0.9367 |
| PC 37:5/PE 40:5 | 793.5976 | 24.882019 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1456 | 0.0831 | 0.079698 | 0.3333 | -0.0704 | 0.128 | 0.582651 | 0.8296 | -0.1789 | 0.1092 | 0.101224 | 0.4331 | NaN | -0.0908 | 0.0777 | 0.242846 | 0.6038 | -0.0278 | 0.1128 | 0.805068 | 0.9336 | -0.123 | 0.1041 | 0.237398 | 0.6818 | NaN | -0.0613 | 0.059 | 0.298643 | 0.782 | -0.0336 | 0.0896 | 0.707748 | 0.8816 | -0.087 | 0.0783 | 0.266643 | 0.66 | NaN | -0.0778 | 0.0438 | 0.075497 | 0.3995 | -0.0682 | 0.0684 | 0.318981 | 0.6334 | -0.0799 | 0.0566 | 0.157699 | 0.9514 | NaN | -0.0193 | 0.0355 | 0.58676 | 0.9708 | 0.0029 | 0.0572 | 0.959935 | 0.9977 | -0.0346 | 0.0449 | 0.441262 | 0.9967 | NaN | -0.0629 | 0.0436 | 0.149062 | 0.7516 | -0.0473 | 0.068 | 0.487271 | 0.7613 | -0.0714 | 0.0568 | 0.209106 | 0.7294 |
| PC 39:5/PE 42:5 | 821.5945 | 25.4785 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0629 | 0.0844 | 0.455836 | 0.7718 | -0.0015 | 0.1264 | 0.990328 | 0.9938 | 0.1384 | 0.1129 | 0.220141 | 0.587 | NaN | 0.0339 | 0.0782 | 0.665287 | 0.9303 | 0.0095 | 0.1109 | 0.932009 | 0.9707 | 0.0904 | 0.107 | 0.39811 | 0.8005 | NaN | 0.0771 | 0.0592 | 0.192514 | 0.6946 | 0.1543 | 0.0882 | 0.080192 | 0.549 | 0.013 | 0.0814 | 0.873388 | 0.9662 | NaN | -0.0702 | 0.0445 | 0.114967 | 0.4618 | -0.094 | 0.0673 | 0.162808 | 0.4427 | -0.0414 | 0.0592 | 0.484412 | 0.9759 | NaN | -0.0429 | 0.0357 | 0.229265 | 0.9708 | -0.0925 | 0.0556 | 0.09619 | 0.7937 | -0.0018 | 0.0463 | 0.969067 | 0.9967 | NaN | -0.0411 | 0.0442 | 0.352808 | 0.7843 | -0.0969 | 0.0668 | 0.146707 | 0.5225 | 0.0116 | 0.059 | 0.843952 | 0.9809 |
| PC 40:5/PE 43:5 | 835.6077 | 25.139347 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0836 | 0.088 | 0.342083 | 0.6908 | 0.2979 | 0.1443 | 0.038958 | 0.2428 | -0.0161 | 0.1097 | 0.883656 | 0.9697 | NaN | 0.0505 | 0.0817 | 0.536499 | 0.8366 | 0.3116 | 0.1255 | 0.013007 | 0.2909 | -0.061 | 0.1034 | 0.555288 | 0.8762 | NaN | 0.0767 | 0.0618 | 0.214754 | 0.7098 | 0.2485 | 0.0999 | 0.012885 | 0.2845 | -0.0189 | 0.0777 | 0.80781 | 0.9477 | NaN | -0.0195 | 0.0466 | 0.674768 | 0.846 | 0.0478 | 0.0807 | 0.553455 | 0.772 | -0.0529 | 0.0562 | 0.346577 | 0.9622 | NaN | -0.0221 | 0.0373 | 0.554419 | 0.9708 | 0.0366 | 0.0669 | 0.584348 | 0.9977 | -0.0525 | 0.0441 | 0.233626 | 0.9967 | NaN | -0.0355 | 0.0463 | 0.443058 | 0.8178 | 0.045 | 0.08 | 0.573536 | 0.8075 | -0.0768 | 0.0561 | 0.170907 | 0.7294 |
| PC 36:6/PE 39:6 | 777.5297 | 24.070581 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.049 | 0.0857 | 0.567719 | 0.8447 | -0.1119 | 0.1243 | 0.36771 | 0.6951 | 0.1897 | 0.1152 | 0.099751 | 0.4331 | NaN | 0.0024 | 0.0797 | 0.976069 | 0.9933 | -0.1024 | 0.109 | 0.347744 | 0.702 | 0.1236 | 0.1103 | 0.262406 | 0.6818 | NaN | 0.0292 | 0.0603 | 0.628382 | 0.9288 | 0.0083 | 0.088 | 0.925072 | 0.9721 | 0.053 | 0.0836 | 0.526233 | 0.826 | NaN | -0.0142 | 0.0451 | 0.752738 | 0.8904 | -0.085 | 0.0664 | 0.20038 | 0.4973 | 0.0464 | 0.0604 | 0.442318 | 0.9735 | NaN | 0.032 | 0.0361 | 0.374923 | 0.9708 | 0.0203 | 0.0559 | 0.7161 | 0.9977 | 0.0462 | 0.0473 | 0.328927 | 0.9967 | NaN | -0.0108 | 0.0448 | 0.809408 | 0.9499 | -0.0738 | 0.066 | 0.263515 | 0.6028 | 0.0443 | 0.0605 | 0.46458 | 0.8635 |
| PC 38:6/PE 41:6 | 805.5625 | 24.26375 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0874 | 0.0896 | 0.329376 | 0.6891 | -0.2305 | 0.1301 | 0.076521 | 0.313 | 0.0237 | 0.1217 | 0.845717 | 0.9565 | NaN | -0.0323 | 0.0836 | 0.699132 | 0.9341 | -0.0397 | 0.1222 | 0.745244 | 0.89 | 0.0282 | 0.1141 | 0.805099 | 0.9546 | NaN | -0.0173 | 0.0634 | 0.784216 | 0.9577 | -0.07 | 0.0936 | 0.454458 | 0.7964 | 0.0171 | 0.0862 | 0.842529 | 0.953 | NaN | -0.0363 | 0.0472 | 0.441674 | 0.7278 | -0.0277 | 0.0721 | 0.700425 | 0.8597 | -0.0353 | 0.0626 | 0.572376 | 0.9885 | NaN | -0.0104 | 0.0379 | 0.783136 | 0.9722 | -0.0224 | 0.0598 | 0.708388 | 0.9977 | -0.002 | 0.0492 | 0.967963 | 0.9967 | NaN | -0.0316 | 0.0469 | 0.499424 | 0.8283 | -0.0224 | 0.0716 | 0.754157 | 0.884 | -0.0335 | 0.0627 | 0.592525 | 0.9367 |
| PC 34:7/PE 37:7 | 747.5202 | 24.72982 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0361 | 0.0851 | 0.671573 | 0.8782 | -0.0124 | 0.1402 | 0.929519 | 0.9682 | -0.0308 | 0.1069 | 0.773615 | 0.9398 | NaN | -0.0657 | 0.0788 | 0.403952 | 0.7538 | -0.0298 | 0.1231 | 0.808512 | 0.9349 | -0.0645 | 0.1005 | 0.520775 | 0.8742 | NaN | -0.0264 | 0.0599 | 0.659161 | 0.9288 | -0.0066 | 0.098 | 0.946117 | 0.9762 | -0.0411 | 0.0757 | 0.586577 | 0.8601 | NaN | -0.0307 | 0.0447 | 0.492871 | 0.7557 | 0.0099 | 0.0752 | 0.895673 | 0.9435 | -0.0504 | 0.0548 | 0.357505 | 0.9622 | NaN | 0.0081 | 0.0359 | 0.821819 | 0.9722 | 0.0168 | 0.0624 | 0.787918 | 0.9977 | 0.0051 | 0.0432 | 0.906533 | 0.9967 | NaN | -0.0176 | 0.0444 | 0.691306 | 0.8979 | -0.0185 | 0.0746 | 0.804365 | 0.9086 | -0.0142 | 0.055 | 0.79655 | 0.9748 |
| PC 37:7/PE 40:7 | 789.5631 | 24.907656 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0278 | 0.0802 | 0.728318 | 0.9158 | 0.0375 | 0.1202 | 0.754811 | 0.9222 | -0.0607 | 0.1074 | 0.572088 | 0.8352 | NaN | -0.0091 | 0.0742 | 0.902448 | 0.9933 | 0.0465 | 0.1055 | 0.659172 | 0.8561 | -0.0429 | 0.1009 | 0.670752 | 0.9031 | NaN | -0.0159 | 0.0564 | 0.778031 | 0.9569 | 0.0286 | 0.084 | 0.733295 | 0.8816 | -0.0636 | 0.0759 | 0.402192 | 0.7682 | NaN | -0.0455 | 0.042 | 0.278946 | 0.5838 | -0.0092 | 0.0646 | 0.88721 | 0.94 | -0.0632 | 0.055 | 0.250172 | 0.9622 | NaN | 0.0009 | 0.0338 | 0.979415 | 0.9915 | 0.028 | 0.0534 | 0.600146 | 0.9977 | -0.0204 | 0.0434 | 0.638147 | 0.9967 | NaN | -0.0259 | 0.0418 | 0.53504 | 0.8373 | 0.0011 | 0.064 | 0.986602 | 0.9974 | -0.0394 | 0.0553 | 0.475427 | 0.8651 |
| PC 41:7/PE 44:7 | 845.6306 | 26.31067 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0885 | 0.087 | 0.30906 | 0.675 | 0.0281 | 0.1194 | 0.814196 | 0.9324 | 0.15 | 0.1254 | 0.231883 | 0.596 | NaN | 0.0717 | 0.0806 | 0.373397 | 0.7361 | -0.0205 | 0.1052 | 0.845363 | 0.9389 | 0.1454 | 0.1176 | 0.216321 | 0.6714 | NaN | 0.1391 | 0.0607 | 0.021954 | 0.2578 | 0.1051 | 0.0831 | 0.205702 | 0.6538 | 0.1769 | 0.0878 | 0.043987 | 0.3772 | NaN | -0.0606 | 0.0461 | 0.189208 | 0.5115 | -0.0725 | 0.0639 | 0.256703 | 0.5687 | -0.0465 | 0.0657 | 0.47987 | 0.9759 | NaN | -0.0472 | 0.0369 | 0.200602 | 0.9708 | -0.0566 | 0.053 | 0.285256 | 0.9834 | -0.0369 | 0.0515 | 0.473783 | 0.9967 | NaN | -0.0323 | 0.0458 | 0.479986 | 0.8239 | -0.0377 | 0.0635 | 0.553109 | 0.7972 | -0.0252 | 0.0658 | 0.70112 | 0.9666 |
| PC 43:7/PE 46:7 | 873.657 | 28.227638 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1828 | 0.0795 | 0.021416 | 0.1665 | -0.2423 | 0.1252 | 0.052947 | 0.2788 | -0.1184 | 0.1046 | 0.257546 | 0.6326 | NaN | -0.1304 | 0.0745 | 0.079949 | 0.3825 | -0.1471 | 0.1126 | 0.191202 | 0.5409 | -0.0827 | 0.0988 | 0.402394 | 0.8019 | NaN | -0.1075 | 0.0564 | 0.056513 | 0.4216 | -0.0533 | 0.0911 | 0.558692 | 0.8202 | -0.1586 | 0.073 | 0.029909 | 0.3354 | NaN | -0.0375 | 0.0427 | 0.380026 | 0.6745 | -0.0767 | 0.0689 | 0.265295 | 0.5788 | 0.0022 | 0.0545 | 0.967085 | 0.9994 | NaN | -0.012 | 0.0344 | 0.726853 | 0.971 | -0.0002 | 0.0582 | 0.997706 | 0.9977 | -0.0172 | 0.0427 | 0.686331 | 0.9967 | NaN | -0.0351 | 0.0424 | 0.407645 | 0.8117 | -0.052 | 0.0688 | 0.449575 | 0.7348 | -0.0151 | 0.0545 | 0.781756 | 0.9748 |
| PC 40:7/PE 43:7 | 831.5581 | 22.282125 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0535 | 0.0831 | 0.519468 | 0.8173 | -0.0528 | 0.1158 | 0.648727 | 0.8671 | -0.0454 | 0.12 | 0.704894 | 0.8959 | NaN | -0.0143 | 0.0772 | 0.853337 | 0.9933 | -0.0183 | 0.1019 | 0.857331 | 0.9418 | 0.008 | 0.1134 | 0.944091 | 0.9876 | NaN | -0.0639 | 0.0583 | 0.273247 | 0.7604 | -0.0001 | 0.0812 | 0.998724 | 0.9998 | -0.1111 | 0.0846 | 0.189046 | 0.5997 | NaN | 0.0035 | 0.0438 | 0.93634 | 0.9731 | -0.0513 | 0.0619 | 0.407374 | 0.6798 | 0.0444 | 0.0618 | 0.472149 | 0.9735 | NaN | -0.0064 | 0.0351 | 0.855393 | 0.9722 | 0.0011 | 0.0517 | 0.983166 | 0.9977 | -0.0095 | 0.0485 | 0.844077 | 0.9967 | NaN | -0.0222 | 0.0434 | 0.609467 | 0.8587 | -0.0907 | 0.061 | 0.137061 | 0.4977 | 0.0377 | 0.0619 | 0.542625 | 0.9124 |
| PC 42:7/PE 45:7 | 859.5929 | 22.454245 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0834 | 0.0859 | 0.331521 | 0.6906 | 0.0385 | 0.1238 | 0.75575 | 0.9222 | 0.1224 | 0.1179 | 0.299023 | 0.6793 | NaN | 0.109 | 0.0794 | 0.169421 | 0.5196 | 0.0531 | 0.1086 | 0.62496 | 0.8459 | 0.1529 | 0.1104 | 0.166097 | 0.6552 | NaN | 0.0253 | 0.0607 | 0.676195 | 0.9288 | 0.0886 | 0.0862 | 0.303932 | 0.7522 | -0.036 | 0.0852 | 0.672736 | 0.8905 | NaN | -0.0663 | 0.0455 | 0.144865 | 0.4845 | -0.1153 | 0.0661 | 0.08108 | 0.3118 | -0.0191 | 0.0614 | 0.756346 | 0.9994 | NaN | 0.0418 | 0.0362 | 0.247859 | 0.9708 | 0.0444 | 0.0549 | 0.419054 | 0.9977 | 0.0397 | 0.0478 | 0.406412 | 0.9967 | NaN | -0.0511 | 0.0451 | 0.257776 | 0.7516 | -0.1155 | 0.0655 | 0.078107 | 0.3895 | 0.0091 | 0.0613 | 0.882078 | 0.993 |
| PC 38:8/PE 41:8 | 801.5294 | 24.024508 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0247 | 0.082 | 0.763168 | 0.9192 | 0.0444 | 0.1155 | 0.70087 | 0.8949 | 0.0072 | 0.1163 | 0.950409 | 0.9916 | NaN | 0.0282 | 0.0759 | 0.710565 | 0.9423 | 0.0576 | 0.1013 | 0.57005 | 0.8131 | 0.001 | 0.1091 | 0.992653 | 0.9993 | NaN | 0.0022 | 0.0578 | 0.969967 | 0.9971 | 0.0875 | 0.0804 | 0.276324 | 0.7263 | -0.1016 | 0.0825 | 0.218265 | 0.6205 | NaN | -0.0434 | 0.0431 | 0.314186 | 0.6261 | -0.0674 | 0.062 | 0.277192 | 0.5869 | -0.0044 | 0.0598 | 0.941925 | 0.9994 | NaN | -0.0199 | 0.0346 | 0.565617 | 0.9708 | 0.0109 | 0.0515 | 0.832036 | 0.9977 | -0.0536 | 0.0468 | 0.251764 | 0.9967 | NaN | -0.0066 | 0.0428 | 0.877456 | 0.9668 | -0.0241 | 0.0616 | 0.695885 | 0.8461 | 0.0218 | 0.0599 | 0.716038 | 0.968 |
| PC 39:8/PE 42:8 | 815.5796 | 25.336128 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1813 | 0.0892 | 0.042223 | 0.2354 | -0.2424 | 0.1331 | 0.068488 | 0.3 | -0.1117 | 0.1214 | 0.357322 | 0.7082 | NaN | -0.148 | 0.0829 | 0.074245 | 0.3627 | -0.1632 | 0.1186 | 0.168788 | 0.5189 | -0.1004 | 0.1139 | 0.378185 | 0.7878 | NaN | -0.0629 | 0.0638 | 0.324421 | 0.782 | -0.0339 | 0.0969 | 0.726103 | 0.8816 | -0.1024 | 0.0857 | 0.232095 | 0.6205 | NaN | -0.027 | 0.0478 | 0.572948 | 0.8059 | -0.0188 | 0.0741 | 0.799085 | 0.8869 | -0.0141 | 0.0629 | 0.823122 | 0.9994 | NaN | -0.0338 | 0.0382 | 0.37696 | 0.9708 | -0.0633 | 0.0606 | 0.29626 | 0.9835 | -0.0106 | 0.0494 | 0.829454 | 0.9967 | NaN | -0.0295 | 0.0474 | 0.533987 | 0.8373 | -0.0405 | 0.0731 | 0.579322 | 0.8075 | -0.0079 | 0.063 | 0.900628 | 0.9953 |
| PC 40:8/PE 43:8 | 829.5607 | 24.46232 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0646 | 0.0901 | 0.473535 | 0.7897 | 0.1509 | 0.1306 | 0.248006 | 0.552 | 0.0094 | 0.1233 | 0.939017 | 0.9916 | NaN | 0.0982 | 0.0834 | 0.238777 | 0.6038 | 0.2767 | 0.1141 | 0.015283 | 0.2909 | 0.0105 | 0.1156 | 0.927694 | 0.9876 | NaN | 0.0758 | 0.0633 | 0.231069 | 0.7309 | 0.1491 | 0.0906 | 0.099857 | 0.577 | 0.007 | 0.0873 | 0.935722 | 0.9766 | NaN | -0.0565 | 0.0476 | 0.234627 | 0.5455 | -0.0216 | 0.0714 | 0.762018 | 0.8754 | -0.0814 | 0.0631 | 0.197345 | 0.9514 | NaN | 0.0152 | 0.0381 | 0.689391 | 0.9708 | 0.0473 | 0.0586 | 0.419061 | 0.9977 | -0.0113 | 0.0498 | 0.820123 | 0.9967 | NaN | -0.06 | 0.0472 | 0.20389 | 0.7516 | -0.0044 | 0.0707 | 0.950315 | 0.9788 | -0.1044 | 0.063 | 0.097586 | 0.7232 |
| PC 41:8/PE 44:8 | 843.6115 | 25.703169 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1213 | 0.0843 | 0.150314 | 0.4635 | -0.2379 | 0.1336 | 0.074906 | 0.313 | -0.0497 | 0.1112 | 0.654708 | 0.885 | NaN | -0.0695 | 0.0787 | 0.37712 | 0.7403 | -0.1193 | 0.1208 | 0.323533 | 0.6906 | -0.0257 | 0.1046 | 0.805862 | 0.9546 | NaN | -0.0335 | 0.0599 | 0.575299 | 0.9166 | -0.0967 | 0.0954 | 0.310944 | 0.7581 | -0.0235 | 0.0788 | 0.76522 | 0.9437 | NaN | -0.0361 | 0.0446 | 0.419195 | 0.7088 | -0.0576 | 0.0735 | 0.433602 | 0.6955 | 0.0038 | 0.0573 | 0.947595 | 0.9994 | NaN | -0.0182 | 0.0359 | 0.61139 | 0.9708 | 0.0116 | 0.0618 | 0.851083 | 0.9977 | -0.0418 | 0.0448 | 0.350606 | 0.9967 | NaN | -0.0313 | 0.0443 | 0.479568 | 0.8239 | -0.0225 | 0.0735 | 0.759279 | 0.8842 | -0.0202 | 0.0573 | 0.72485 | 0.968 |
| PC 43:8/PE 46:8 | 871.6412 | 26.845314 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.157 | 0.0773 | 0.04221 | 0.2354 | -0.1399 | 0.1163 | 0.228653 | 0.5281 | -0.1537 | 0.1035 | 0.13759 | 0.4932 | NaN | -0.1033 | 0.0725 | 0.153898 | 0.491 | -0.0368 | 0.1046 | 0.725008 | 0.8829 | -0.1181 | 0.0979 | 0.227452 | 0.6764 | NaN | -0.0546 | 0.0553 | 0.323376 | 0.782 | -0.0609 | 0.082 | 0.457518 | 0.7964 | -0.0575 | 0.0745 | 0.439923 | 0.7876 | NaN | -0.037 | 0.0413 | 0.370362 | 0.6693 | -0.002 | 0.0635 | 0.97514 | 0.9823 | -0.0548 | 0.0538 | 0.308772 | 0.9622 | NaN | -0.0176 | 0.0332 | 0.59714 | 0.9708 | 0.0271 | 0.0527 | 0.607224 | 0.9977 | -0.0512 | 0.0422 | 0.225227 | 0.9967 | NaN | -0.0445 | 0.0409 | 0.276787 | 0.7695 | 0.0048 | 0.063 | 0.93931 | 0.9728 | -0.0767 | 0.0535 | 0.151897 | 0.7294 |
| PS 39.0 | 833.6163 | 25.583288 | Lipid | Phosphatidylserine | -0.0011 | 0.0857 | 0.989453 | 0.9949 | -0.1437 | 0.1325 | 0.278165 | 0.592 | 0.1153 | 0.111 | 0.298953 | 0.6793 | NaN | -0.0469 | 0.0795 | 0.555501 | 0.8543 | -0.0929 | 0.117 | 0.426991 | 0.7515 | 0.0439 | 0.1063 | 0.679477 | 0.9126 | NaN | 0.0191 | 0.0603 | 0.751841 | 0.9454 | 0.0153 | 0.0945 | 0.871258 | 0.9467 | 0.0336 | 0.0794 | 0.672378 | 0.8905 | NaN | -0.0657 | 0.0449 | 0.143276 | 0.4842 | -0.1199 | 0.0704 | 0.088718 | 0.3206 | -0.0359 | 0.0579 | 0.534913 | 0.9885 | NaN | -0.035 | 0.036 | 0.331318 | 0.9708 | -0.0704 | 0.059 | 0.232635 | 0.9728 | -0.0058 | 0.0454 | 0.897621 | 0.9967 | NaN | -0.0338 | 0.0447 | 0.44971 | 0.8178 | -0.0909 | 0.0704 | 0.19657 | 0.5437 | 0.002 | 0.0578 | 0.972392 | 0.996 |
| PS 40:3 | 841.5442 | 22.668882 | Lipid | Phosphatidylserine | 0.0088 | 0.0894 | 0.921924 | 0.9635 | 0.0426 | 0.1173 | 0.716406 | 0.9045 | -0.0396 | 0.1361 | 0.771196 | 0.9398 | NaN | 0.0154 | 0.0827 | 0.852002 | 0.9933 | 0.0967 | 0.103 | 0.348221 | 0.702 | -0.0597 | 0.1277 | 0.639924 | 0.8939 | NaN | -0.0061 | 0.0629 | 0.922496 | 0.9965 | 0.0486 | 0.0819 | 0.552967 | 0.8202 | -0.0842 | 0.0962 | 0.381714 | 0.7419 | NaN | -0.1065 | 0.0467 | 0.02253 | 0.3584 | -0.1349 | 0.0625 | 0.030784 | 0.2296 | -0.0673 | 0.0697 | 0.334341 | 0.9622 | NaN | -0.0468 | 0.0376 | 0.213885 | 0.9708 | -0.0443 | 0.0522 | 0.396037 | 0.9977 | -0.0525 | 0.0548 | 0.337798 | 0.9967 | NaN | -0.0538 | 0.0466 | 0.248053 | 0.7516 | -0.0871 | 0.0624 | 0.162246 | 0.5359 | -0.0082 | 0.0701 | 0.906629 | 0.9953 |
| PS 41:3 | 855.5623 | 24.634058 | Lipid | Phosphatidylserine | -0.1477 | 0.079 | 0.061597 | 0.2974 | -0.1564 | 0.1001 | 0.118117 | 0.3717 | -0.1211 | 0.1282 | 0.344836 | 0.7068 | NaN | -0.1122 | 0.0735 | 0.127244 | 0.4437 | -0.1018 | 0.089 | 0.252588 | 0.6142 | -0.0953 | 0.1206 | 0.429516 | 0.8249 | NaN | -0.0432 | 0.0565 | 0.444239 | 0.8554 | -0.0513 | 0.0714 | 0.472793 | 0.799 | -0.0485 | 0.0914 | 0.595276 | 0.8601 | NaN | -0.051 | 0.042 | 0.224639 | 0.5407 | -0.0096 | 0.0552 | 0.862059 | 0.9258 | -0.0973 | 0.0655 | 0.137472 | 0.9514 | NaN | -0.0511 | 0.0336 | 0.128121 | 0.9708 | -0.0834 | 0.0444 | 0.060537 | 0.6733 | -0.0017 | 0.0523 | 0.973896 | 0.9967 | NaN | -0.0524 | 0.0416 | 0.207867 | 0.7516 | -0.0314 | 0.0544 | 0.564424 | 0.8024 | -0.0731 | 0.066 | 0.268001 | 0.7827 |
| PS 42:3 | 869.6301 | 25.986755 | Lipid | Phosphatidylserine | -0.039 | 0.0821 | 0.634434 | 0.8777 | -0.0473 | 0.1145 | 0.679767 | 0.8879 | -0.0133 | 0.1191 | 0.911358 | 0.9854 | NaN | -0.0246 | 0.076 | 0.745986 | 0.964 | -0.0021 | 0.101 | 0.983719 | 0.989 | -0.0201 | 0.1117 | 0.856877 | 0.9708 | NaN | -0.0295 | 0.0578 | 0.609947 | 0.9199 | -0.0286 | 0.0801 | 0.720604 | 0.8816 | -0.0572 | 0.0843 | 0.497332 | 0.8203 | NaN | -0.0377 | 0.0431 | 0.382339 | 0.6745 | -0.0414 | 0.0613 | 0.499467 | 0.7431 | -0.0108 | 0.0612 | 0.859973 | 0.9994 | NaN | 0.0122 | 0.0347 | 0.725395 | 0.971 | 0.0497 | 0.051 | 0.329312 | 0.9977 | -0.0274 | 0.048 | 0.56881 | 0.9967 | NaN | -0.0241 | 0.0428 | 0.574533 | 0.8527 | -0.0162 | 0.061 | 0.790002 | 0.9029 | -0.0165 | 0.0613 | 0.787246 | 0.9748 |
| PS 42:3 | 869.633 | 26.532726 | Lipid | Phosphatidylserine | -0.203 | 0.0808 | 0.011984 | 0.1141 | -0.2596 | 0.1275 | 0.041794 | 0.2428 | -0.1644 | 0.1035 | 0.112099 | 0.4498 | NaN | -0.1364 | 0.0762 | 0.073648 | 0.3627 | -0.1114 | 0.1177 | 0.343874 | 0.702 | -0.1212 | 0.0982 | 0.217179 | 0.6714 | NaN | -0.0916 | 0.0579 | 0.113759 | 0.5674 | -0.0518 | 0.0934 | 0.579266 | 0.8355 | -0.1108 | 0.0735 | 0.131935 | 0.5272 | NaN | -0.0298 | 0.0438 | 0.495998 | 0.7563 | -0.0822 | 0.0703 | 0.242675 | 0.5571 | 0.0036 | 0.0547 | 0.947058 | 0.9994 | NaN | -0.0384 | 0.0349 | 0.271218 | 0.9708 | -0.0397 | 0.0589 | 0.50085 | 0.9977 | -0.037 | 0.0425 | 0.383871 | 0.9967 | NaN | -0.0441 | 0.0433 | 0.308385 | 0.7695 | -0.0727 | 0.07 | 0.298902 | 0.6411 | -0.0266 | 0.0544 | 0.624594 | 0.9472 |
| PS 44:3 | 897.665 | 27.227468 | Lipid | Phosphatidylserine | -0.0693 | 0.081 | 0.392128 | 0.7224 | -0.0013 | 0.1226 | 0.991825 | 0.9938 | -0.0972 | 0.1084 | 0.369696 | 0.7082 | NaN | 0.0048 | 0.0761 | 0.949292 | 0.9933 | 0.0801 | 0.1083 | 0.459894 | 0.7623 | -0.0281 | 0.1037 | 0.786231 | 0.9535 | NaN | -0.0005 | 0.0573 | 0.993179 | 0.9992 | 0.0075 | 0.0856 | 0.930145 | 0.9734 | -0.0177 | 0.0774 | 0.819278 | 0.9488 | NaN | 0.0008 | 0.0428 | 0.984976 | 0.9995 | 0.0198 | 0.0657 | 0.76305 | 0.8754 | -0.0014 | 0.0562 | 0.979522 | 0.9994 | NaN | 0.0198 | 0.0343 | 0.563528 | 0.9708 | 0.1018 | 0.0538 | 0.058467 | 0.6733 | -0.0412 | 0.0438 | 0.347608 | 0.9967 | NaN | -0.011 | 0.0424 | 0.795512 | 0.9482 | 0.0282 | 0.0652 | 0.664933 | 0.8393 | -0.0335 | 0.056 | 0.549447 | 0.9167 |
| PS 38:4 | 811.5485 | 24.525646 | Lipid | Phosphatidylserine | -0.1515 | 0.0896 | 0.090963 | 0.3578 | -0.3064 | 0.1427 | 0.03178 | 0.2396 | -0.0475 | 0.1141 | 0.676949 | 0.8876 | NaN | -0.1369 | 0.083 | 0.098845 | 0.4077 | -0.2166 | 0.1275 | 0.089396 | 0.4459 | -0.0527 | 0.107 | 0.621946 | 0.8939 | NaN | -0.0976 | 0.0632 | 0.122865 | 0.5898 | -0.1596 | 0.1019 | 0.117207 | 0.577 | -0.0536 | 0.0807 | 0.506198 | 0.8218 | NaN | -0.0213 | 0.0478 | 0.655276 | 0.846 | -0.0396 | 0.0802 | 0.621759 | 0.8019 | -0.0154 | 0.0587 | 0.793165 | 0.9994 | NaN | -0.0111 | 0.0383 | 0.771784 | 0.9722 | -0.053 | 0.0661 | 0.42293 | 0.9977 | 0.0165 | 0.0462 | 0.720799 | 0.9967 | NaN | -0.0314 | 0.0473 | 0.506955 | 0.8283 | -0.0711 | 0.0789 | 0.367703 | 0.6653 | -0.0112 | 0.0588 | 0.848473 | 0.9809 |
| PS 39:4 | 825.5579 | 25.606718 | Lipid | Phosphatidylserine | -0.0474 | 0.0853 | 0.578902 | 0.8499 | -0.0336 | 0.1243 | 0.786858 | 0.9222 | -0.0282 | 0.1185 | 0.812132 | 0.9518 | NaN | -0.0651 | 0.0789 | 0.408992 | 0.7538 | -0.0228 | 0.1091 | 0.83476 | 0.9389 | -0.0581 | 0.1113 | 0.601682 | 0.8877 | NaN | -0.0445 | 0.06 | 0.45839 | 0.863 | 0.0973 | 0.0873 | 0.264911 | 0.7133 | -0.1641 | 0.0835 | 0.049378 | 0.3839 | NaN | -0.0413 | 0.0448 | 0.357051 | 0.6636 | -0.1112 | 0.0659 | 0.091388 | 0.3255 | 0.0154 | 0.061 | 0.800321 | 0.9994 | NaN | -0.0671 | 0.0357 | 0.06014 | 0.9656 | -0.0824 | 0.0547 | 0.132268 | 0.8645 | -0.0507 | 0.0477 | 0.287813 | 0.9967 | NaN | -0.0293 | 0.0445 | 0.509813 | 0.8283 | -0.1112 | 0.0653 | 0.088841 | 0.4046 | 0.0402 | 0.061 | 0.509894 | 0.8952 |
| PS 35:5 | 767.4737 | 23.664724 | Lipid | Phosphatidylserine | 0.017 | 0.0838 | 0.83889 | 0.9457 | 0.0742 | 0.1148 | 0.518133 | 0.8001 | -0.0029 | 0.124 | 0.981161 | 0.9945 | NaN | -0.0323 | 0.0779 | 0.678761 | 0.9303 | 0.0621 | 0.1008 | 0.538126 | 0.7816 | -0.0833 | 0.1178 | 0.479524 | 0.8484 | NaN | -0.005 | 0.059 | 0.933078 | 0.9968 | 0.0084 | 0.0806 | 0.91682 | 0.9695 | -0.0203 | 0.0878 | 0.81714 | 0.9488 | NaN | 0.0472 | 0.0439 | 0.282422 | 0.5883 | 0.0476 | 0.0615 | 0.43888 | 0.6962 | 0.0513 | 0.0636 | 0.419642 | 0.9735 | NaN | 0.041 | 0.0352 | 0.243908 | 0.9708 | 0.055 | 0.0509 | 0.27983 | 0.9834 | 0.033 | 0.05 | 0.509053 | 0.9967 | NaN | 0.0274 | 0.0437 | 0.530351 | 0.8373 | 0.0175 | 0.0613 | 0.775251 | 0.8958 | 0.042 | 0.0637 | 0.509697 | 0.8952 |
| PS 37:5 | 795.5063 | 24.099264 | Lipid | Phosphatidylserine | 0.0547 | 0.0851 | 0.520451 | 0.8173 | 0.1163 | 0.1237 | 0.347354 | 0.675 | 0.0344 | 0.1175 | 0.769572 | 0.9398 | NaN | 0.0164 | 0.079 | 0.835761 | 0.99 | 0.0806 | 0.109 | 0.459321 | 0.7623 | -0.0097 | 0.1108 | 0.930225 | 0.9876 | NaN | 0.0766 | 0.0597 | 0.199567 | 0.7091 | 0.1349 | 0.0857 | 0.115665 | 0.577 | 0.0285 | 0.0832 | 0.732167 | 0.9305 | NaN | 0.0307 | 0.0447 | 0.492383 | 0.7557 | 0.0132 | 0.067 | 0.844319 | 0.9174 | 0.0497 | 0.0602 | 0.409107 | 0.9735 | NaN | 0.01 | 0.0359 | 0.78171 | 0.9722 | -0.0073 | 0.0557 | 0.895548 | 0.9977 | 0.0289 | 0.0474 | 0.542287 | 0.9967 | NaN | 0.0032 | 0.0445 | 0.942633 | 0.9786 | -0.0266 | 0.0667 | 0.689535 | 0.8461 | 0.0311 | 0.0604 | 0.607191 | 0.9367 |
| PS 39:5 | 823.5315 | 24.665892 | Lipid | Phosphatidylserine | -0.205 | 0.0838 | 0.014488 | 0.1311 | -0.314 | 0.1319 | 0.017269 | 0.1833 | -0.1482 | 0.1083 | 0.170966 | 0.5263 | NaN | -0.1543 | 0.0784 | 0.04922 | 0.3365 | -0.3295 | 0.1143 | 0.003949 | 0.1817 | -0.0838 | 0.1036 | 0.418651 | 0.8166 | NaN | -0.0951 | 0.06 | 0.112683 | 0.5674 | -0.2109 | 0.0929 | 0.023248 | 0.3282 | -0.0345 | 0.0781 | 0.658854 | 0.8899 | NaN | -0.0447 | 0.0452 | 0.322171 | 0.6354 | -0.0581 | 0.0746 | 0.435679 | 0.6955 | -0.0251 | 0.0565 | 0.656501 | 0.9994 | NaN | -0.0584 | 0.036 | 0.104276 | 0.9708 | -0.0738 | 0.0612 | 0.227828 | 0.96 | -0.0532 | 0.044 | 0.226754 | 0.9967 | NaN | -0.0536 | 0.0447 | 0.230511 | 0.7516 | -0.0477 | 0.0742 | 0.520549 | 0.7787 | -0.0508 | 0.0563 | 0.366972 | 0.8297 |
| PS 41:5 | 851.5624 | 25.434872 | Lipid | Phosphatidylserine | -0.0392 | 0.0878 | 0.655171 | 0.8782 | -0.0816 | 0.1391 | 0.557394 | 0.8118 | 0.0017 | 0.1135 | 0.988329 | 0.9955 | NaN | -0.0107 | 0.0813 | 0.895722 | 0.9933 | -0.0494 | 0.1224 | 0.686382 | 0.8728 | 0.0225 | 0.1065 | 0.832419 | 0.9674 | NaN | 0.0369 | 0.0619 | 0.551599 | 0.902 | 0.1247 | 0.0987 | 0.206213 | 0.6538 | -0.0309 | 0.0804 | 0.700187 | 0.9093 | NaN | -0.0405 | 0.0461 | 0.379506 | 0.6745 | -0.1351 | 0.0735 | 0.066087 | 0.2844 | 0.0382 | 0.0582 | 0.512071 | 0.9885 | NaN | 0.0019 | 0.037 | 0.95853 | 0.9897 | -0.0892 | 0.0613 | 0.146081 | 0.8645 | 0.0604 | 0.0455 | 0.184398 | 0.9967 | NaN | 0.0093 | 0.0459 | 0.839728 | 0.9557 | -0.0986 | 0.0734 | 0.179313 | 0.5427 | 0.0932 | 0.0579 | 0.107739 | 0.7232 |
| PS 37:6 | 793.4957 | 24.084814 | Lipid | Phosphatidylserine | 0.0441 | 0.0892 | 0.620786 | 0.8777 | 0.0308 | 0.1337 | 0.818046 | 0.9335 | 0.0616 | 0.1187 | 0.603801 | 0.8469 | NaN | 0.005 | 0.0828 | 0.951744 | 0.9933 | 0.1136 | 0.1178 | 0.334977 | 0.6989 | -0.0225 | 0.1136 | 0.842949 | 0.9708 | NaN | 0.0767 | 0.0626 | 0.220467 | 0.7201 | 0.2483 | 0.0924 | 0.00717 | 0.2454 | -0.052 | 0.0847 | 0.539482 | 0.8318 | NaN | -0.0625 | 0.0469 | 0.183046 | 0.5115 | -0.1636 | 0.0709 | 0.020954 | 0.2134 | 0.0214 | 0.0611 | 0.726132 | 0.9994 | NaN | -0.0137 | 0.0377 | 0.715578 | 0.971 | -0.0605 | 0.0594 | 0.308193 | 0.9977 | 0.022 | 0.048 | 0.646119 | 0.9967 | NaN | -0.0487 | 0.0466 | 0.296079 | 0.7695 | -0.1585 | 0.0703 | 0.024188 | 0.2725 | 0.0395 | 0.0611 | 0.51773 | 0.8961 |
| PS 39:6 | 821.5289 | 24.635998 | Lipid | Phosphatidylserine | -0.1608 | 0.0895 | 0.072324 | 0.3144 | -0.2237 | 0.1427 | 0.116853 | 0.3717 | -0.1602 | 0.1158 | 0.166673 | 0.5263 | NaN | -0.1442 | 0.0828 | 0.0817 | 0.3825 | -0.2591 | 0.1242 | 0.036939 | 0.395 | -0.1229 | 0.1094 | 0.261563 | 0.6818 | NaN | -0.047 | 0.0639 | 0.46204 | 0.8642 | -0.1165 | 0.1008 | 0.247973 | 0.6984 | 0.0153 | 0.0845 | 0.855935 | 0.9569 | NaN | -0.0292 | 0.0477 | 0.541093 | 0.7923 | -0.0195 | 0.0786 | 0.804358 | 0.8898 | -0.0536 | 0.0602 | 0.372937 | 0.9665 | NaN | 0.0009 | 0.0384 | 0.9823 | 0.9915 | -0.0949 | 0.0639 | 0.137601 | 0.8645 | 0.0614 | 0.0478 | 0.199106 | 0.9967 | NaN | -0.0582 | 0.0471 | 0.216181 | 0.7516 | -0.0502 | 0.0775 | 0.517427 | 0.7783 | -0.0784 | 0.0599 | 0.190339 | 0.7294 |
| PS 41:6 | 849.5462 | 24.797037 | Lipid | Phosphatidylserine | -0.0266 | 0.0851 | 0.754529 | 0.9192 | -0.0202 | 0.1219 | 0.868206 | 0.9547 | -0.0541 | 0.1183 | 0.647666 | 0.8806 | NaN | 0.019 | 0.0791 | 0.810306 | 0.9803 | -0.0564 | 0.107 | 0.597926 | 0.8293 | 0.0299 | 0.1132 | 0.791421 | 0.9535 | NaN | -0.0063 | 0.0599 | 0.915769 | 0.9951 | -0.0718 | 0.085 | 0.397855 | 0.7775 | 0.0536 | 0.0844 | 0.524888 | 0.826 | NaN | -0.0539 | 0.0446 | 0.227536 | 0.5414 | -0.0281 | 0.0653 | 0.666743 | 0.8422 | -0.0804 | 0.0604 | 0.183377 | 0.9514 | NaN | 0.0069 | 0.0359 | 0.847596 | 0.9722 | -0.021 | 0.0542 | 0.698732 | 0.9977 | 0.0295 | 0.0479 | 0.53793 | 0.9967 | NaN | -0.0688 | 0.0442 | 0.11974 | 0.7516 | -0.0258 | 0.0648 | 0.69 | 0.8461 | -0.1114 | 0.0601 | 0.063769 | 0.7232 |
| PS 46:6 | 919.6415 | 26.437166 | Lipid | Phosphatidylserine | -0.0158 | 0.0874 | 0.856664 | 0.9457 | -0.1551 | 0.1428 | 0.277503 | 0.592 | 0.073 | 0.1098 | 0.505996 | 0.8016 | NaN | 0.0036 | 0.0809 | 0.964306 | 0.9933 | -0.045 | 0.1278 | 0.724512 | 0.8829 | 0.0636 | 0.1031 | 0.536897 | 0.8742 | NaN | -0.0766 | 0.0614 | 0.211954 | 0.7091 | -0.0913 | 0.1002 | 0.362237 | 0.7705 | -0.0858 | 0.079 | 0.277757 | 0.6725 | NaN | 0 | 0.046 | 0.999939 | 0.9999 | -0.0715 | 0.0769 | 0.352837 | 0.6514 | 0.0551 | 0.0563 | 0.327803 | 0.9622 | NaN | -0.0186 | 0.0368 | 0.614306 | 0.9708 | -0.0192 | 0.0643 | 0.765713 | 0.9977 | -0.0182 | 0.0446 | 0.682685 | 0.9967 | NaN | 0.0251 | 0.0456 | 0.582264 | 0.8527 | -0.0558 | 0.0765 | 0.46597 | 0.7446 | 0.0819 | 0.0561 | 0.14411 | 0.7232 |
| PS 38:7 | 805.502 | 23.481342 | Lipid | Phosphatidylserine | 0.122 | 0.0793 | 0.124067 | 0.4101 | 0.033 | 0.1365 | 0.808913 | 0.9283 | 0.1806 | 0.0963 | 0.060652 | 0.3614 | NaN | 0.0811 | 0.0739 | 0.272763 | 0.6455 | 0.0526 | 0.1198 | 0.660761 | 0.8562 | 0.1302 | 0.092 | 0.157047 | 0.652 | NaN | 0.1302 | 0.0554 | 0.018768 | 0.2387 | 0.1684 | 0.0947 | 0.075576 | 0.549 | 0.1149 | 0.0687 | 0.094584 | 0.4637 | NaN | -0.0199 | 0.0424 | 0.637953 | 0.846 | -0.1291 | 0.0728 | 0.076071 | 0.3014 | 0.0372 | 0.0509 | 0.464004 | 0.9735 | NaN | 0.0438 | 0.0336 | 0.192794 | 0.9708 | 0.1169 | 0.0597 | 0.050245 | 0.6733 | 0.0107 | 0.0402 | 0.789251 | 0.9967 | NaN | -0.0148 | 0.042 | 0.72398 | 0.9166 | -0.1036 | 0.0724 | 0.15214 | 0.5225 | 0.0326 | 0.051 | 0.523475 | 0.8961 |
| PS 40:7 | 833.5156 | 24.11669 | Lipid | Phosphatidylserine | 0.0394 | 0.0853 | 0.644253 | 0.8782 | -0.0058 | 0.122 | 0.962239 | 0.9746 | 0.0894 | 0.1198 | 0.455478 | 0.755 | NaN | 0.0858 | 0.0791 | 0.277897 | 0.6471 | 0.1148 | 0.1087 | 0.290808 | 0.6717 | 0.1031 | 0.1123 | 0.35866 | 0.7716 | NaN | 0.0947 | 0.0598 | 0.113637 | 0.5674 | 0.0913 | 0.0853 | 0.284326 | 0.73 | 0.0809 | 0.0847 | 0.33956 | 0.7154 | NaN | -0.0178 | 0.0449 | 0.69141 | 0.8519 | -0.0629 | 0.0652 | 0.33475 | 0.6487 | 0.0459 | 0.0616 | 0.456263 | 0.9735 | NaN | 0.0575 | 0.0358 | 0.10806 | 0.9708 | 0.0803 | 0.0538 | 0.136064 | 0.8645 | 0.0366 | 0.0485 | 0.450454 | 0.9967 | NaN | -0.0318 | 0.0446 | 0.47534 | 0.8239 | -0.0633 | 0.0647 | 0.327948 | 0.6453 | 0.0119 | 0.062 | 0.847657 | 0.9809 |
| PS 41:7 | 847.5315 | 24.377514 | Lipid | Phosphatidylserine | 0.0728 | 0.086 | 0.397486 | 0.7289 | 0.1123 | 0.1233 | 0.362155 | 0.6924 | 0.0176 | 0.1193 | 0.882912 | 0.9697 | NaN | 0.1007 | 0.0795 | 0.205408 | 0.5669 | 0.0944 | 0.1083 | 0.383048 | 0.7136 | 0.0668 | 0.1125 | 0.552291 | 0.8762 | NaN | 0.0335 | 0.0607 | 0.58088 | 0.9166 | 0.0112 | 0.0871 | 0.897285 | 0.9599 | 0.0506 | 0.0845 | 0.54907 | 0.8359 | NaN | 0.0265 | 0.0453 | 0.559333 | 0.802 | 0.0572 | 0.0662 | 0.387376 | 0.6687 | -0.0024 | 0.0614 | 0.968856 | 0.9994 | NaN | -0.0116 | 0.0364 | 0.749972 | 0.9722 | -0.0247 | 0.0555 | 0.655457 | 0.9977 | -0.0037 | 0.0482 | 0.939324 | 0.9967 | NaN | 0.0018 | 0.0451 | 0.967517 | 0.9927 | 0.0655 | 0.0656 | 0.318017 | 0.6453 | -0.0579 | 0.0613 | 0.344949 | 0.8286 |
| PS 42:7 | 861.5447 | 24.69211 | Lipid | Phosphatidylserine | -0.1503 | 0.087 | 0.084103 | 0.3439 | -0.1704 | 0.1139 | 0.134523 | 0.3992 | -0.1189 | 0.1333 | 0.372202 | 0.7082 | NaN | -0.0653 | 0.0823 | 0.427407 | 0.7682 | -0.1424 | 0.1002 | 0.155193 | 0.5063 | 0.0168 | 0.1306 | 0.897661 | 0.9798 | NaN | -0.0491 | 0.062 | 0.428417 | 0.8487 | -0.0694 | 0.0808 | 0.390241 | 0.7775 | -0.032 | 0.0951 | 0.736623 | 0.9305 | NaN | -0.0145 | 0.0465 | 0.754372 | 0.8904 | 0.009 | 0.0629 | 0.885577 | 0.94 | -0.0327 | 0.0689 | 0.634977 | 0.9994 | NaN | 0.028 | 0.0374 | 0.453131 | 0.9708 | 0.0365 | 0.0522 | 0.484073 | 0.9977 | 0.0175 | 0.0543 | 0.746711 | 0.9967 | NaN | -0.0258 | 0.046 | 0.575125 | 0.8527 | -0.0173 | 0.062 | 0.780198 | 0.8991 | -0.0285 | 0.069 | 0.679272 | 0.9564 |
| PS 39:8 | 817.4908 | 23.6556 | Lipid | Phosphatidylserine | 0.0263 | 0.085 | 0.756802 | 0.9192 | -0.0764 | 0.1231 | 0.535232 | 0.8052 | 0.1365 | 0.1159 | 0.239005 | 0.6101 | NaN | 0.0041 | 0.0787 | 0.95877 | 0.9933 | -0.0576 | 0.1082 | 0.594516 | 0.8266 | 0.0975 | 0.1095 | 0.373259 | 0.7878 | NaN | 0.0717 | 0.0597 | 0.229838 | 0.7309 | 0.0889 | 0.0873 | 0.308316 | 0.7564 | 0.0661 | 0.0827 | 0.423712 | 0.7865 | NaN | -0.0833 | 0.0446 | 0.061598 | 0.3995 | -0.1707 | 0.0641 | 0.007759 | 0.1672 | -0.0072 | 0.0605 | 0.905143 | 0.9994 | NaN | -0.0158 | 0.0359 | 0.660487 | 0.9708 | -0.0107 | 0.055 | 0.846045 | 0.9977 | -0.0157 | 0.0476 | 0.741227 | 0.9967 | NaN | -0.0834 | 0.0442 | 0.059281 | 0.7347 | -0.1807 | 0.0633 | 0.004312 | 0.2424 | 0.0024 | 0.0606 | 0.968662 | 0.996 |
| 16-bromo-9E-hexadecenoic acid | 332.1376 | 11.983191 | Lipid | Halogenated Fatty Acids | -0.1339 | 0.0834 | 0.108377 | 0.381 | -0.205 | 0.1176 | 0.081328 | 0.3252 | -0.0889 | 0.117 | 0.447365 | 0.7518 | NaN | -0.0731 | 0.0782 | 0.349632 | 0.7175 | -0.1479 | 0.1043 | 0.156385 | 0.5063 | -0.0171 | 0.1117 | 0.878403 | 0.9756 | NaN | -0.0698 | 0.059 | 0.237039 | 0.7392 | -0.1096 | 0.0833 | 0.187907 | 0.652 | -0.0237 | 0.0833 | 0.776519 | 0.9437 | NaN | -0.0396 | 0.0442 | 0.370243 | 0.6693 | -0.0621 | 0.0644 | 0.33515 | 0.6487 | -0.027 | 0.0604 | 0.654617 | 0.9994 | NaN | 0.0142 | 0.0357 | 0.690856 | 0.9708 | 0.0004 | 0.0542 | 0.993464 | 0.9977 | 0.0264 | 0.0476 | 0.579554 | 0.9967 | NaN | -0.0426 | 0.0439 | 0.331805 | 0.7759 | -0.0886 | 0.0633 | 0.161843 | 0.5359 | -0.0051 | 0.0606 | 0.932487 | 0.996 |
| myo-inositol | 180.0635 | 0.624334 | Lipid | Inositol Metabolism | -0.017 | 0.0951 | 0.858111 | 0.9457 | -0.0344 | 0.1309 | 0.792695 | 0.9222 | -0.0041 | 0.1367 | 0.976297 | 0.994 | NaN | -0.1365 | 0.0896 | 0.127634 | 0.4437 | -0.0783 | 0.1149 | 0.495438 | 0.7769 | -0.1817 | 0.1343 | 0.176004 | 0.6632 | NaN | 0.0222 | 0.0669 | 0.739977 | 0.9415 | -0.0314 | 0.0914 | 0.730972 | 0.8816 | 0.0784 | 0.0968 | 0.418098 | 0.7823 | NaN | -0.0463 | 0.0499 | 0.35362 | 0.6617 | -0.0959 | 0.0696 | 0.168689 | 0.4506 | 0.0088 | 0.0702 | 0.900669 | 0.9994 | NaN | 0.0187 | 0.0401 | 0.641629 | 0.9708 | 0.0393 | 0.0582 | 0.500176 | 0.9977 | -0.0038 | 0.0552 | 0.945237 | 0.9967 | NaN | -0.0346 | 0.0496 | 0.484683 | 0.8258 | -0.0468 | 0.0695 | 0.500615 | 0.7761 | -0.0206 | 0.0703 | 0.769922 | 0.9748 |
| LysoPA 20.5 | 456.2297 | 14.845019 | Lipid | Lysolipid, PA | 0.1815 | 0.0798 | 0.022911 | 0.1738 | 0.3058 | 0.1128 | 0.0067 | 0.1275 | 0.0686 | 0.1103 | 0.534032 | 0.8099 | NaN | 0.1215 | 0.075 | 0.105199 | 0.4118 | 0.1731 | 0.105 | 0.099037 | 0.4459 | 0.0355 | 0.104 | 0.732993 | 0.9342 | NaN | -0.0263 | 0.0587 | 0.654744 | 0.9288 | 0.1055 | 0.0838 | 0.207911 | 0.6538 | -0.1455 | 0.0797 | 0.06782 | 0.4364 | NaN | 0.1128 | 0.0419 | 0.007054 | 0.3584 | 0.1553 | 0.0615 | 0.011654 | 0.1777 | 0.0751 | 0.0563 | 0.182602 | 0.9514 | NaN | 0.0415 | 0.0343 | 0.225648 | 0.9708 | 0.0845 | 0.0527 | 0.108473 | 0.7937 | 0.0044 | 0.0447 | 0.922511 | 0.9967 | NaN | 0.1127 | 0.0415 | 0.006619 | 0.7271 | 0.1281 | 0.062 | 0.038844 | 0.3022 | 0.1002 | 0.0561 | 0.073918 | 0.7232 |
| LysoPC 15:0 | 481.3168 | 21.947886 | Lipid | Lysolipid, PC | 0.1776 | 0.0837 | 0.033909 | 0.2202 | 0.1184 | 0.102 | 0.245605 | 0.5511 | 0.2912 | 0.1438 | 0.042916 | 0.3531 | NaN | 0.1441 | 0.0779 | 0.064157 | 0.3472 | 0.1166 | 0.0894 | 0.192048 | 0.5409 | 0.2195 | 0.1373 | 0.109762 | 0.577 | NaN | 0.1224 | 0.0591 | 0.03828 | 0.3464 | 0.1337 | 0.0705 | 0.057856 | 0.499 | 0.1042 | 0.105 | 0.320781 | 0.6944 | NaN | 0.0282 | 0.045 | 0.529845 | 0.7799 | -0.0049 | 0.0557 | 0.930118 | 0.9554 | 0.0924 | 0.0757 | 0.222098 | 0.9578 | NaN | 0.0465 | 0.0358 | 0.194538 | 0.9708 | 0.0352 | 0.0458 | 0.441557 | 0.9977 | 0.0697 | 0.0596 | 0.242313 | 0.9967 | NaN | 0.0537 | 0.0443 | 0.225612 | 0.7516 | 0.0199 | 0.055 | 0.716924 | 0.8584 | 0.1208 | 0.0752 | 0.108258 | 0.7232 |
| LysoPC 16:0 | 495.3327 | 22.244642 | Lipid | Lysolipid, PC | 0.0968 | 0.0842 | 0.250123 | 0.6074 | -0.0722 | 0.1223 | 0.554862 | 0.8103 | 0.2552 | 0.1146 | 0.025939 | 0.2796 | NaN | 0.0686 | 0.0781 | 0.379562 | 0.7403 | 0.0085 | 0.1086 | 0.937316 | 0.9726 | 0.1814 | 0.1106 | 0.100956 | 0.5686 | NaN | 0.0587 | 0.0593 | 0.322633 | 0.782 | 0.0165 | 0.086 | 0.847764 | 0.9285 | 0.083 | 0.0844 | 0.325262 | 0.7013 | NaN | -0.0557 | 0.0447 | 0.212818 | 0.5221 | -0.1114 | 0.0647 | 0.085178 | 0.3135 | 0.0139 | 0.0619 | 0.821726 | 0.9994 | NaN | 0.045 | 0.0355 | 0.205454 | 0.9708 | -0.0057 | 0.0546 | 0.916699 | 0.9977 | 0.0935 | 0.047 | 0.046715 | 0.9967 | NaN | -0.0208 | 0.0443 | 0.638764 | 0.8685 | -0.083 | 0.0646 | 0.198656 | 0.5437 | 0.0508 | 0.0613 | 0.407175 | 0.8463 |
| LysoPC 18:0 | 523.3636 | 22.659883 | Lipid | Lysolipid, PC | 0.1157 | 0.0857 | 0.177051 | 0.5051 | 0.0384 | 0.1274 | 0.762979 | 0.9222 | 0.1881 | 0.116 | 0.104958 | 0.4389 | NaN | 0.0754 | 0.0798 | 0.344729 | 0.7127 | 0.0814 | 0.1118 | 0.466817 | 0.7643 | 0.1113 | 0.1117 | 0.319204 | 0.7194 | NaN | 0.0426 | 0.0607 | 0.483079 | 0.8859 | 0.0833 | 0.0887 | 0.347848 | 0.7705 | -0.0123 | 0.0855 | 0.886046 | 0.9707 | NaN | -0.0803 | 0.0457 | 0.079016 | 0.4034 | -0.1566 | 0.0676 | 0.020539 | 0.2134 | 0.0013 | 0.0613 | 0.983531 | 0.9994 | NaN | 0.0697 | 0.036 | 0.05294 | 0.9656 | 0.0852 | 0.0561 | 0.128946 | 0.8645 | 0.0585 | 0.0474 | 0.217827 | 0.9967 | NaN | -0.0073 | 0.0452 | 0.87183 | 0.9644 | -0.0897 | 0.0677 | 0.184835 | 0.5427 | 0.0755 | 0.0604 | 0.210869 | 0.7294 |
| LysoPC 16:1 | 493.3177 | 21.817492 | Lipid | Lysolipid, PC | 0.1996 | 0.0857 | 0.019801 | 0.1584 | 0.0561 | 0.1413 | 0.691471 | 0.892 | 0.2929 | 0.1072 | 0.006291 | 0.1158 | NaN | 0.1486 | 0.0801 | 0.063528 | 0.3472 | 0.1293 | 0.1241 | 0.297426 | 0.6731 | 0.2126 | 0.1048 | 0.042493 | 0.4527 | NaN | 0.1348 | 0.0605 | 0.025877 | 0.28 | 0.1673 | 0.0979 | 0.087369 | 0.549 | 0.1067 | 0.0801 | 0.183215 | 0.5977 | NaN | -0.0204 | 0.0466 | 0.661696 | 0.846 | -0.1172 | 0.0757 | 0.121577 | 0.3875 | 0.0584 | 0.0584 | 0.317471 | 0.9622 | NaN | 0.0696 | 0.0365 | 0.056829 | 0.9656 | 0.0519 | 0.0627 | 0.407714 | 0.9977 | 0.0834 | 0.045 | 0.063762 | 0.9967 | NaN | 0.0287 | 0.0459 | 0.531513 | 0.8373 | -0.0437 | 0.0753 | 0.561612 | 0.8024 | 0.089 | 0.0577 | 0.123302 | 0.7232 |
| LysoPC 18:1 | 521.3471 | 22.368698 | Lipid | Lysolipid, PC | -0.0788 | 0.0857 | 0.357762 | 0.7053 | -0.2342 | 0.11 | 0.033298 | 0.2428 | 0.1847 | 0.1349 | 0.171066 | 0.5263 | NaN | -0.0798 | 0.0792 | 0.313799 | 0.6816 | -0.1738 | 0.0979 | 0.075936 | 0.4408 | 0.1321 | 0.1278 | 0.301248 | 0.7079 | NaN | -0.0274 | 0.0605 | 0.650247 | 0.9288 | -0.0609 | 0.0804 | 0.448938 | 0.7964 | -0.0109 | 0.0983 | 0.912074 | 0.9738 | NaN | -0.0151 | 0.0452 | 0.738899 | 0.8848 | -0.0336 | 0.0618 | 0.586634 | 0.7765 | 0.0405 | 0.0704 | 0.564524 | 0.9885 | NaN | -0.0416 | 0.0361 | 0.248747 | 0.9708 | -0.1218 | 0.0489 | 0.012724 | 0.5742 | 0.0731 | 0.0547 | 0.18143 | 0.9967 | NaN | 0.0322 | 0.045 | 0.474546 | 0.8239 | 0.0086 | 0.062 | 0.89021 | 0.9587 | 0.0931 | 0.0697 | 0.181784 | 0.7294 |
| LysoPC 18:3 | 517.4306 | 23.745913 | Lipid | Lysolipid, PC | -0.0096 | 0.0837 | 0.909159 | 0.9586 | -0.1957 | 0.1234 | 0.112783 | 0.3717 | 0.1537 | 0.1111 | 0.166317 | 0.5263 | NaN | -0.0424 | 0.0776 | 0.58453 | 0.8776 | -0.1279 | 0.1097 | 0.243495 | 0.6054 | 0.0855 | 0.1064 | 0.421711 | 0.8197 | NaN | 0.0202 | 0.0589 | 0.731235 | 0.9415 | -0.0164 | 0.0892 | 0.854011 | 0.9316 | 0.0498 | 0.0799 | 0.532675 | 0.826 | NaN | -0.0611 | 0.0439 | 0.163652 | 0.5058 | -0.1185 | 0.0661 | 0.073183 | 0.297 | -0.0126 | 0.0584 | 0.829442 | 0.9994 | NaN | -0.0117 | 0.0353 | 0.741161 | 0.9722 | -0.0231 | 0.0563 | 0.681518 | 0.9977 | 0.0013 | 0.0457 | 0.977246 | 0.9967 | NaN | -0.027 | 0.0437 | 0.536266 | 0.8373 | -0.0947 | 0.0661 | 0.151921 | 0.5225 | 0.0303 | 0.0581 | 0.601436 | 0.9367 |
| LysoPC 20:3 | 545.3462 | 22.560707 | Lipid | Lysolipid, PC | 0.1599 | 0.0823 | 0.05205 | 0.2644 | 0.0919 | 0.149 | 0.537212 | 0.8052 | 0.1969 | 0.0986 | 0.045784 | 0.3531 | NaN | 0.1225 | 0.0766 | 0.110074 | 0.4199 | 0.105 | 0.1306 | 0.42159 | 0.7507 | 0.1491 | 0.094 | 0.112632 | 0.5865 | NaN | 0.0259 | 0.0592 | 0.661764 | 0.9288 | 0.1086 | 0.1037 | 0.295006 | 0.7436 | -0.0301 | 0.0746 | 0.686646 | 0.903 | NaN | 0.0033 | 0.0442 | 0.941325 | 0.9731 | -0.0845 | 0.0804 | 0.29325 | 0.6018 | 0.0571 | 0.052 | 0.272274 | 0.9622 | NaN | 0.0114 | 0.0354 | 0.747553 | 0.9722 | -0.0012 | 0.0666 | 0.985705 | 0.9977 | 0.017 | 0.0413 | 0.681179 | 0.9967 | NaN | 0.0081 | 0.0438 | 0.854298 | 0.9644 | -0.087 | 0.0797 | 0.27501 | 0.6201 | 0.0612 | 0.052 | 0.238823 | 0.7365 |
| LysoPC 20:4 | 543.3407 | 19.784397 | Lipid | Lysolipid, PC | -0.0583 | 0.0873 | 0.504677 | 0.8075 | -0.2067 | 0.1307 | 0.113851 | 0.3717 | 0.0916 | 0.1171 | 0.433693 | 0.7481 | NaN | -0.081 | 0.0807 | 0.31564 | 0.6816 | -0.1337 | 0.1163 | 0.250064 | 0.6132 | 0.0331 | 0.1111 | 0.765982 | 0.9436 | NaN | 0.0028 | 0.0616 | 0.964046 | 0.9971 | -0.0219 | 0.0944 | 0.816418 | 0.9217 | 0.0235 | 0.0834 | 0.777852 | 0.9437 | NaN | -0.0804 | 0.0456 | 0.078056 | 0.4034 | -0.099 | 0.0706 | 0.16096 | 0.4399 | -0.0673 | 0.0607 | 0.267166 | 0.9622 | NaN | -0.01 | 0.0369 | 0.786297 | 0.9722 | -0.0364 | 0.0595 | 0.540458 | 0.9977 | 0.0163 | 0.0475 | 0.730915 | 0.9967 | NaN | -0.0361 | 0.0455 | 0.42847 | 0.8178 | -0.0787 | 0.0705 | 0.264277 | 0.6028 | -0.001 | 0.0607 | 0.987216 | 0.996 |
| LysoPE 16:0 | 453.2871 | 22.236048 | Lipid | Lysolipid, PE | 0.0327 | 0.0825 | 0.691757 | 0.8901 | -0.1773 | 0.1281 | 0.166595 | 0.4386 | 0.189 | 0.105 | 0.071899 | 0.3709 | NaN | -0.0167 | 0.0767 | 0.827675 | 0.9848 | -0.0999 | 0.1141 | 0.381288 | 0.7136 | 0.1058 | 0.1022 | 0.300762 | 0.7079 | NaN | 0.0205 | 0.058 | 0.724233 | 0.9415 | -0.0101 | 0.092 | 0.912148 | 0.9695 | 0.0389 | 0.0768 | 0.612947 | 0.8637 | NaN | -0.054 | 0.0434 | 0.212692 | 0.5221 | -0.1219 | 0.0684 | 0.074477 | 0.2979 | -0.0024 | 0.0559 | 0.965753 | 0.9994 | NaN | 0.0167 | 0.0348 | 0.630969 | 0.9708 | -0.0163 | 0.0581 | 0.779297 | 0.9977 | 0.0433 | 0.0433 | 0.317435 | 0.9967 | NaN | -0.0012 | 0.0431 | 0.97703 | 0.9951 | -0.0672 | 0.0689 | 0.329148 | 0.6453 | 0.0492 | 0.0553 | 0.373834 | 0.8297 |
| LysoPE 18:0 | 481.3184 | 22.637491 | Lipid | Lysolipid, PE | 0.0565 | 0.0827 | 0.494135 | 0.8017 | -0.1787 | 0.1255 | 0.15436 | 0.4298 | 0.2443 | 0.1061 | 0.021326 | 0.2559 | NaN | 0.0027 | 0.0771 | 0.972172 | 0.9933 | -0.1123 | 0.1114 | 0.313325 | 0.6823 | 0.1583 | 0.104 | 0.127835 | 0.6104 | NaN | 0.0313 | 0.0582 | 0.590492 | 0.9166 | -0.0173 | 0.0901 | 0.847795 | 0.9285 | 0.0675 | 0.0788 | 0.391566 | 0.7576 | NaN | -0.0627 | 0.0436 | 0.150205 | 0.4906 | -0.1297 | 0.0668 | 0.051956 | 0.2572 | -0.0088 | 0.0579 | 0.879743 | 0.9994 | NaN | 0.0168 | 0.0349 | 0.630189 | 0.9708 | -0.0266 | 0.0569 | 0.640523 | 0.9977 | 0.0544 | 0.0444 | 0.220256 | 0.9967 | NaN | -0.0118 | 0.0433 | 0.785362 | 0.9466 | -0.0925 | 0.067 | 0.167435 | 0.5381 | 0.0537 | 0.0569 | 0.345236 | 0.8286 |
| LysoPE 18:0 | 481.3465 | 22.425735 | Lipid | Lysolipid, PE | -0.0707 | 0.0793 | 0.37312 | 0.7078 | -0.1462 | 0.1131 | 0.196207 | 0.4734 | 0.009 | 0.1103 | 0.935288 | 0.9916 | NaN | -0.0624 | 0.0734 | 0.395198 | 0.7491 | -0.0964 | 0.1001 | 0.335536 | 0.6989 | -0.0038 | 0.1035 | 0.970489 | 0.9948 | NaN | 0.0259 | 0.0563 | 0.645319 | 0.9288 | -0.0368 | 0.0804 | 0.647391 | 0.8476 | 0.0734 | 0.0781 | 0.347491 | 0.7211 | NaN | -0.0648 | 0.0415 | 0.118797 | 0.4618 | -0.0188 | 0.0617 | 0.760849 | 0.8754 | -0.0984 | 0.0563 | 0.080349 | 0.8712 | NaN | -0.0476 | 0.0334 | 0.153444 | 0.9708 | -0.1036 | 0.0497 | 0.037074 | 0.6602 | 0.0034 | 0.0446 | 0.939677 | 0.9967 | NaN | -0.0642 | 0.0412 | 0.119745 | 0.7516 | -0.0427 | 0.0609 | 0.482909 | 0.7613 | -0.0773 | 0.0565 | 0.171407 | 0.7294 |
| LysoPE 18:2 | 477.2847 | 22.108313 | Lipid | Lysolipid, PE | -0.0072 | 0.0797 | 0.927998 | 0.9641 | -0.2336 | 0.1202 | 0.051984 | 0.2786 | 0.1478 | 0.1032 | 0.152043 | 0.5142 | NaN | -0.0184 | 0.0738 | 0.803423 | 0.979 | -0.1452 | 0.108 | 0.178662 | 0.5274 | 0.1082 | 0.0977 | 0.267903 | 0.6818 | NaN | 0.0292 | 0.0561 | 0.602752 | 0.9166 | 0.092 | 0.0915 | 0.314705 | 0.7586 | 0.0054 | 0.0751 | 0.942266 | 0.9766 | NaN | -0.0669 | 0.0417 | 0.108983 | 0.4618 | -0.2432 | 0.0609 | 0.000064 | 0.0355 | 0.0543 | 0.0535 | 0.31024 | 0.9622 | NaN | -0.0466 | 0.0335 | 0.164216 | 0.9708 | -0.1555 | 0.0523 | 0.002961 | 0.2724 | 0.033 | 0.0422 | 0.434979 | 0.9967 | NaN | -0.0549 | 0.0415 | 0.185609 | 0.7516 | -0.2617 | 0.0595 | 0.000011 | 0.006 | 0.0899 | 0.053 | 0.089865 | 0.7232 |
| LysoPS 21:0 | 567.3552 | 22.364582 | Lipid | Lysolipid, PS | -0.0859 | 0.0857 | 0.316157 | 0.6791 | -0.3302 | 0.1254 | 0.008466 | 0.146 | 0.1305 | 0.1141 | 0.252918 | 0.6289 | NaN | -0.0904 | 0.0792 | 0.253451 | 0.6274 | -0.1748 | 0.1173 | 0.136102 | 0.4744 | 0.0665 | 0.1089 | 0.541636 | 0.8742 | NaN | -0.0379 | 0.0605 | 0.530919 | 0.9005 | -0.0856 | 0.094 | 0.362416 | 0.7705 | -0.0057 | 0.0824 | 0.944788 | 0.9766 | NaN | -0.0958 | 0.0447 | 0.031994 | 0.3584 | -0.1786 | 0.068 | 0.008597 | 0.1672 | -0.0323 | 0.0597 | 0.587893 | 0.9975 | NaN | 0.0104 | 0.0363 | 0.77456 | 0.9722 | -0.0021 | 0.0603 | 0.972202 | 0.9977 | 0.0272 | 0.0465 | 0.558767 | 0.9967 | NaN | -0.0325 | 0.0448 | 0.46825 | 0.8239 | -0.1142 | 0.0696 | 0.10083 | 0.438 | 0.0319 | 0.0593 | 0.590873 | 0.9367 |
| rac-glycerol-1-myristate | 302.2458 | 22.129429 | Lipid | Monoacylglycerol | 0.0742 | 0.0831 | 0.371683 | 0.7078 | 0.1727 | 0.1138 | 0.128973 | 0.3869 | -0.0154 | 0.1194 | 0.89708 | 0.9806 | NaN | 0.0085 | 0.0778 | 0.913347 | 0.9933 | 0.0738 | 0.1026 | 0.472176 | 0.7643 | -0.0772 | 0.1128 | 0.493726 | 0.8652 | NaN | -0.0283 | 0.059 | 0.631628 | 0.9288 | -0.0692 | 0.0838 | 0.40903 | 0.784 | -0.0045 | 0.0846 | 0.957459 | 0.9766 | NaN | 0.0528 | 0.0436 | 0.226287 | 0.5407 | 0.1094 | 0.0609 | 0.072262 | 0.297 | 0.0005 | 0.0614 | 0.994107 | 0.9994 | NaN | 0.0171 | 0.0351 | 0.625313 | 0.9708 | 0.0177 | 0.0518 | 0.732209 | 0.9977 | 0.016 | 0.0482 | 0.740708 | 0.9967 | NaN | 0.0319 | 0.0434 | 0.462102 | 0.8239 | 0.0947 | 0.0607 | 0.118575 | 0.4609 | -0.0294 | 0.0614 | 0.63197 | 0.9483 |
| 1-octadecanoyl-rac-glycerol | 358.3087 | 22.912283 | Lipid | Monoacylglycerol | -0.063 | 0.0812 | 0.437815 | 0.7648 | 0.0882 | 0.1385 | 0.524087 | 0.8001 | -0.1321 | 0.0992 | 0.183055 | 0.5263 | NaN | -0.0591 | 0.0751 | 0.430901 | 0.7698 | 0.05 | 0.1219 | 0.681964 | 0.8726 | -0.1231 | 0.0931 | 0.186184 | 0.6674 | NaN | -0.0679 | 0.057 | 0.233182 | 0.7313 | -0.1664 | 0.0987 | 0.091788 | 0.5507 | -0.0384 | 0.0714 | 0.590215 | 0.8601 | NaN | 0.0184 | 0.0429 | 0.667507 | 0.846 | 0.1483 | 0.073 | 0.042105 | 0.2513 | -0.038 | 0.0516 | 0.460893 | 0.9735 | NaN | -0.0057 | 0.0343 | 0.868093 | 0.9722 | 0.0265 | 0.0618 | 0.667442 | 0.9977 | -0.0245 | 0.0406 | 0.546203 | 0.9967 | NaN | 0.0124 | 0.0425 | 0.770976 | 0.9353 | 0.1725 | 0.0719 | 0.01644 | 0.2658 | -0.063 | 0.0513 | 0.219269 | 0.7294 |
| 1-oleoyl-rac-glycerol | 356.2929 | 22.690039 | Lipid | Monoacylglycerol | 0.1622 | 0.0828 | 0.05023 | 0.2616 | 0.1536 | 0.1196 | 0.199219 | 0.4761 | 0.1776 | 0.1152 | 0.122925 | 0.4648 | NaN | 0.1319 | 0.077 | 0.086537 | 0.3825 | 0.1706 | 0.1045 | 0.102478 | 0.449 | 0.1206 | 0.1097 | 0.271716 | 0.6818 | NaN | 0.0366 | 0.0594 | 0.53834 | 0.9005 | 0.0611 | 0.0846 | 0.470078 | 0.799 | -0.0101 | 0.0845 | 0.904893 | 0.9707 | NaN | 0.0296 | 0.0443 | 0.504321 | 0.7669 | 0.0239 | 0.0652 | 0.714101 | 0.8608 | 0.0544 | 0.06 | 0.364885 | 0.9622 | NaN | 0.0848 | 0.0348 | 0.014932 | 0.7645 | 0.0792 | 0.0532 | 0.136792 | 0.8645 | 0.09 | 0.0464 | 0.052394 | 0.9967 | NaN | 0.05 | 0.0438 | 0.253585 | 0.7516 | 0.0483 | 0.0643 | 0.452824 | 0.7368 | 0.0661 | 0.0599 | 0.270332 | 0.7854 |
| 9,10,13-Trihydroxy-11-octadecenoic acid | 330.2412 | 20.380095 | Lipid | Octadecanoids | 0.0566 | 0.0857 | 0.508717 | 0.8116 | 0.1869 | 0.1174 | 0.111262 | 0.3717 | -0.0716 | 0.1236 | 0.562599 | 0.8352 | NaN | 0.0138 | 0.0797 | 0.862656 | 0.9933 | 0.0827 | 0.106 | 0.435269 | 0.7515 | -0.0856 | 0.1159 | 0.459935 | 0.8416 | NaN | -0.069 | 0.0608 | 0.256385 | 0.7568 | 0.0714 | 0.0836 | 0.393112 | 0.7775 | -0.2074 | 0.0863 | 0.016281 | 0.2643 | NaN | 0.0629 | 0.0449 | 0.160975 | 0.5058 | 0.0837 | 0.0635 | 0.187694 | 0.4797 | 0.0293 | 0.0638 | 0.646226 | 0.9994 | NaN | 0.0215 | 0.0362 | 0.551941 | 0.9708 | 0.0349 | 0.0534 | 0.513189 | 0.9977 | 0.01 | 0.0501 | 0.841336 | 0.9967 | NaN | 0.0734 | 0.0445 | 0.098982 | 0.7516 | 0.0481 | 0.0637 | 0.449904 | 0.7348 | 0.0954 | 0.0638 | 0.134679 | 0.7232 |
| PG 31.4 | 700.4412 | 22.19887 | Lipid | Phosphatidylglycerol | 0.0926 | 0.0842 | 0.271325 | 0.6373 | 0.1383 | 0.1169 | 0.236768 | 0.5379 | 0.0442 | 0.121 | 0.714836 | 0.9018 | NaN | 0.0821 | 0.0779 | 0.29167 | 0.6598 | 0.1065 | 0.1029 | 0.300701 | 0.6747 | 0.0486 | 0.1135 | 0.668311 | 0.902 | NaN | 0.0101 | 0.0597 | 0.865924 | 0.9805 | 0.0999 | 0.0817 | 0.221615 | 0.6655 | -0.066 | 0.0862 | 0.443739 | 0.7876 | NaN | 0.0359 | 0.0444 | 0.41895 | 0.7088 | 0.0491 | 0.0632 | 0.437471 | 0.6959 | 0.0049 | 0.0623 | 0.937057 | 0.9994 | NaN | 0.0583 | 0.0354 | 0.099115 | 0.9708 | 0.066 | 0.0521 | 0.205183 | 0.9357 | 0.0539 | 0.0487 | 0.268342 | 0.9967 | NaN | 0.0508 | 0.0439 | 0.248152 | 0.7516 | 0.0084 | 0.0632 | 0.89442 | 0.9587 | 0.0843 | 0.0619 | 0.173154 | 0.7294 |
| PI 34:1 | 696.3705 | 21.316105 | Lipid | Phosphatidylinositol | -0.0346 | 0.0803 | 0.666299 | 0.8782 | 0.0501 | 0.1312 | 0.702789 | 0.8949 | -0.0722 | 0.1023 | 0.480306 | 0.7821 | NaN | -0.0189 | 0.0743 | 0.799183 | 0.976 | 0.083 | 0.1151 | 0.470706 | 0.7643 | -0.0568 | 0.096 | 0.554338 | 0.8762 | NaN | -0.0013 | 0.0566 | 0.981284 | 0.9992 | 0.1082 | 0.0912 | 0.235441 | 0.6783 | -0.0498 | 0.0725 | 0.491555 | 0.8203 | NaN | 0.0186 | 0.0423 | 0.659329 | 0.846 | -0.0625 | 0.0705 | 0.375684 | 0.6609 | 0.0566 | 0.0529 | 0.28484 | 0.9622 | NaN | 0.0457 | 0.0338 | 0.176731 | 0.9708 | 0.05 | 0.0582 | 0.390071 | 0.9977 | 0.0483 | 0.0415 | 0.24412 | 0.9967 | NaN | 0.0042 | 0.0419 | 0.919592 | 0.9724 | -0.1116 | 0.0697 | 0.109064 | 0.4527 | 0.0655 | 0.053 | 0.216072 | 0.7294 |
| PI 35:1 | 710.3856 | 21.509493 | Lipid | Phosphatidylinositol | -0.0357 | 0.0836 | 0.669176 | 0.8782 | 0.0011 | 0.1291 | 0.993109 | 0.9938 | -0.0431 | 0.1127 | 0.702072 | 0.8959 | NaN | -0.028 | 0.0774 | 0.717844 | 0.945 | 0.0217 | 0.1133 | 0.847847 | 0.9398 | -0.0322 | 0.1058 | 0.760617 | 0.9436 | NaN | -0.0347 | 0.0588 | 0.554935 | 0.9023 | 0.0768 | 0.0901 | 0.394135 | 0.7775 | -0.0942 | 0.0795 | 0.236208 | 0.6205 | NaN | 0.054 | 0.044 | 0.21954 | 0.5339 | -0.0206 | 0.0692 | 0.765959 | 0.8754 | 0.0957 | 0.0578 | 0.097853 | 0.8712 | NaN | 0.0036 | 0.0353 | 0.91987 | 0.9722 | -0.0075 | 0.0574 | 0.896001 | 0.9977 | 0.0186 | 0.0456 | 0.683235 | 0.9967 | NaN | 0.0347 | 0.0437 | 0.427519 | 0.8178 | -0.0824 | 0.0683 | 0.227796 | 0.5642 | 0.1141 | 0.0577 | 0.048042 | 0.6979 |
| PI 36:1 | 724.4045 | 21.826448 | Lipid | Phosphatidylinositol | -0.0157 | 0.0793 | 0.842681 | 0.9457 | 0.0415 | 0.1185 | 0.726538 | 0.9045 | -0.058 | 0.1079 | 0.591091 | 0.8413 | NaN | -0.0062 | 0.0734 | 0.933154 | 0.9933 | 0.0678 | 0.104 | 0.51445 | 0.7797 | -0.0464 | 0.1013 | 0.646573 | 0.8939 | NaN | -0.0296 | 0.0558 | 0.595313 | 0.9166 | 0.0558 | 0.0827 | 0.499456 | 0.807 | -0.0772 | 0.0762 | 0.310597 | 0.6892 | NaN | 0.0299 | 0.0417 | 0.473081 | 0.7483 | -0.0136 | 0.0637 | 0.831489 | 0.9053 | 0.0477 | 0.0557 | 0.39117 | 0.9735 | NaN | 0.0311 | 0.0334 | 0.352222 | 0.9708 | 0.0429 | 0.0526 | 0.415025 | 0.9977 | 0.0264 | 0.0437 | 0.545334 | 0.9967 | NaN | 0.0381 | 0.0414 | 0.356641 | 0.7843 | -0.0468 | 0.0631 | 0.458973 | 0.743 | 0.0979 | 0.0555 | 0.077944 | 0.7232 |
| PI 37:1 | 738.421 | 21.882294 | Lipid | Phosphatidylinositol | -0.0412 | 0.085 | 0.627629 | 0.8777 | -0.0372 | 0.1251 | 0.765906 | 0.9222 | -0.0375 | 0.1159 | 0.746021 | 0.9233 | NaN | -0.0025 | 0.0789 | 0.974295 | 0.9933 | 0.0237 | 0.1104 | 0.830092 | 0.9389 | 0.0004 | 0.1092 | 0.997234 | 0.9993 | NaN | -0.0074 | 0.0599 | 0.901052 | 0.9908 | 0.0826 | 0.0878 | 0.346911 | 0.7705 | -0.0627 | 0.082 | 0.444342 | 0.7876 | NaN | -0.0003 | 0.0447 | 0.994858 | 0.9999 | -0.1037 | 0.0664 | 0.118516 | 0.3845 | 0.0746 | 0.0595 | 0.210319 | 0.9514 | NaN | 0.0179 | 0.0359 | 0.617619 | 0.9708 | 0.0109 | 0.0557 | 0.845186 | 0.9977 | 0.0278 | 0.0469 | 0.552614 | 0.9967 | NaN | -0.0236 | 0.0443 | 0.594611 | 0.8527 | -0.1525 | 0.0651 | 0.019188 | 0.2716 | 0.0752 | 0.0596 | 0.207219 | 0.7294 |
| PI 38:1 | 752.4347 | 22.042263 | Lipid | Phosphatidylinositol | -0.0443 | 0.0846 | 0.600524 | 0.8708 | 0.0337 | 0.1287 | 0.793492 | 0.9222 | -0.0925 | 0.1139 | 0.416791 | 0.7446 | NaN | -0.0113 | 0.0785 | 0.88531 | 0.9933 | 0.0611 | 0.113 | 0.588292 | 0.8258 | -0.0494 | 0.1076 | 0.646498 | 0.8939 | NaN | -0.013 | 0.0596 | 0.827865 | 0.9805 | 0.1085 | 0.0896 | 0.225828 | 0.6655 | -0.0819 | 0.0805 | 0.309137 | 0.6892 | NaN | 0.0114 | 0.0446 | 0.798801 | 0.9092 | -0.0753 | 0.069 | 0.275062 | 0.5862 | 0.0614 | 0.0591 | 0.299164 | 0.9622 | NaN | 0.0185 | 0.0357 | 0.605541 | 0.9708 | 0.0298 | 0.0572 | 0.602992 | 0.9977 | 0.0153 | 0.0464 | 0.742091 | 0.9967 | NaN | -0.0146 | 0.0442 | 0.740804 | 0.9202 | -0.1182 | 0.0681 | 0.082554 | 0.3918 | 0.0511 | 0.0592 | 0.387571 | 0.8324 |
| PI 39:1 | 766.4491 | 22.154734 | Lipid | Phosphatidylinositol | -0.0463 | 0.0798 | 0.561401 | 0.8421 | -0.0111 | 0.1188 | 0.925366 | 0.9682 | -0.0613 | 0.1086 | 0.572663 | 0.8352 | NaN | -0.016 | 0.074 | 0.828441 | 0.9848 | 0.0247 | 0.1045 | 0.81301 | 0.9349 | -0.0262 | 0.1024 | 0.798315 | 0.9546 | NaN | -0.0293 | 0.0561 | 0.601469 | 0.9166 | 0.0812 | 0.0831 | 0.328481 | 0.7705 | -0.1009 | 0.0765 | 0.187335 | 0.5977 | NaN | -0.0078 | 0.042 | 0.852286 | 0.9461 | -0.0953 | 0.0632 | 0.131496 | 0.4016 | 0.0506 | 0.0561 | 0.367148 | 0.9622 | NaN | 0.0124 | 0.0337 | 0.712997 | 0.971 | 0.0213 | 0.0529 | 0.686618 | 0.9977 | 0.01 | 0.044 | 0.820215 | 0.9967 | NaN | -0.0201 | 0.0416 | 0.628655 | 0.8654 | -0.1271 | 0.0623 | 0.041361 | 0.3085 | 0.0574 | 0.0561 | 0.306843 | 0.8042 |
| PI 40:1 | 780.4654 | 22.279175 | Lipid | Phosphatidylinositol | -0.0393 | 0.0856 | 0.646569 | 0.8782 | 0.0146 | 0.1192 | 0.902223 | 0.9573 | -0.0897 | 0.1228 | 0.465191 | 0.7642 | NaN | -0.0115 | 0.0793 | 0.884597 | 0.9933 | 0.0039 | 0.1046 | 0.970463 | 0.9835 | -0.0358 | 0.1163 | 0.757933 | 0.9436 | NaN | -0.0297 | 0.0602 | 0.621516 | 0.9285 | 0.0585 | 0.0832 | 0.482116 | 0.8009 | -0.1032 | 0.0866 | 0.233393 | 0.6205 | NaN | -0.0155 | 0.045 | 0.730531 | 0.8817 | -0.0598 | 0.0638 | 0.348866 | 0.6506 | 0.0154 | 0.0636 | 0.808212 | 0.9994 | NaN | -0.018 | 0.0361 | 0.618451 | 0.9708 | -0.0226 | 0.053 | 0.669657 | 0.9977 | -0.0109 | 0.0498 | 0.827298 | 0.9967 | NaN | -0.0442 | 0.0446 | 0.321349 | 0.7727 | -0.0893 | 0.0631 | 0.157025 | 0.5311 | -0.0097 | 0.0635 | 0.878892 | 0.993 |
| PI 41:1 | 794.4758 | 22.366863 | Lipid | Phosphatidylinositol | -0.0251 | 0.0853 | 0.768452 | 0.9192 | -0.0696 | 0.1248 | 0.577186 | 0.8295 | 0.0275 | 0.1158 | 0.812089 | 0.9518 | NaN | -0.0052 | 0.0789 | 0.947858 | 0.9933 | -0.0919 | 0.1094 | 0.400971 | 0.7257 | 0.0638 | 0.1088 | 0.557932 | 0.8762 | NaN | -0.0781 | 0.0599 | 0.191946 | 0.6946 | -0.0095 | 0.0875 | 0.913925 | 0.9695 | -0.1385 | 0.0825 | 0.093143 | 0.4632 | NaN | -0.0131 | 0.0448 | 0.770511 | 0.8919 | -0.0939 | 0.0664 | 0.157224 | 0.4339 | 0.0559 | 0.0593 | 0.345473 | 0.9622 | NaN | 0.0117 | 0.036 | 0.744861 | 0.9722 | 0.0014 | 0.0557 | 0.980169 | 0.9977 | 0.0234 | 0.0467 | 0.616056 | 0.9967 | NaN | -0.0005 | 0.0445 | 0.991543 | 0.9972 | -0.0826 | 0.0659 | 0.210332 | 0.5528 | 0.0699 | 0.0593 | 0.238516 | 0.7365 |
| PI 42:1 | 808.4955 | 22.451042 | Lipid | Phosphatidylinositol | 0.127 | 0.0856 | 0.137766 | 0.4388 | 0.0828 | 0.1293 | 0.522115 | 0.8001 | 0.1671 | 0.1129 | 0.138618 | 0.4937 | NaN | 0.1218 | 0.0791 | 0.123714 | 0.4437 | 0.0373 | 0.114 | 0.743461 | 0.89 | 0.1739 | 0.1056 | 0.099552 | 0.5686 | NaN | 0.0234 | 0.061 | 0.700779 | 0.9414 | 0.1216 | 0.0897 | 0.175346 | 0.6496 | -0.058 | 0.0835 | 0.487575 | 0.8181 | NaN | -0.0361 | 0.0457 | 0.429916 | 0.7148 | -0.1177 | 0.0696 | 0.091095 | 0.3255 | 0.0277 | 0.0591 | 0.639343 | 0.9994 | NaN | 0.0403 | 0.0363 | 0.266718 | 0.9708 | 0.0234 | 0.0577 | 0.684847 | 0.9977 | 0.0547 | 0.046 | 0.234678 | 0.9967 | NaN | -0.0153 | 0.0453 | 0.735075 | 0.918 | -0.099 | 0.0691 | 0.152391 | 0.5225 | 0.0499 | 0.0589 | 0.396849 | 0.8425 |
| PI 43:1 | 822.5134 | 22.551065 | Lipid | Phosphatidylinositol | 0.0398 | 0.0853 | 0.641239 | 0.8782 | 0.0287 | 0.1309 | 0.82622 | 0.9363 | 0.0539 | 0.1115 | 0.628658 | 0.859 | NaN | 0.0682 | 0.0789 | 0.38731 | 0.7434 | 0.1084 | 0.1153 | 0.347318 | 0.702 | 0.0647 | 0.1045 | 0.536017 | 0.8742 | NaN | -0.0223 | 0.0602 | 0.7113 | 0.9414 | 0.0862 | 0.0912 | 0.345038 | 0.7705 | -0.1081 | 0.0799 | 0.175823 | 0.5812 | NaN | -0.0346 | 0.0449 | 0.441412 | 0.7278 | -0.1122 | 0.0699 | 0.108372 | 0.3712 | 0.0257 | 0.0573 | 0.654436 | 0.9994 | NaN | 0.0131 | 0.036 | 0.716617 | 0.971 | 0.055 | 0.058 | 0.343093 | 0.9977 | -0.0163 | 0.0451 | 0.718386 | 0.9967 | NaN | -0.0262 | 0.0446 | 0.556199 | 0.8505 | -0.0934 | 0.0694 | 0.178668 | 0.5427 | 0.0252 | 0.0574 | 0.661262 | 0.9564 |
| choline | 104.1083 | 0.63293 | Lipid | Phospholipid Metabolism | 0.1547 | 0.0837 | 0.064381 | 0.3054 | 0.1818 | 0.1176 | 0.122342 | 0.3746 | 0.1031 | 0.1196 | 0.388859 | 0.7131 | NaN | 0.1403 | 0.0774 | 0.070074 | 0.3516 | 0.0814 | 0.106 | 0.442565 | 0.7563 | 0.1242 | 0.1121 | 0.26766 | 0.6818 | NaN | 0.04 | 0.0598 | 0.503624 | 0.8921 | 0.0789 | 0.0835 | 0.344495 | 0.7705 | -0.0103 | 0.0857 | 0.904559 | 0.9707 | NaN | -0.0062 | 0.0449 | 0.890777 | 0.9579 | 0.02 | 0.0647 | 0.757329 | 0.8746 | -0.0275 | 0.0621 | 0.658307 | 0.9994 | NaN | -0.0174 | 0.036 | 0.62846 | 0.9708 | 0.0133 | 0.0537 | 0.80402 | 0.9977 | -0.0542 | 0.0487 | 0.265763 | 0.9967 | NaN | -0.004 | 0.0445 | 0.927683 | 0.9724 | 0.027 | 0.0641 | 0.673635 | 0.8407 | -0.032 | 0.0622 | 0.607525 | 0.9367 |
| 3,7-dihydroxy-5-cholestanoic acid | 434.3391 | 22.831043 | Lipid | Primary Bile Acid Metabolism | -0.1567 | 0.0884 | 0.076261 | 0.3238 | -0.0916 | 0.12 | 0.44547 | 0.7474 | -0.2046 | 0.1322 | 0.121695 | 0.4648 | NaN | -0.203 | 0.0815 | 0.012723 | 0.1561 | -0.1445 | 0.1051 | 0.169174 | 0.5189 | -0.2554 | 0.1236 | 0.038803 | 0.4527 | NaN | -0.0402 | 0.0631 | 0.524635 | 0.8998 | 0.02 | 0.0848 | 0.813423 | 0.9217 | -0.0985 | 0.0948 | 0.298487 | 0.6808 | NaN | -0.083 | 0.0466 | 0.074597 | 0.3995 | -0.0531 | 0.0644 | 0.409619 | 0.6798 | -0.1309 | 0.0677 | 0.053139 | 0.8712 | NaN | -0.0166 | 0.0378 | 0.661342 | 0.9708 | -0.0212 | 0.0537 | 0.692973 | 0.9977 | -0.0055 | 0.0547 | 0.919374 | 0.9967 | NaN | -0.0642 | 0.0464 | 0.166672 | 0.7516 | -0.0389 | 0.064 | 0.543324 | 0.7934 | -0.1028 | 0.0684 | 0.132473 | 0.7232 |
| dihomoursodeoxycholic acid | 420.3245 | 22.660122 | Lipid | Primary Bile Acid Metabolism | -0.1742 | 0.081 | 0.031474 | 0.2145 | -0.2098 | 0.1353 | 0.120902 | 0.3728 | -0.1394 | 0.1013 | 0.168666 | 0.5263 | NaN | -0.145 | 0.0752 | 0.053958 | 0.3365 | -0.205 | 0.1184 | 0.083361 | 0.4425 | -0.1094 | 0.0956 | 0.252068 | 0.6818 | NaN | -0.1403 | 0.0568 | 0.013597 | 0.2028 | -0.0854 | 0.0961 | 0.37436 | 0.775 | -0.1799 | 0.0704 | 0.010541 | 0.1877 | NaN | -0.0184 | 0.0436 | 0.673432 | 0.846 | -0.0476 | 0.0741 | 0.520132 | 0.7556 | 0.0078 | 0.0532 | 0.883998 | 0.9994 | NaN | -0.034 | 0.0348 | 0.328331 | 0.9708 | -0.0149 | 0.0618 | 0.809011 | 0.9977 | -0.0436 | 0.0413 | 0.290537 | 0.9967 | NaN | -0.0105 | 0.0433 | 0.809056 | 0.9499 | -0.0642 | 0.0732 | 0.380583 | 0.6777 | 0.0262 | 0.0534 | 0.62352 | 0.9472 |
| glycochenodeoxycholate | 449.315 | 20.243961 | Lipid | Primary Bile Acid Metabolism | 0.0113 | 0.0846 | 0.893311 | 0.9586 | -0.1106 | 0.1179 | 0.34849 | 0.675 | 0.1422 | 0.1187 | 0.230753 | 0.596 | NaN | -0.1749 | 0.0828 | 0.034712 | 0.2777 | -0.2526 | 0.1037 | 0.014866 | 0.2909 | -0.0652 | 0.1254 | 0.602887 | 0.8877 | NaN | -0.0297 | 0.0595 | 0.617642 | 0.9265 | -0.075 | 0.0825 | 0.362919 | 0.7705 | 0.0208 | 0.0854 | 0.807572 | 0.9477 | NaN | 0.0443 | 0.0444 | 0.31839 | 0.6322 | -0.0113 | 0.0638 | 0.859907 | 0.9253 | 0.0978 | 0.0607 | 0.107473 | 0.8962 | NaN | -0.0151 | 0.0357 | 0.672204 | 0.9708 | -0.0522 | 0.0525 | 0.3204 | 0.9977 | 0.0259 | 0.0484 | 0.593279 | 0.9967 | NaN | 0.0323 | 0.0441 | 0.463027 | 0.8239 | -0.0741 | 0.0626 | 0.236143 | 0.5717 | 0.1385 | 0.06 | 0.02104 | 0.6979 |
| glycocholate | 465.309 | 18.850445 | Lipid | Primary Bile Acid Metabolism | 0.0293 | 0.085 | 0.730439 | 0.916 | -0.0924 | 0.1236 | 0.454777 | 0.7561 | 0.1552 | 0.1153 | 0.178198 | 0.5263 | NaN | -0.1386 | 0.0827 | 0.093854 | 0.3985 | -0.2682 | 0.1095 | 0.014341 | 0.2909 | -0.0061 | 0.118 | 0.958846 | 0.9893 | NaN | -0.0234 | 0.0599 | 0.695932 | 0.9393 | -0.1074 | 0.0859 | 0.21084 | 0.6538 | 0.0527 | 0.0828 | 0.524559 | 0.826 | NaN | 0.0764 | 0.0444 | 0.085681 | 0.4113 | 0.0217 | 0.0668 | 0.745731 | 0.873 | 0.1243 | 0.0586 | 0.033858 | 0.8712 | NaN | 0.0111 | 0.0358 | 0.756573 | 0.9722 | -0.0832 | 0.0545 | 0.12662 | 0.8645 | 0.0976 | 0.0461 | 0.034173 | 0.9432 | NaN | 0.0513 | 0.0442 | 0.245648 | 0.7516 | -0.0382 | 0.0659 | 0.561928 | 0.8024 | 0.1302 | 0.0585 | 0.026142 | 0.6979 |
| taurocholate | 515.2836 | 24.507624 | Lipid | Primary Bile Acid Metabolism | 0.0684 | 0.085 | 0.421199 | 0.7549 | 0.2278 | 0.1103 | 0.038872 | 0.2428 | -0.177 | 0.1291 | 0.170401 | 0.5263 | NaN | 0.1294 | 0.0789 | 0.100957 | 0.4077 | 0.1506 | 0.0989 | 0.127719 | 0.4744 | -0.0235 | 0.1295 | 0.855875 | 0.9708 | NaN | 0.0345 | 0.0599 | 0.565063 | 0.912 | 0.1159 | 0.0787 | 0.140562 | 0.5905 | -0.0666 | 0.0926 | 0.472067 | 0.8005 | NaN | 0.0234 | 0.0448 | 0.601254 | 0.818 | 0.0485 | 0.0614 | 0.429595 | 0.6954 | -0.0158 | 0.0676 | 0.814904 | 0.9994 | NaN | 0.0062 | 0.036 | 0.863643 | 0.9722 | 0.0179 | 0.0513 | 0.726505 | 0.9977 | -0.0166 | 0.053 | 0.753766 | 0.9967 | NaN | -0.0141 | 0.0446 | 0.751532 | 0.9221 | 0.023 | 0.0614 | 0.708475 | 0.8511 | -0.0704 | 0.067 | 0.2935 | 0.8042 |
| ursodeoxycholic acid | 392.2928 | 20.447248 | Lipid | Primary Bile Acid Metabolism | 0.0351 | 0.082 | 0.668551 | 0.8782 | 0.0477 | 0.1125 | 0.671685 | 0.8849 | 0.0231 | 0.1194 | 0.846891 | 0.9565 | NaN | 0.0296 | 0.0759 | 0.69618 | 0.9341 | 0.0423 | 0.0988 | 0.668379 | 0.864 | 0.0111 | 0.1121 | 0.921072 | 0.9876 | NaN | 0.0588 | 0.0576 | 0.30736 | 0.782 | 0.0979 | 0.0782 | 0.210619 | 0.6538 | 0.0009 | 0.0846 | 0.991889 | 0.9973 | NaN | -0.018 | 0.0432 | 0.6774 | 0.846 | 0.0008 | 0.0605 | 0.989634 | 0.9914 | -0.0238 | 0.0614 | 0.698814 | 0.9994 | NaN | -0.0686 | 0.0344 | 0.046422 | 0.9656 | -0.0622 | 0.05 | 0.213552 | 0.9357 | -0.0798 | 0.0478 | 0.095196 | 0.9967 | NaN | -0.0429 | 0.0429 | 0.317127 | 0.7708 | -0.058 | 0.06 | 0.333662 | 0.6463 | -0.0165 | 0.0615 | 0.788504 | 0.9748 |
| hyodeoxycholic acid | 392.2958 | 22.847624 | Lipid | Secondary Bile Acid Metabolism | 0.1553 | 0.0867 | 0.073307 | 0.3161 | 0.1658 | 0.1195 | 0.165423 | 0.4386 | 0.1003 | 0.1292 | 0.437573 | 0.7481 | NaN | 0.1469 | 0.0802 | 0.066951 | 0.3516 | 0.1336 | 0.1053 | 0.204191 | 0.5525 | 0.1048 | 0.1211 | 0.386808 | 0.7982 | NaN | 0.0575 | 0.0617 | 0.351452 | 0.793 | 0.0866 | 0.0843 | 0.304255 | 0.7522 | 0.0238 | 0.092 | 0.795905 | 0.9477 | NaN | 0.0631 | 0.0459 | 0.16894 | 0.5068 | 0.0905 | 0.0643 | 0.15894 | 0.4365 | 0.0328 | 0.0666 | 0.62282 | 0.9994 | NaN | 0.0145 | 0.0371 | 0.695825 | 0.971 | 0.0038 | 0.0544 | 0.94445 | 0.9977 | 0.019 | 0.0524 | 0.716718 | 0.9967 | NaN | 0.0626 | 0.0456 | 0.169692 | 0.7516 | 0.1113 | 0.0633 | 0.078819 | 0.3895 | 0.008 | 0.0669 | 0.905178 | 0.9953 |
| taurolithocholate | 483.298 | 21.677956 | Lipid | Secondary Bile Acid Metabolism | -0.0636 | 0.0859 | 0.458843 | 0.7746 | -0.1404 | 0.1383 | 0.310297 | 0.6377 | -0.0125 | 0.1086 | 0.908323 | 0.9854 | NaN | -0.0186 | 0.0799 | 0.816274 | 0.9803 | -0.0751 | 0.1225 | 0.539458 | 0.7816 | 0.0236 | 0.1023 | 0.817718 | 0.9616 | NaN | -0.0117 | 0.0606 | 0.846368 | 0.9805 | 0.0228 | 0.0985 | 0.817063 | 0.9217 | -0.0352 | 0.0769 | 0.64674 | 0.8837 | NaN | -0.0436 | 0.0451 | 0.333655 | 0.6417 | -0.1576 | 0.0728 | 0.030501 | 0.2296 | 0.0315 | 0.0558 | 0.573023 | 0.9885 | NaN | -0.0446 | 0.0361 | 0.216576 | 0.9708 | -0.0145 | 0.0622 | 0.815349 | 0.9977 | -0.0622 | 0.0435 | 0.152886 | 0.9967 | NaN | -0.0546 | 0.0447 | 0.22236 | 0.7516 | -0.1563 | 0.0722 | 0.030443 | 0.2981 | 0.0109 | 0.0559 | 0.845561 | 0.9809 |
| sphingosine | 299.2791 | 20.533209 | Lipid | Sphingolipid Metabolism | 0.1914 | 0.0801 | 0.0169 | 0.1377 | 0.1132 | 0.168 | 0.500477 | 0.7964 | 0.2264 | 0.0905 | 0.012399 | 0.1816 | NaN | 0.1451 | 0.0749 | 0.052715 | 0.3365 | 0.1451 | 0.1472 | 0.324034 | 0.6906 | 0.1742 | 0.087 | 0.045408 | 0.4545 | NaN | 0.081 | 0.0574 | 0.158355 | 0.6546 | 0.0291 | 0.1179 | 0.805134 | 0.9217 | 0.0858 | 0.067 | 0.200241 | 0.6141 | NaN | 0.0029 | 0.0435 | 0.946917 | 0.977 | -0.0804 | 0.0908 | 0.375725 | 0.6609 | 0.0415 | 0.049 | 0.397108 | 0.9735 | NaN | 0.0621 | 0.0342 | 0.069563 | 0.9708 | 0.1344 | 0.0737 | 0.068188 | 0.6957 | 0.043 | 0.0382 | 0.260397 | 0.9967 | NaN | 0.0511 | 0.0427 | 0.230946 | 0.7516 | 0.0376 | 0.0896 | 0.674664 | 0.8407 | 0.0664 | 0.0485 | 0.17082 | 0.7294 |
| C16 Sphinganine | 273.267 | 16.9842 | Lipid | Sphingolipids | -0.0712 | 0.0898 | 0.427726 | 0.7595 | -0.0995 | 0.1421 | 0.483772 | 0.7831 | -0.0209 | 0.1168 | 0.858339 | 0.9597 | NaN | -0.11 | 0.0831 | 0.185489 | 0.5452 | -0.0629 | 0.125 | 0.615069 | 0.8425 | -0.0864 | 0.1106 | 0.43431 | 0.8249 | NaN | -0.0393 | 0.0633 | 0.534774 | 0.9005 | -0.0802 | 0.0992 | 0.418946 | 0.792 | -0.0186 | 0.0828 | 0.822414 | 0.9492 | NaN | -0.0906 | 0.0469 | 0.053127 | 0.3914 | -0.1906 | 0.0741 | 0.010092 | 0.1688 | -0.0197 | 0.06 | 0.743286 | 0.9994 | NaN | -0.0415 | 0.0378 | 0.272794 | 0.9708 | -0.0474 | 0.0632 | 0.453833 | 0.9977 | -0.0348 | 0.0471 | 0.459463 | 0.9967 | NaN | -0.0448 | 0.0468 | 0.338955 | 0.7759 | -0.1006 | 0.075 | 0.180176 | 0.5427 | -0.0032 | 0.0602 | 0.958086 | 0.996 |
| C17 Sphinganine | 287.2825 | 16.69317 | Lipid | Sphingolipids | -0.0015 | 0.085 | 0.986041 | 0.9936 | 0.0662 | 0.1192 | 0.578512 | 0.8295 | -0.0599 | 0.1203 | 0.618593 | 0.8559 | NaN | 0.0202 | 0.0787 | 0.797204 | 0.976 | 0.1272 | 0.1046 | 0.223934 | 0.5831 | -0.0574 | 0.1128 | 0.610602 | 0.8917 | NaN | 0.061 | 0.0598 | 0.307649 | 0.782 | 0.0282 | 0.0835 | 0.735212 | 0.8816 | 0.0809 | 0.086 | 0.346857 | 0.7211 | NaN | -0.0573 | 0.0446 | 0.19847 | 0.5115 | -0.0607 | 0.0643 | 0.34524 | 0.6506 | -0.0417 | 0.0618 | 0.499353 | 0.988 | NaN | 0.013 | 0.0358 | 0.717824 | 0.971 | 0.0573 | 0.0528 | 0.2782 | 0.9834 | -0.0329 | 0.0486 | 0.498233 | 0.9967 | NaN | -0.0466 | 0.0443 | 0.292917 | 0.7695 | 0.0052 | 0.0636 | 0.935303 | 0.9719 | -0.0902 | 0.0614 | 0.141801 | 0.7232 |
| SM d32:1 | 674.5378 | 23.6049 | Lipid | Sphingomyelin | 0.1204 | 0.0978 | 0.218635 | 0.5715 | 0.0583 | 0.1257 | 0.642832 | 0.8665 | 0.2505 | 0.1555 | 0.107211 | 0.4416 | NaN | 0.0831 | 0.0909 | 0.360545 | 0.7308 | 0.0402 | 0.1105 | 0.716118 | 0.8811 | 0.1807 | 0.1478 | 0.221409 | 0.6714 | NaN | 0.0941 | 0.0688 | 0.17143 | 0.6546 | 0.1212 | 0.0873 | 0.165027 | 0.6267 | 0.0325 | 0.1135 | 0.774473 | 0.9437 | NaN | -0.0761 | 0.0521 | 0.143849 | 0.4842 | -0.1005 | 0.0675 | 0.136684 | 0.4056 | -0.014 | 0.0823 | 0.865171 | 0.9994 | NaN | 0.006 | 0.0416 | 0.886054 | 0.9722 | -0.0047 | 0.0561 | 0.933407 | 0.9977 | 0.0241 | 0.0643 | 0.707892 | 0.9967 | NaN | -0.0606 | 0.0517 | 0.240885 | 0.7516 | -0.1072 | 0.0669 | 0.108945 | 0.4527 | 0.0285 | 0.082 | 0.727843 | 0.968 |
| SM d33:1 | 688.5525 | 23.80148 | Lipid | Sphingomyelin | 0.059 | 0.0868 | 0.496762 | 0.8017 | 0.0194 | 0.1372 | 0.887513 | 0.9558 | 0.1082 | 0.1117 | 0.332899 | 0.7038 | NaN | 0.0547 | 0.0802 | 0.495845 | 0.7987 | 0.0602 | 0.1205 | 0.617568 | 0.8436 | 0.0873 | 0.105 | 0.406058 | 0.8023 | NaN | 0.061 | 0.061 | 0.317442 | 0.782 | 0.1485 | 0.0955 | 0.119992 | 0.577 | -0.0003 | 0.0802 | 0.99659 | 0.9994 | NaN | -0.0651 | 0.0458 | 0.155099 | 0.4949 | -0.1325 | 0.073 | 0.06952 | 0.2929 | -0.013 | 0.0581 | 0.823444 | 0.9994 | NaN | -0.0175 | 0.0367 | 0.633012 | 0.9708 | -0.0032 | 0.0611 | 0.957718 | 0.9977 | -0.0247 | 0.0456 | 0.587852 | 0.9967 | NaN | -0.0598 | 0.0454 | 0.188285 | 0.7516 | -0.1509 | 0.0722 | 0.036432 | 0.3022 | 0.0055 | 0.0581 | 0.925048 | 0.996 |
| SM d34:1 | 702.5686 | 24.01544 | Lipid | Sphingomyelin | -0.0618 | 0.0884 | 0.484585 | 0.7986 | -0.1798 | 0.143 | 0.20853 | 0.4927 | 0.0211 | 0.1125 | 0.851022 | 0.9565 | NaN | -0.0349 | 0.082 | 0.670657 | 0.9303 | -0.0971 | 0.1271 | 0.445265 | 0.7586 | 0.0264 | 0.1055 | 0.802657 | 0.9546 | NaN | -0.0073 | 0.0624 | 0.907342 | 0.9918 | -0.0145 | 0.1021 | 0.886719 | 0.9527 | -0.0178 | 0.0798 | 0.823692 | 0.9492 | NaN | -0.0925 | 0.0461 | 0.044948 | 0.3914 | -0.1085 | 0.0767 | 0.157091 | 0.4339 | -0.0698 | 0.0577 | 0.22628 | 0.9622 | NaN | -0.0125 | 0.0373 | 0.738261 | 0.9722 | -0.0331 | 0.0645 | 0.607763 | 0.9977 | -0.0004 | 0.0455 | 0.993061 | 0.9967 | NaN | -0.0541 | 0.046 | 0.240265 | 0.7516 | -0.0824 | 0.0765 | 0.281493 | 0.6236 | -0.0271 | 0.0579 | 0.639981 | 0.9483 |
| SM d36:1 | 730.6008 | 24.56354 | Lipid | Sphingomyelin | 0.0994 | 0.0838 | 0.235606 | 0.588 | 0.053 | 0.1308 | 0.685304 | 0.8901 | 0.105 | 0.1109 | 0.34379 | 0.7068 | NaN | 0.1027 | 0.0774 | 0.184806 | 0.5452 | 0.0032 | 0.1152 | 0.978151 | 0.9853 | 0.1234 | 0.1038 | 0.234682 | 0.6818 | NaN | 0.0945 | 0.0588 | 0.10782 | 0.5674 | 0.0598 | 0.0912 | 0.511749 | 0.8105 | 0.1132 | 0.0781 | 0.147199 | 0.5464 | NaN | -0.0415 | 0.0445 | 0.351356 | 0.6617 | 0.0486 | 0.07 | 0.487512 | 0.7333 | -0.1059 | 0.0576 | 0.065947 | 0.8712 | NaN | 0.0345 | 0.0354 | 0.329724 | 0.9708 | 0.0746 | 0.0577 | 0.196313 | 0.9357 | 0.0025 | 0.0452 | 0.956152 | 0.9967 | NaN | -0.0197 | 0.0441 | 0.656074 | 0.8716 | 0.0884 | 0.069 | 0.200596 | 0.5437 | -0.0973 | 0.0577 | 0.091885 | 0.7232 |
| SM d40:1 | 786.6598 | 26.323471 | Lipid | Sphingomyelin | 0.0645 | 0.0854 | 0.450449 | 0.7691 | -0.1313 | 0.1312 | 0.316828 | 0.6383 | 0.2023 | 0.111 | 0.068433 | 0.3664 | NaN | 0.0537 | 0.079 | 0.497003 | 0.7987 | -0.116 | 0.1151 | 0.31364 | 0.6823 | 0.1785 | 0.1045 | 0.087692 | 0.5595 | NaN | 0.0451 | 0.0601 | 0.452967 | 0.8592 | 0.0453 | 0.0937 | 0.628955 | 0.8438 | 0.035 | 0.0815 | 0.667688 | 0.8903 | NaN | -0.0937 | 0.045 | 0.037337 | 0.3817 | -0.1768 | 0.0684 | 0.009778 | 0.1687 | -0.0195 | 0.0594 | 0.742278 | 0.9994 | NaN | -0.0153 | 0.0361 | 0.67169 | 0.9708 | -0.0729 | 0.0583 | 0.211112 | 0.9357 | 0.0256 | 0.0461 | 0.579218 | 0.9967 | NaN | -0.053 | 0.0448 | 0.236698 | 0.7516 | -0.1559 | 0.0683 | 0.022501 | 0.2725 | 0.0327 | 0.0588 | 0.577814 | 0.9367 |
| SM d42:1 | 814.6936 | 27.731535 | Lipid | Sphingomyelin | -0.008 | 0.0854 | 0.925057 | 0.9635 | -0.2189 | 0.1398 | 0.117451 | 0.3717 | 0.1062 | 0.1067 | 0.31939 | 0.6905 | NaN | -0.0137 | 0.079 | 0.862305 | 0.9933 | -0.1909 | 0.1229 | 0.120132 | 0.4674 | 0.0884 | 0.1003 | 0.37782 | 0.7878 | NaN | -0.0218 | 0.0601 | 0.716875 | 0.9414 | -0.0555 | 0.1001 | 0.57973 | 0.8355 | -0.0157 | 0.0768 | 0.837931 | 0.9506 | NaN | -0.0874 | 0.0446 | 0.050013 | 0.3914 | -0.1643 | 0.0741 | 0.026735 | 0.2227 | -0.0343 | 0.0556 | 0.53738 | 0.9885 | NaN | -0.0154 | 0.036 | 0.66861 | 0.9708 | -0.0861 | 0.0628 | 0.170156 | 0.8945 | 0.0228 | 0.0434 | 0.599299 | 0.9967 | NaN | -0.0428 | 0.0445 | 0.335937 | 0.7759 | -0.1307 | 0.0743 | 0.078702 | 0.3895 | 0.0145 | 0.0554 | 0.79339 | 0.9748 |
| SM d34:2 | 700.5532 | 23.705383 | Lipid | Sphingomyelin | 0.2242 | 0.0882 | 0.011083 | 0.1096 | 0.1983 | 0.1395 | 0.155091 | 0.4298 | 0.2508 | 0.1128 | 0.026217 | 0.2796 | NaN | 0.188 | 0.0821 | 0.021998 | 0.2168 | 0.2197 | 0.1217 | 0.071024 | 0.4408 | 0.198 | 0.1076 | 0.065615 | 0.4962 | NaN | 0.1514 | 0.0624 | 0.015181 | 0.2205 | 0.2387 | 0.0955 | 0.012396 | 0.2845 | 0.0889 | 0.0829 | 0.283606 | 0.6732 | NaN | -0.0355 | 0.0484 | 0.463968 | 0.7407 | -0.0772 | 0.0773 | 0.317694 | 0.6331 | -0.0009 | 0.0612 | 0.988063 | 0.9994 | NaN | -0.0065 | 0.0386 | 0.866598 | 0.9722 | -0.0381 | 0.0638 | 0.550102 | 0.9977 | 0.0155 | 0.0477 | 0.744982 | 0.9967 | NaN | -0.0171 | 0.0479 | 0.72137 | 0.9166 | -0.0661 | 0.0766 | 0.387877 | 0.6841 | 0.0211 | 0.0609 | 0.729606 | 0.968 |
| SM d41:2 | 798.6609 | 26.103058 | Lipid | Sphingomyelin | 0.1906 | 0.0884 | 0.030996 | 0.2145 | 0.203 | 0.1294 | 0.11655 | 0.3717 | 0.1929 | 0.1228 | 0.116401 | 0.4525 | NaN | 0.1823 | 0.0817 | 0.025592 | 0.2243 | 0.2111 | 0.113 | 0.061641 | 0.4362 | 0.1679 | 0.1156 | 0.14629 | 0.6249 | NaN | 0.1131 | 0.0626 | 0.070827 | 0.4654 | 0.1538 | 0.0903 | 0.088476 | 0.549 | 0.0509 | 0.089 | 0.567549 | 0.8507 | NaN | -0.0203 | 0.0479 | 0.671486 | 0.846 | 0.0079 | 0.0714 | 0.911721 | 0.9514 | -0.019 | 0.065 | 0.77018 | 0.9994 | NaN | 0.0347 | 0.0379 | 0.360231 | 0.9708 | 0.0626 | 0.0584 | 0.283737 | 0.9834 | 0.0078 | 0.0508 | 0.877588 | 0.9967 | NaN | 0.0254 | 0.0471 | 0.589449 | 0.8527 | 0.0308 | 0.0705 | 0.66244 | 0.8393 | 0.0413 | 0.0645 | 0.521635 | 0.8961 |
| SM d42:2 | 812.6772 | 26.441246 | Lipid | Sphingomyelin | 0.0269 | 0.0882 | 0.760109 | 0.9192 | -0.0639 | 0.1413 | 0.650903 | 0.8679 | 0.0881 | 0.1125 | 0.433602 | 0.7481 | NaN | 0.0353 | 0.0816 | 0.665124 | 0.9303 | -0.0015 | 0.1247 | 0.99013 | 0.9919 | 0.0766 | 0.1056 | 0.468519 | 0.8416 | NaN | 0.0506 | 0.062 | 0.414184 | 0.8406 | 0.1206 | 0.0997 | 0.226434 | 0.6655 | -0.0023 | 0.0804 | 0.976873 | 0.9894 | NaN | -0.0534 | 0.0464 | 0.249343 | 0.5618 | -0.1402 | 0.0746 | 0.060326 | 0.2766 | 0.0144 | 0.0581 | 0.803786 | 0.9994 | NaN | -0.0342 | 0.0372 | 0.357613 | 0.9708 | -0.0886 | 0.0623 | 0.155021 | 0.8645 | -0.0015 | 0.0457 | 0.974258 | 0.9967 | NaN | -0.0157 | 0.0461 | 0.733939 | 0.918 | -0.0953 | 0.0746 | 0.201446 | 0.5437 | 0.0442 | 0.058 | 0.446042 | 0.8627 |
| 17-alpha-hydroxyprogesterone | 330.2045 | 18.162195 | Lipid | Steroid | 0.0868 | 0.0863 | 0.314646 | 0.6791 | 0.1954 | 0.1172 | 0.095432 | 0.3536 | -0.0252 | 0.1252 | 0.840374 | 0.9565 | NaN | 0.0399 | 0.0804 | 0.619809 | 0.9037 | 0.0784 | 0.1066 | 0.462047 | 0.7636 | -0.0409 | 0.1174 | 0.727599 | 0.9342 | NaN | -0.0784 | 0.0617 | 0.204078 | 0.7091 | 0.0531 | 0.0841 | 0.52752 | 0.8173 | -0.2187 | 0.088 | 0.013001 | 0.2243 | NaN | 0.115 | 0.0448 | 0.010251 | 0.3584 | 0.147 | 0.062 | 0.017756 | 0.2 | 0.073 | 0.0642 | 0.255769 | 0.9622 | NaN | 0.026 | 0.0365 | 0.476344 | 0.9708 | 0.0531 | 0.0531 | 0.317646 | 0.9977 | -0.0019 | 0.0506 | 0.97026 | 0.9967 | NaN | 0.1206 | 0.0444 | 0.006583 | 0.7271 | 0.1204 | 0.0622 | 0.052864 | 0.3516 | 0.118 | 0.064 | 0.064981 | 0.7232 |
| cortisol | 362.2099 | 13.811827 | Lipid | Steroid | -0.0484 | 0.0868 | 0.576829 | 0.8499 | -0.0586 | 0.1358 | 0.665984 | 0.8808 | -0.0221 | 0.1129 | 0.844686 | 0.9565 | NaN | -0.0725 | 0.0802 | 0.36622 | 0.7351 | -0.1203 | 0.1192 | 0.312869 | 0.6823 | -0.0404 | 0.106 | 0.703141 | 0.9241 | NaN | -0.0479 | 0.061 | 0.431903 | 0.8488 | -0.0581 | 0.0947 | 0.539489 | 0.8173 | -0.0541 | 0.0799 | 0.498484 | 0.8203 | NaN | -0.0137 | 0.0457 | 0.76414 | 0.8918 | -0.0066 | 0.0729 | 0.927458 | 0.9554 | -0.0063 | 0.0581 | 0.913428 | 0.9994 | NaN | -0.0011 | 0.0366 | 0.975749 | 0.9915 | -0.0296 | 0.0604 | 0.623934 | 0.9977 | 0.019 | 0.0456 | 0.67693 | 0.9967 | NaN | -0.0444 | 0.0452 | 0.32615 | 0.7727 | -0.0677 | 0.0719 | 0.346351 | 0.6513 | -0.0205 | 0.0581 | 0.72381 | 0.968 |
| cortisol 21-acetate | 404.2041 | 15.652845 | Lipid | Steroid | 0.0318 | 0.0864 | 0.712699 | 0.9027 | 0.1691 | 0.1261 | 0.180125 | 0.4582 | -0.078 | 0.118 | 0.508387 | 0.8016 | NaN | 0.0089 | 0.08 | 0.911784 | 0.9933 | 0.0744 | 0.113 | 0.509874 | 0.7797 | -0.0695 | 0.1107 | 0.530215 | 0.8742 | NaN | -0.0412 | 0.061 | 0.498694 | 0.8921 | 0.0813 | 0.089 | 0.360823 | 0.7705 | -0.1287 | 0.083 | 0.120959 | 0.5136 | NaN | 0.057 | 0.0453 | 0.208333 | 0.5183 | 0.0882 | 0.0679 | 0.193829 | 0.49 | 0.0159 | 0.061 | 0.794713 | 0.9994 | NaN | -0.0136 | 0.0365 | 0.708648 | 0.971 | -0.0199 | 0.0574 | 0.729367 | 0.9977 | -0.0076 | 0.0479 | 0.874602 | 0.9967 | NaN | 0.049 | 0.045 | 0.275883 | 0.7695 | 0.0288 | 0.0682 | 0.673132 | 0.8407 | 0.0574 | 0.0611 | 0.347683 | 0.8297 |
| testosterone | 288.1938 | 17.07625 | Lipid | Steroid | -0.0575 | 0.0839 | 0.493279 | 0.8017 | 0.0614 | 0.1392 | 0.659425 | 0.8771 | -0.1153 | 0.1078 | 0.284807 | 0.6662 | NaN | -0.0604 | 0.0776 | 0.435943 | 0.7723 | 0.048 | 0.1222 | 0.694525 | 0.8728 | -0.108 | 0.1011 | 0.285706 | 0.6902 | NaN | -0.0196 | 0.0591 | 0.740244 | 0.9415 | 0.1201 | 0.0968 | 0.214384 | 0.6538 | -0.0762 | 0.0765 | 0.319077 | 0.6934 | NaN | 0.0491 | 0.0443 | 0.267119 | 0.5828 | -0.0262 | 0.0749 | 0.726483 | 0.8643 | 0.0788 | 0.0563 | 0.161938 | 0.9514 | NaN | 0.0258 | 0.0355 | 0.466883 | 0.9708 | 0.0168 | 0.062 | 0.786774 | 0.9977 | 0.0386 | 0.0441 | 0.381183 | 0.9967 | NaN | 0.0289 | 0.0439 | 0.510181 | 0.8283 | -0.089 | 0.0742 | 0.230323 | 0.5676 | 0.0892 | 0.0564 | 0.113462 | 0.7232 |
| cholesterol | 386.3549 | 24.565115 | Lipid | Sterol | 0.0555 | 0.0924 | 0.547977 | 0.8315 | 0.0939 | 0.1476 | 0.524558 | 0.8001 | 0.0455 | 0.1179 | 0.699759 | 0.8959 | NaN | 0.0676 | 0.0854 | 0.428644 | 0.7682 | 0.165 | 0.1294 | 0.202417 | 0.5505 | 0.0378 | 0.1106 | 0.732289 | 0.9342 | NaN | 0.0531 | 0.065 | 0.414191 | 0.8406 | 0.1697 | 0.1022 | 0.09668 | 0.5738 | -0.0278 | 0.0838 | 0.739782 | 0.9323 | NaN | -0.0344 | 0.0487 | 0.479908 | 0.7505 | -0.0718 | 0.0797 | 0.367565 | 0.659 | -0.0021 | 0.0607 | 0.972673 | 0.9994 | NaN | -0.0104 | 0.0391 | 0.789062 | 0.9722 | -0.0081 | 0.066 | 0.9024 | 0.9977 | -0.0118 | 0.0477 | 0.80536 | 0.9967 | NaN | -0.0349 | 0.0484 | 0.469887 | 0.8239 | -0.0806 | 0.079 | 0.308134 | 0.6453 | -0.0004 | 0.0608 | 0.994191 | 0.996 |
| cholesterol hydrogen sulfate | 466.3126 | 23.898865 | Lipid | Sterol | 0.1641 | 0.0956 | 0.086023 | 0.3466 | 0.1282 | 0.1453 | 0.377545 | 0.6978 | 0.1643 | 0.1273 | 0.196998 | 0.5464 | NaN | 0.1706 | 0.0882 | 0.053111 | 0.3365 | 0.1702 | 0.1271 | 0.180549 | 0.5289 | 0.1621 | 0.1193 | 0.174227 | 0.6632 | NaN | 0.0961 | 0.0676 | 0.154902 | 0.6546 | 0.1571 | 0.1007 | 0.118533 | 0.577 | 0.0547 | 0.0914 | 0.549206 | 0.8359 | NaN | 0.0063 | 0.0511 | 0.902386 | 0.9579 | -0.0433 | 0.0789 | 0.582704 | 0.7765 | 0.0387 | 0.0663 | 0.558757 | 0.9885 | NaN | 0.0491 | 0.0406 | 0.226807 | 0.9708 | 0.016 | 0.0651 | 0.805689 | 0.9977 | 0.0718 | 0.0515 | 0.163734 | 0.9967 | NaN | 0.0278 | 0.0505 | 0.581718 | 0.8527 | -0.0241 | 0.0782 | 0.757946 | 0.8842 | 0.0642 | 0.066 | 0.330925 | 0.8205 |
| TG 49:8 | 804.6346 | 25.35286 | Lipid | Triacylglycerol | -0.024 | 0.0828 | 0.771847 | 0.9192 | -0.2567 | 0.1215 | 0.034639 | 0.2428 | 0.1618 | 0.1101 | 0.141782 | 0.4985 | NaN | -0.0204 | 0.0766 | 0.789457 | 0.9749 | -0.1922 | 0.108 | 0.075198 | 0.4408 | 0.1385 | 0.1036 | 0.181546 | 0.6637 | NaN | 0.0201 | 0.0583 | 0.729699 | 0.9415 | -0.0817 | 0.0883 | 0.354886 | 0.7705 | 0.0857 | 0.0787 | 0.2764 | 0.6721 | NaN | -0.0934 | 0.0431 | 0.030466 | 0.3584 | -0.1385 | 0.0656 | 0.034748 | 0.2355 | -0.0479 | 0.0583 | 0.410676 | 0.9735 | NaN | -0.0151 | 0.0349 | 0.664715 | 0.9708 | -0.0907 | 0.0552 | 0.100334 | 0.7937 | 0.0434 | 0.045 | 0.334555 | 0.9967 | NaN | -0.0539 | 0.0431 | 0.210866 | 0.7516 | -0.1179 | 0.0656 | 0.07231 | 0.3895 | 0.0054 | 0.058 | 0.925946 | 0.996 |
| TG 50:8 | 818.6476 | 25.808493 | Lipid | Triacylglycerol | -0.0278 | 0.0842 | 0.741121 | 0.9192 | -0.3435 | 0.1243 | 0.005737 | 0.1275 | 0.2073 | 0.1088 | 0.05678 | 0.3614 | NaN | -0.0286 | 0.0778 | 0.713554 | 0.9423 | -0.2567 | 0.1117 | 0.021549 | 0.3387 | 0.174 | 0.1028 | 0.090421 | 0.5595 | NaN | 0.0303 | 0.0593 | 0.609863 | 0.9199 | -0.1181 | 0.0926 | 0.202032 | 0.6538 | 0.126 | 0.0778 | 0.105328 | 0.4845 | NaN | -0.1079 | 0.0437 | 0.01361 | 0.3584 | -0.1769 | 0.0678 | 0.009087 | 0.1672 | -0.055 | 0.0587 | 0.348268 | 0.9622 | NaN | -0.0257 | 0.0354 | 0.468923 | 0.9708 | -0.1209 | 0.0574 | 0.035054 | 0.6466 | 0.043 | 0.0451 | 0.339679 | 0.9967 | NaN | -0.0767 | 0.0436 | 0.07889 | 0.7496 | -0.1683 | 0.0675 | 0.012699 | 0.265 | -0.006 | 0.0583 | 0.917696 | 0.996 |
| TG 52:8 | 846.6828 | 26.959837 | Lipid | Triacylglycerol | -0.0357 | 0.0857 | 0.676659 | 0.8795 | -0.3174 | 0.1267 | 0.012216 | 0.1645 | 0.1832 | 0.1121 | 0.102129 | 0.4331 | NaN | -0.0333 | 0.0792 | 0.674471 | 0.9303 | -0.2192 | 0.1143 | 0.055092 | 0.4173 | 0.1485 | 0.1058 | 0.160559 | 0.6552 | NaN | 0.0363 | 0.0605 | 0.548222 | 0.9017 | -0.0723 | 0.0947 | 0.445081 | 0.7964 | 0.1046 | 0.0801 | 0.191535 | 0.6042 | NaN | -0.1343 | 0.0443 | 0.002422 | 0.2657 | -0.2019 | 0.0674 | 0.002756 | 0.1525 | -0.0784 | 0.0598 | 0.190144 | 0.9514 | NaN | -0.0336 | 0.0361 | 0.351145 | 0.9708 | -0.1248 | 0.0577 | 0.030447 | 0.6225 | 0.0337 | 0.0462 | 0.465479 | 0.9967 | NaN | -0.0861 | 0.0444 | 0.052204 | 0.7271 | -0.1782 | 0.0677 | 0.008538 | 0.265 | -0.0112 | 0.0595 | 0.851148 | 0.9809 |
| 2-deoxyinosine | 252.0976 | 6.110615 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.1543 | 0.0845 | 0.067783 | 0.3125 | 0.2798 | 0.1396 | 0.044999 | 0.2535 | 0.0781 | 0.1057 | 0.459937 | 0.7601 | NaN | 0.1506 | 0.078 | 0.053664 | 0.3365 | 0.1617 | 0.1261 | 0.199864 | 0.5489 | 0.1006 | 0.0991 | 0.310132 | 0.7142 | NaN | 0.0522 | 0.0602 | 0.385765 | 0.8287 | 0.1207 | 0.1001 | 0.22787 | 0.6655 | 0.0033 | 0.0754 | 0.964826 | 0.979 | NaN | 0.0289 | 0.0451 | 0.521049 | 0.7773 | 0.0287 | 0.0781 | 0.713795 | 0.8608 | 0.0376 | 0.0544 | 0.489336 | 0.9822 | NaN | 0.0297 | 0.0361 | 0.410685 | 0.9708 | 0.013 | 0.0649 | 0.84098 | 0.9977 | 0.0352 | 0.0427 | 0.409882 | 0.9967 | NaN | 0.0447 | 0.0446 | 0.315821 | 0.7708 | 0.0406 | 0.0773 | 0.5993 | 0.8122 | 0.053 | 0.0543 | 0.329268 | 0.8205 |
| hypoxanthine | 136.039 | 1.085038 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.1354 | 0.0834 | 0.104389 | 0.3755 | 0.1662 | 0.1201 | 0.166348 | 0.4386 | 0.1009 | 0.1151 | 0.380699 | 0.7082 | NaN | 0.1729 | 0.0769 | 0.024556 | 0.2243 | 0.1853 | 0.1048 | 0.07699 | 0.4408 | 0.1449 | 0.108 | 0.179989 | 0.6637 | NaN | 0.1098 | 0.0585 | 0.060703 | 0.4352 | 0.0514 | 0.0853 | 0.547148 | 0.8202 | 0.1504 | 0.0807 | 0.062357 | 0.4338 | NaN | 0.0735 | 0.0439 | 0.093919 | 0.4393 | 0.0715 | 0.0649 | 0.270717 | 0.5824 | 0.0858 | 0.0588 | 0.1449 | 0.9514 | NaN | 0.0866 | 0.0349 | 0.013079 | 0.7645 | 0.1607 | 0.0514 | 0.001772 | 0.2446 | 0.0186 | 0.0468 | 0.691601 | 0.9967 | NaN | 0.078 | 0.0435 | 0.073126 | 0.7496 | 0.1132 | 0.0635 | 0.074817 | 0.3895 | 0.0533 | 0.0593 | 0.369385 | 0.8297 |
| inosine | 268.0812 | 1.800299 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.0368 | 0.0832 | 0.657897 | 0.8782 | 0.0984 | 0.1214 | 0.417867 | 0.7231 | -0.0059 | 0.1129 | 0.958223 | 0.9916 | NaN | 0.0911 | 0.0772 | 0.237956 | 0.6038 | 0.1908 | 0.1064 | 0.07297 | 0.4408 | 0.0373 | 0.1064 | 0.725773 | 0.9342 | NaN | 0.0444 | 0.0585 | 0.447838 | 0.8554 | -0.0004 | 0.0857 | 0.996379 | 0.9998 | 0.0835 | 0.08 | 0.296439 | 0.679 | NaN | 0.078 | 0.0434 | 0.072609 | 0.3995 | 0.107 | 0.0644 | 0.096659 | 0.3408 | 0.0524 | 0.0579 | 0.365573 | 0.9622 | NaN | 0.0305 | 0.035 | 0.38437 | 0.9708 | 0.1116 | 0.053 | 0.035143 | 0.6466 | -0.0365 | 0.0455 | 0.422178 | 0.9967 | NaN | 0.0532 | 0.0433 | 0.21848 | 0.7516 | 0.089 | 0.0641 | 0.165125 | 0.5362 | 0.022 | 0.0581 | 0.705 | 0.9666 |
| xanthine | 152.0335 | 1.282354 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.1726 | 0.0979 | 0.077925 | 0.3284 | 0.2378 | 0.1432 | 0.096921 | 0.3566 | 0.1342 | 0.1345 | 0.318692 | 0.6905 | NaN | 0.1473 | 0.0907 | 0.10447 | 0.4118 | 0.1055 | 0.1297 | 0.416032 | 0.7456 | 0.1386 | 0.1261 | 0.27141 | 0.6818 | NaN | 0.0884 | 0.0694 | 0.202361 | 0.7091 | 0.1318 | 0.1012 | 0.192523 | 0.652 | 0.0256 | 0.0963 | 0.79018 | 0.9477 | NaN | 0.0273 | 0.0522 | 0.600676 | 0.818 | 0.0741 | 0.0783 | 0.344194 | 0.6506 | 0.0123 | 0.0698 | 0.859694 | 0.9994 | NaN | 0.0178 | 0.0419 | 0.670179 | 0.9708 | 0.0916 | 0.0644 | 0.155053 | 0.8645 | -0.0471 | 0.055 | 0.390966 | 0.9967 | NaN | 0.029 | 0.0518 | 0.575628 | 0.8527 | 0.0306 | 0.0784 | 0.695878 | 0.8461 | 0.0454 | 0.0696 | 0.514709 | 0.8961 |
| xanthosine | 284.0758 | 2.258693 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.0756 | 0.084 | 0.368525 | 0.7078 | 0.1376 | 0.1223 | 0.260494 | 0.5698 | 0.027 | 0.1149 | 0.81395 | 0.9519 | NaN | 0.1431 | 0.078 | 0.0666 | 0.3516 | 0.1948 | 0.1067 | 0.067942 | 0.4408 | 0.0964 | 0.1088 | 0.375548 | 0.7878 | NaN | 0.0676 | 0.059 | 0.252541 | 0.7568 | 0.1032 | 0.0854 | 0.227081 | 0.6655 | 0.0225 | 0.0814 | 0.781945 | 0.9449 | NaN | -0.0229 | 0.0444 | 0.607102 | 0.8214 | -0.0147 | 0.0667 | 0.825678 | 0.9029 | -0.0171 | 0.0591 | 0.771961 | 0.9994 | NaN | 0.0626 | 0.0352 | 0.075683 | 0.9708 | 0.1496 | 0.0526 | 0.00445 | 0.307 | -0.0131 | 0.0464 | 0.778562 | 0.9967 | NaN | 0.0072 | 0.044 | 0.8693 | 0.9644 | 0.0422 | 0.0656 | 0.519988 | 0.7787 | -0.0138 | 0.0592 | 0.815752 | 0.9748 |
| 1-methyladenosine | 281.113 | 1.018368 | Nucleotide | Purine Metabolism, Adenine containing | -0.0613 | 0.0848 | 0.469783 | 0.7858 | -0.1763 | 0.1835 | 0.336595 | 0.6612 | -0.0228 | 0.0953 | 0.810973 | 0.9518 | NaN | -0.065 | 0.0784 | 0.406897 | 0.7538 | -0.1261 | 0.1616 | 0.434951 | 0.7515 | -0.0315 | 0.0894 | 0.724774 | 0.9342 | NaN | -0.0209 | 0.0598 | 0.726572 | 0.9415 | -0.0207 | 0.1297 | 0.872913 | 0.9467 | -0.0161 | 0.0675 | 0.811364 | 0.9488 | NaN | -0.0233 | 0.0447 | 0.602511 | 0.818 | -0.148 | 0.0977 | 0.129862 | 0.4016 | 0.0074 | 0.049 | 0.88055 | 0.9994 | NaN | -0.0397 | 0.0357 | 0.265967 | 0.9708 | -0.0491 | 0.0821 | 0.550153 | 0.9977 | -0.0353 | 0.0384 | 0.356971 | 0.9967 | NaN | -0.0411 | 0.0442 | 0.353199 | 0.7843 | -0.1763 | 0.0964 | 0.067399 | 0.3895 | -0.007 | 0.0491 | 0.886166 | 0.9942 |
| guanine | 151.0494 | 0.977411 | Nucleotide | Purine Metabolism, Adenine containing | 0.1615 | 0.0775 | 0.037162 | 0.2244 | -0.0432 | 0.2702 | 0.873038 | 0.9553 | 0.1848 | 0.0795 | 0.020136 | 0.251 | NaN | 0.1099 | 0.0726 | 0.130209 | 0.4437 | -0.3416 | 0.2407 | 0.155894 | 0.5063 | 0.1527 | 0.0755 | 0.043232 | 0.4527 | NaN | 0.089 | 0.055 | 0.105696 | 0.5671 | -0.1045 | 0.1886 | 0.579474 | 0.8355 | 0.1058 | 0.0573 | 0.065139 | 0.4338 | NaN | 0.0596 | 0.0412 | 0.147984 | 0.4862 | -0.1558 | 0.1442 | 0.280004 | 0.5899 | 0.0813 | 0.0416 | 0.050796 | 0.8712 | NaN | 0.0336 | 0.0332 | 0.310842 | 0.9708 | 0.0051 | 0.1203 | 0.966452 | 0.9977 | 0.0391 | 0.0333 | 0.240661 | 0.9967 | NaN | 0.0526 | 0.041 | 0.198782 | 0.7516 | -0.0758 | 0.1435 | 0.597276 | 0.8122 | 0.0667 | 0.042 | 0.112532 | 0.7232 |
| guanosine | 283.092 | 1.791455 | Nucleotide | Purine Metabolism, Adenine containing | 0.0427 | 0.0783 | 0.58576 | 0.8554 | 0.1182 | 0.1195 | 0.322434 | 0.6425 | -0.0178 | 0.1027 | 0.862301 | 0.9597 | NaN | 0.0792 | 0.0725 | 0.27482 | 0.6455 | 0.1985 | 0.1044 | 0.057322 | 0.4173 | 0.0091 | 0.0966 | 0.924873 | 0.9876 | NaN | 0.0499 | 0.055 | 0.363957 | 0.8068 | 0.0389 | 0.0842 | 0.643908 | 0.8476 | 0.0673 | 0.073 | 0.356184 | 0.7319 | NaN | 0.0715 | 0.0409 | 0.080321 | 0.4034 | 0.0963 | 0.0637 | 0.130214 | 0.4016 | 0.0456 | 0.0528 | 0.387285 | 0.9735 | NaN | 0.0104 | 0.033 | 0.752423 | 0.9722 | 0.0775 | 0.0529 | 0.142893 | 0.8645 | -0.0376 | 0.0414 | 0.363935 | 0.9967 | NaN | 0.0386 | 0.0408 | 0.344376 | 0.7759 | 0.0739 | 0.0635 | 0.244666 | 0.5776 | 0.007 | 0.0529 | 0.894393 | 0.9953 |
| beta-alanine | 89.0478 | 0.671792 | Nucleotide | Pyrimidine Metabolism, Uracil containing | -0.0262 | 0.0774 | 0.735091 | 0.916 | 0.0132 | 0.1168 | 0.90987 | 0.9622 | -0.0563 | 0.1033 | 0.585311 | 0.8382 | NaN | -0.1003 | 0.0723 | 0.16523 | 0.5124 | -0.0403 | 0.1029 | 0.695409 | 0.8728 | -0.1365 | 0.0981 | 0.16426 | 0.6552 | NaN | -0.0023 | 0.0545 | 0.965705 | 0.9971 | 0.0384 | 0.0815 | 0.638005 | 0.8476 | -0.0178 | 0.0733 | 0.808675 | 0.9477 | NaN | -0.0003 | 0.0407 | 0.994766 | 0.9999 | -0.0737 | 0.0624 | 0.237727 | 0.5537 | 0.0439 | 0.0533 | 0.410258 | 0.9735 | NaN | -0.0449 | 0.0325 | 0.166577 | 0.9708 | -0.0426 | 0.0519 | 0.411712 | 0.9977 | -0.0458 | 0.0415 | 0.270273 | 0.9967 | NaN | 0.004 | 0.0404 | 0.922098 | 0.9724 | -0.0772 | 0.0619 | 0.21186 | 0.5528 | 0.0582 | 0.0533 | 0.2755 | 0.7921 |
| deoxyuridine | 228.0759 | 1.666972 | Nucleotide | Pyrimidine Metabolism, Uracil containing | -0.0005 | 0.0855 | 0.995246 | 0.9964 | 0.008 | 0.1483 | 0.956739 | 0.974 | -0.0114 | 0.104 | 0.912473 | 0.9854 | NaN | 0.0066 | 0.0791 | 0.933693 | 0.9933 | -0.0213 | 0.1303 | 0.869852 | 0.942 | 0.0052 | 0.0977 | 0.957583 | 0.9893 | NaN | 0.0106 | 0.0602 | 0.860736 | 0.9805 | 0.0931 | 0.1035 | 0.368569 | 0.7724 | -0.0217 | 0.0737 | 0.768473 | 0.9437 | NaN | -0.0085 | 0.045 | 0.849587 | 0.9461 | -0.0125 | 0.0795 | 0.875236 | 0.9327 | -0.0129 | 0.0535 | 0.809113 | 0.9994 | NaN | -0.016 | 0.036 | 0.656759 | 0.9708 | 0.0493 | 0.0658 | 0.454068 | 0.9977 | -0.0473 | 0.0418 | 0.25772 | 0.9967 | NaN | -0.0104 | 0.0446 | 0.815616 | 0.9499 | -0.0418 | 0.0788 | 0.596163 | 0.8122 | 0.0005 | 0.0536 | 0.993046 | 0.996 |
| uridine | 244.0701 | 1.340193 | Nucleotide | Pyrimidine Metabolism, Uracil containing | 0.1003 | 0.0879 | 0.253806 | 0.6104 | 0.0674 | 0.1193 | 0.57216 | 0.8246 | 0.1387 | 0.1284 | 0.280061 | 0.6622 | NaN | 0.0573 | 0.0818 | 0.483525 | 0.7907 | 0.0161 | 0.1053 | 0.878435 | 0.9471 | 0.0957 | 0.1213 | 0.429986 | 0.8249 | NaN | 0.0663 | 0.0619 | 0.284255 | 0.7662 | 0.0079 | 0.0837 | 0.924901 | 0.9721 | 0.1379 | 0.0905 | 0.127389 | 0.5265 | NaN | 0.0823 | 0.046 | 0.073704 | 0.3995 | 0.0446 | 0.0639 | 0.485476 | 0.7322 | 0.1207 | 0.0654 | 0.064677 | 0.8712 | NaN | -0.0477 | 0.0374 | 0.201128 | 0.9708 | -0.0431 | 0.0533 | 0.418603 | 0.9977 | -0.0516 | 0.0526 | 0.326308 | 0.9967 | NaN | 0.0351 | 0.046 | 0.445356 | 0.8178 | 0.0239 | 0.0636 | 0.706692 | 0.8511 | 0.0445 | 0.0666 | 0.503631 | 0.8935 |
| cycloheptanecarboxylic acid | 142.0996 | 10.720997 | Organic acids and derivatives | Carboxylic Acid | 0.1472 | 0.0863 | 0.087845 | 0.3514 | 0.3142 | 0.1294 | 0.015196 | 0.1765 | 0.0305 | 0.1134 | 0.787567 | 0.9451 | NaN | 0.0779 | 0.0811 | 0.336664 | 0.704 | 0.1478 | 0.1211 | 0.222416 | 0.5819 | -0.0079 | 0.1068 | 0.941172 | 0.9876 | NaN | -0.059 | 0.0627 | 0.346109 | 0.793 | 0.0813 | 0.0959 | 0.39684 | 0.7775 | -0.1652 | 0.0809 | 0.041099 | 0.3772 | NaN | 0.1026 | 0.0451 | 0.023034 | 0.3584 | 0.1744 | 0.0699 | 0.012556 | 0.1777 | 0.0546 | 0.0581 | 0.3469 | 0.9622 | NaN | 0.0291 | 0.0368 | 0.428615 | 0.9708 | 0.0792 | 0.06 | 0.187069 | 0.9357 | -0.0062 | 0.0458 | 0.892376 | 0.9967 | NaN | 0.1092 | 0.0447 | 0.014562 | 0.7271 | 0.152 | 0.07 | 0.0299 | 0.2981 | 0.0818 | 0.0579 | 0.157626 | 0.7294 |
| indole-3-acetaldehyde | 159.0686 | 1.769727 | Organic Compound | 3-alkylindoles | 0.0195 | 0.0847 | 0.818032 | 0.9391 | 0.1705 | 0.1164 | 0.142945 | 0.415 | -0.113 | 0.122 | 0.354373 | 0.7082 | NaN | 0.0112 | 0.0784 | 0.885843 | 0.9933 | 0.1278 | 0.1028 | 0.213906 | 0.5647 | -0.1049 | 0.1144 | 0.35925 | 0.7716 | NaN | 0.0396 | 0.0596 | 0.505882 | 0.8921 | 0.0898 | 0.0821 | 0.27414 | 0.7263 | -0.0058 | 0.0873 | 0.947424 | 0.9766 | NaN | 0.0634 | 0.0444 | 0.153102 | 0.4947 | 0.0484 | 0.0634 | 0.445303 | 0.7003 | 0.0804 | 0.0635 | 0.205196 | 0.9514 | NaN | -0.0008 | 0.0357 | 0.982539 | 0.9915 | -0.0135 | 0.0532 | 0.799623 | 0.9977 | 0.0145 | 0.0497 | 0.770675 | 0.9967 | NaN | 0.0165 | 0.0442 | 0.70818 | 0.9124 | 0.042 | 0.063 | 0.504953 | 0.7764 | -0.0133 | 0.0633 | 0.833901 | 0.9809 |
| porphobilinogen | 226.0821 | 6.687804 | Organic nitrogen compounds | Amines | 0.1314 | 0.084 | 0.117884 | 0.4014 | 0.2498 | 0.1375 | 0.06916 | 0.3006 | 0.0727 | 0.1055 | 0.490979 | 0.7878 | NaN | 0.1022 | 0.078 | 0.189939 | 0.548 | 0.1936 | 0.1216 | 0.111344 | 0.4674 | 0.0542 | 0.0992 | 0.584488 | 0.8877 | NaN | 0.0036 | 0.0601 | 0.951956 | 0.997 | 0.1633 | 0.0966 | 0.091026 | 0.5507 | -0.0806 | 0.076 | 0.288725 | 0.6745 | NaN | 0.0356 | 0.0446 | 0.423874 | 0.709 | -0.0072 | 0.0769 | 0.925187 | 0.9554 | 0.0513 | 0.0542 | 0.343109 | 0.9622 | NaN | 0.029 | 0.0357 | 0.417524 | 0.9708 | 0.0308 | 0.0632 | 0.625682 | 0.9977 | 0.0302 | 0.0427 | 0.479267 | 0.9967 | NaN | 0.038 | 0.0442 | 0.390155 | 0.8116 | -0.0515 | 0.0768 | 0.501945 | 0.7761 | 0.0811 | 0.0539 | 0.132339 | 0.7232 |
| methyl beta-D-galactoside | 194.0788 | 0.883257 | Organic oxygen compounds | Carbohydrates and carbohydrate conjugates | -0.0573 | 0.0844 | 0.49753 | 0.8017 | -0.0997 | 0.1252 | 0.42589 | 0.7255 | -0.0316 | 0.1137 | 0.781283 | 0.9437 | NaN | -0.026 | 0.0783 | 0.740064 | 0.9612 | -0.0532 | 0.1104 | 0.62986 | 0.8459 | -0.0076 | 0.1068 | 0.943471 | 0.9876 | NaN | -0.1145 | 0.059 | 0.052481 | 0.4157 | -0.0603 | 0.0876 | 0.49153 | 0.8029 | -0.1744 | 0.0799 | 0.02909 | 0.3354 | NaN | -0.0562 | 0.0443 | 0.204485 | 0.5151 | -0.1145 | 0.0663 | 0.08423 | 0.313 | 0.0006 | 0.0585 | 0.991911 | 0.9994 | NaN | 0.0064 | 0.0357 | 0.857457 | 0.9722 | -0.0078 | 0.0561 | 0.889902 | 0.9977 | 0.0153 | 0.046 | 0.738428 | 0.9967 | NaN | -0.024 | 0.0441 | 0.585766 | 0.8527 | -0.0864 | 0.0662 | 0.191992 | 0.5437 | 0.0332 | 0.0586 | 0.571401 | 0.9321 |
| 3-hydroxybenzaldehyde | 122.0371 | 4.799146 | Organic oxygen compounds | Carbonyl compounds | -0.0462 | 0.0838 | 0.581265 | 0.8511 | -0.1668 | 0.1194 | 0.162236 | 0.4369 | 0.0809 | 0.1157 | 0.484616 | 0.7845 | NaN | -0.0429 | 0.0775 | 0.579711 | 0.8743 | -0.1417 | 0.1049 | 0.177054 | 0.5254 | 0.0717 | 0.1086 | 0.508968 | 0.8742 | NaN | 0.019 | 0.0591 | 0.748287 | 0.9454 | -0.0376 | 0.0852 | 0.659066 | 0.852 | 0.0644 | 0.0819 | 0.432045 | 0.7865 | NaN | -0.0307 | 0.044 | 0.485429 | 0.7545 | -0.0574 | 0.0648 | 0.375971 | 0.6609 | 0.0018 | 0.0598 | 0.976505 | 0.9994 | NaN | -0.0342 | 0.0353 | 0.332235 | 0.9708 | -0.0501 | 0.0537 | 0.350964 | 0.9977 | -0.0177 | 0.047 | 0.706263 | 0.9967 | NaN | -0.0092 | 0.0438 | 0.833523 | 0.9535 | -0.0763 | 0.0639 | 0.232686 | 0.5691 | 0.0588 | 0.0595 | 0.323052 | 0.8205 |
| 2,3-dihydroxybenzoate | 154.0262 | 4.700874 | Organoheterocyclic compounds | Benzoate and derivatives | 0.0159 | 0.0815 | 0.845347 | 0.9457 | 0.107 | 0.121 | 0.376518 | 0.6978 | -0.0766 | 0.1105 | 0.488128 | 0.7856 | NaN | -0.0317 | 0.0758 | 0.675853 | 0.9303 | -0.0126 | 0.109 | 0.907694 | 0.9654 | -0.1058 | 0.1036 | 0.307323 | 0.7128 | NaN | -0.0393 | 0.0574 | 0.494118 | 0.8921 | 0.0614 | 0.0847 | 0.468729 | 0.799 | -0.1414 | 0.0775 | 0.067986 | 0.4364 | NaN | -0.0144 | 0.0429 | 0.737767 | 0.8848 | -0.0345 | 0.0657 | 0.6 | 0.7883 | 0.0153 | 0.0571 | 0.788543 | 0.9994 | NaN | -0.0012 | 0.0344 | 0.972842 | 0.9915 | -0.0002 | 0.0543 | 0.996991 | 0.9977 | -0.0086 | 0.0448 | 0.847365 | 0.9967 | NaN | 0.0003 | 0.0425 | 0.994628 | 0.9972 | -0.0404 | 0.0652 | 0.535444 | 0.7903 | 0.0424 | 0.0573 | 0.45904 | 0.8635 |
| 5-methoxytryptophol | 191.0925 | 10.292022 | Organoheterocyclic compounds | Indoles | 0.1024 | 0.084 | 0.22259 | 0.5715 | 0.2465 | 0.1389 | 0.0759 | 0.313 | 0.0304 | 0.1046 | 0.771542 | 0.9398 | NaN | 0.0815 | 0.0778 | 0.294935 | 0.6634 | 0.1901 | 0.1228 | 0.121686 | 0.4674 | 0.0217 | 0.0982 | 0.825146 | 0.9616 | NaN | -0.0115 | 0.0598 | 0.847971 | 0.9805 | 0.1687 | 0.0974 | 0.083315 | 0.549 | -0.1037 | 0.0746 | 0.164381 | 0.5601 | NaN | 0.0248 | 0.0444 | 0.577253 | 0.8067 | -0.0439 | 0.078 | 0.573643 | 0.7754 | 0.0533 | 0.0536 | 0.319599 | 0.9622 | NaN | 0.0201 | 0.0356 | 0.57214 | 0.9708 | 0.0229 | 0.0638 | 0.720079 | 0.9977 | 0.0201 | 0.0422 | 0.633973 | 0.9967 | NaN | 0.0355 | 0.044 | 0.419846 | 0.8132 | -0.066 | 0.0775 | 0.394542 | 0.687 | 0.0834 | 0.0534 | 0.118197 | 0.7232 |
| 3-indolepropionic acid | 189.0794 | 10.379467 | Organoheterocyclic compounds | Indolyl carboxylic acids and derivatives | -0.0847 | 0.0817 | 0.299429 | 0.6636 | -0.2825 | 0.1185 | 0.017124 | 0.1833 | 0.0566 | 0.1107 | 0.609227 | 0.8492 | NaN | -0.0573 | 0.0758 | 0.449183 | 0.7771 | -0.2491 | 0.1042 | 0.016788 | 0.3007 | 0.0901 | 0.1039 | 0.386001 | 0.7982 | NaN | -0.0196 | 0.0578 | 0.734179 | 0.9415 | -0.1492 | 0.0849 | 0.079058 | 0.549 | 0.1031 | 0.078 | 0.186267 | 0.5977 | NaN | -0.0509 | 0.0429 | 0.235918 | 0.5455 | -0.1848 | 0.0629 | 0.003315 | 0.1525 | 0.04 | 0.0568 | 0.481513 | 0.9759 | NaN | -0.1001 | 0.0338 | 0.003059 | 0.5629 | -0.1305 | 0.0532 | 0.014125 | 0.5742 | -0.0785 | 0.0445 | 0.077538 | 0.9967 | NaN | -0.0734 | 0.0424 | 0.083626 | 0.7508 | -0.1865 | 0.0623 | 0.002755 | 0.2424 | 0.0049 | 0.0571 | 0.931063 | 0.996 |
| 5-valerolactone | 100.0525 | 1.741256 | Organoheterocyclic compounds | Lactones | 0.0436 | 0.0842 | 0.604793 | 0.8708 | 0.0767 | 0.1201 | 0.52295 | 0.8001 | 0.0021 | 0.1168 | 0.98579 | 0.9955 | NaN | 0.0215 | 0.078 | 0.782391 | 0.9727 | -0.0215 | 0.1072 | 0.8413 | 0.9389 | 0.0108 | 0.1096 | 0.921358 | 0.9876 | NaN | 0.0007 | 0.0594 | 0.99115 | 0.9992 | 0.0492 | 0.084 | 0.558215 | 0.8202 | -0.0408 | 0.0828 | 0.621763 | 0.8667 | NaN | 0.0055 | 0.0443 | 0.901709 | 0.9579 | -0.0399 | 0.0649 | 0.538507 | 0.7661 | 0.043 | 0.06 | 0.473301 | 0.9735 | NaN | 0.0479 | 0.0354 | 0.175246 | 0.9708 | 0.061 | 0.0532 | 0.251825 | 0.9821 | 0.0348 | 0.0471 | 0.460227 | 0.9967 | NaN | 0.0208 | 0.0439 | 0.635328 | 0.8685 | -0.0613 | 0.0643 | 0.340737 | 0.6499 | 0.0938 | 0.0597 | 0.116074 | 0.7232 |
| 2,4-dihydroxypteridine | 164.0331 | 1.32753 | Organoheterocyclic compounds | Pteridines and derivatives | -0.0106 | 0.089 | 0.905214 | 0.9586 | -0.0588 | 0.1201 | 0.624625 | 0.8596 | 0.0393 | 0.1307 | 0.763965 | 0.9392 | NaN | -0.0054 | 0.0823 | 0.947257 | 0.9933 | -0.0792 | 0.1053 | 0.451715 | 0.7607 | 0.0605 | 0.1227 | 0.622072 | 0.8939 | NaN | -0.028 | 0.0626 | 0.655209 | 0.9288 | -0.041 | 0.0839 | 0.625031 | 0.8438 | -0.006 | 0.0927 | 0.94867 | 0.9766 | NaN | -0.0701 | 0.0466 | 0.132867 | 0.4825 | -0.0588 | 0.0642 | 0.359498 | 0.659 | -0.0911 | 0.0671 | 0.174636 | 0.9514 | NaN | -0.0359 | 0.0375 | 0.337412 | 0.9708 | -0.0385 | 0.0534 | 0.470975 | 0.9977 | -0.0321 | 0.0528 | 0.544079 | 0.9967 | NaN | -0.0884 | 0.0462 | 0.05532 | 0.7271 | -0.0917 | 0.0633 | 0.147609 | 0.5225 | -0.0894 | 0.0672 | 0.183496 | 0.7294 |
| salsolinol | 179.0938 | 1.273321 | Organoheterocyclic compounds | Tetrahydroisoquinolines | -0.0261 | 0.0801 | 0.744621 | 0.9192 | -0.1784 | 0.2604 | 0.493222 | 0.7914 | -0.0023 | 0.084 | 0.97775 | 0.994 | NaN | -0.0331 | 0.0741 | 0.655289 | 0.9303 | -0.0042 | 0.2314 | 0.985404 | 0.989 | -0.0158 | 0.0788 | 0.840626 | 0.9708 | NaN | -0.059 | 0.0563 | 0.2942 | 0.7808 | -0.091 | 0.1823 | 0.617492 | 0.8437 | -0.0542 | 0.0595 | 0.361731 | 0.7368 | NaN | 0.0622 | 0.0421 | 0.139413 | 0.4828 | -0.1345 | 0.1393 | 0.334304 | 0.6487 | 0.083 | 0.0427 | 0.0519 | 0.8712 | NaN | 0.0024 | 0.0338 | 0.944184 | 0.9797 | 0.0057 | 0.1165 | 0.961125 | 0.9977 | 0.0035 | 0.0339 | 0.917059 | 0.9967 | NaN | 0.0241 | 0.0418 | 0.563892 | 0.8527 | -0.1765 | 0.1376 | 0.199783 | 0.5437 | 0.0445 | 0.0431 | 0.301316 | 0.8042 |
| dipepetide (aspartate glutamate) | 262.0823 | 15.655098 | Peptide | Dipeptide | -0.0401 | 0.0842 | 0.633929 | 0.8777 | -0.0731 | 0.1221 | 0.549334 | 0.8065 | -0.0455 | 0.1171 | 0.697773 | 0.8959 | NaN | -0.057 | 0.0779 | 0.463946 | 0.7817 | -0.0847 | 0.107 | 0.428782 | 0.7515 | -0.0603 | 0.1098 | 0.58269 | 0.8877 | NaN | -0.0591 | 0.0592 | 0.317638 | 0.782 | -0.0408 | 0.0854 | 0.632791 | 0.8442 | -0.0658 | 0.0827 | 0.426661 | 0.7865 | NaN | 0.038 | 0.0444 | 0.391759 | 0.6828 | 0.0087 | 0.0658 | 0.895313 | 0.9435 | 0.0541 | 0.0603 | 0.369522 | 0.9622 | NaN | -0.0367 | 0.0354 | 0.300595 | 0.9708 | -0.0205 | 0.0544 | 0.706228 | 0.9977 | -0.055 | 0.047 | 0.242144 | 0.9967 | NaN | 0.0242 | 0.044 | 0.583144 | 0.8527 | -0.0072 | 0.0652 | 0.912314 | 0.9654 | 0.0447 | 0.0604 | 0.459428 | 0.8635 |
| dipeptide (phenylalanine phenylalanine) | 312.1484 | 8.417695 | Peptide | Dipeptide | 0.138 | 0.0819 | 0.092216 | 0.3578 | 0.3256 | 0.1549 | 0.035592 | 0.2428 | 0.0746 | 0.0959 | 0.436643 | 0.7481 | NaN | 0.124 | 0.0758 | 0.101933 | 0.4077 | 0.307 | 0.1355 | 0.023506 | 0.3387 | 0.0645 | 0.09 | 0.473819 | 0.8435 | NaN | 0.0808 | 0.0579 | 0.16287 | 0.6546 | 0.1484 | 0.1111 | 0.181815 | 0.652 | 0.061 | 0.0679 | 0.369096 | 0.7398 | NaN | 0.0955 | 0.0429 | 0.025966 | 0.3584 | 0.0394 | 0.087 | 0.650975 | 0.8261 | 0.1131 | 0.0483 | 0.019125 | 0.8712 | NaN | 0.0209 | 0.035 | 0.550073 | 0.9708 | -0.0486 | 0.073 | 0.505049 | 0.9977 | 0.0453 | 0.0386 | 0.241071 | 0.9967 | NaN | 0.0535 | 0.043 | 0.214062 | 0.7516 | 0.0212 | 0.0866 | 0.806571 | 0.9086 | 0.0623 | 0.0491 | 0.205037 | 0.7294 |
| dipeptide (serine histidine) | 242.1028 | 17.227266 | Peptide | Dipeptide | -0.0136 | 0.0835 | 0.870642 | 0.9457 | -0.0344 | 0.1267 | 0.786101 | 0.9222 | 0.0097 | 0.1119 | 0.930998 | 0.9916 | NaN | -0.0166 | 0.0772 | 0.829556 | 0.9848 | 0.0073 | 0.1115 | 0.947986 | 0.9799 | -0.0022 | 0.105 | 0.983372 | 0.9993 | NaN | -0.056 | 0.0587 | 0.340084 | 0.7921 | -0.066 | 0.0883 | 0.454923 | 0.7964 | -0.0302 | 0.0793 | 0.703512 | 0.9095 | NaN | 0.0001 | 0.0439 | 0.99813 | 0.9999 | 0.1167 | 0.0676 | 0.084474 | 0.313 | -0.1087 | 0.0569 | 0.056346 | 0.8712 | NaN | -0.0229 | 0.0352 | 0.515275 | 0.9708 | -0.0063 | 0.0564 | 0.911071 | 0.9977 | -0.0317 | 0.0451 | 0.48274 | 0.9967 | NaN | 0.0234 | 0.0436 | 0.591692 | 0.8527 | 0.1155 | 0.0671 | 0.084967 | 0.3942 | -0.0576 | 0.0575 | 0.316229 | 0.8169 |
| dipeptide (glutamate isoleucine/leucine) | 262.1323 | 6.182869 | Peptide | Dipeptide | 0.1856 | 0.0849 | 0.028882 | 0.207 | 0.1974 | 0.1184 | 0.095453 | 0.3536 | 0.21 | 0.1217 | 0.084472 | 0.3985 | NaN | 0.1366 | 0.0793 | 0.085257 | 0.3825 | 0.0859 | 0.1073 | 0.423369 | 0.7514 | 0.1768 | 0.1148 | 0.123645 | 0.6104 | NaN | 0.116 | 0.0601 | 0.053609 | 0.4157 | 0.1746 | 0.082 | 0.033178 | 0.3738 | 0.0444 | 0.0888 | 0.616994 | 0.8637 | NaN | 0.0779 | 0.0451 | 0.083982 | 0.407 | 0.0376 | 0.0651 | 0.563394 | 0.7754 | 0.1367 | 0.0622 | 0.027973 | 0.8712 | NaN | 0.0284 | 0.0365 | 0.43695 | 0.9708 | 0.0208 | 0.0542 | 0.700634 | 0.9977 | 0.0395 | 0.0502 | 0.431239 | 0.9967 | NaN | 0.0769 | 0.0448 | 0.085689 | 0.7508 | 0.0141 | 0.065 | 0.828509 | 0.9165 | 0.1545 | 0.0618 | 0.012493 | 0.6979 |
| dipeptide (isoleucine/leucine isoleucine/leucine) | 244.1532 | 5.463248 | Peptide | Dipeptide | 0.2128 | 0.1239 | 0.085931 | 0.3466 | 0.1289 | 0.153 | 0.399395 | 0.7124 | 0.3789 | 0.2072 | 0.067449 | 0.3664 | NaN | 0.1722 | 0.115 | 0.134185 | 0.4462 | 0.142 | 0.134 | 0.289256 | 0.6709 | 0.2857 | 0.1971 | 0.147177 | 0.6249 | NaN | 0.1925 | 0.0868 | 0.026545 | 0.28 | 0.2423 | 0.105 | 0.020979 | 0.3282 | 0.123 | 0.1507 | 0.414246 | 0.7786 | NaN | 0.0878 | 0.0656 | 0.18043 | 0.5115 | 0.0653 | 0.0822 | 0.426599 | 0.6926 | 0.1225 | 0.1085 | 0.258873 | 0.9622 | NaN | 0.077 | 0.0525 | 0.142659 | 0.9708 | 0.0578 | 0.0682 | 0.396722 | 0.9977 | 0.1178 | 0.085 | 0.165547 | 0.9967 | NaN | 0.0919 | 0.065 | 0.157485 | 0.7516 | 0.0381 | 0.0818 | 0.640908 | 0.8247 | 0.1884 | 0.1073 | 0.079172 | 0.7232 |
| dipeptide (isoleucine/leucine valine) | 230.1634 | 3.14795 | Peptide | Dipeptide | 0.0774 | 0.0858 | 0.366806 | 0.7078 | 0.0113 | 0.1253 | 0.927909 | 0.9682 | 0.1093 | 0.1182 | 0.355228 | 0.7082 | NaN | 0.0771 | 0.0793 | 0.33105 | 0.701 | 0.0188 | 0.11 | 0.864295 | 0.942 | 0.1053 | 0.1109 | 0.342452 | 0.7561 | NaN | 0.0834 | 0.0602 | 0.165971 | 0.6546 | 0.0221 | 0.0875 | 0.800642 | 0.9217 | 0.1332 | 0.0831 | 0.109099 | 0.4896 | NaN | 0.0191 | 0.0452 | 0.673353 | 0.846 | -0.0178 | 0.0672 | 0.790873 | 0.8867 | 0.0568 | 0.0608 | 0.350424 | 0.9622 | NaN | -0.0635 | 0.0363 | 0.079953 | 0.9708 | -0.1333 | 0.0546 | 0.014564 | 0.5742 | -0.0087 | 0.0482 | 0.856887 | 0.9967 | NaN | 0.0023 | 0.045 | 0.959508 | 0.9881 | -0.0559 | 0.0666 | 0.400834 | 0.6948 | 0.0567 | 0.0609 | 0.351753 | 0.8297 |
| dipeptide (isoleucine/leucine alanine) | 202.1322 | 2.070814 | Peptide | Dipeptide | 0.0854 | 0.0838 | 0.308397 | 0.675 | 0.0829 | 0.1353 | 0.539985 | 0.8052 | 0.0856 | 0.1059 | 0.41882 | 0.7447 | NaN | 0.0806 | 0.0775 | 0.298737 | 0.6657 | 0.1198 | 0.1186 | 0.312168 | 0.6823 | 0.0719 | 0.0995 | 0.469571 | 0.8416 | NaN | 0.0826 | 0.0589 | 0.160644 | 0.6546 | 0.0871 | 0.0943 | 0.355406 | 0.7705 | 0.085 | 0.0748 | 0.255743 | 0.644 | NaN | 0.1081 | 0.0436 | 0.013046 | 0.3584 | 0.0455 | 0.0726 | 0.530898 | 0.7612 | 0.1429 | 0.053 | 0.006964 | 0.8712 | NaN | -0.026 | 0.0356 | 0.464609 | 0.9708 | -0.0739 | 0.0604 | 0.221085 | 0.9527 | 0.0033 | 0.0431 | 0.938391 | 0.9967 | NaN | 0.0568 | 0.0437 | 0.193843 | 0.7516 | -0.0082 | 0.0723 | 0.909385 | 0.9654 | 0.0933 | 0.054 | 0.083893 | 0.7232 |
| possible peptide | 247.1106 | 4.573735 | Peptide | Dipeptide | 0.0587 | 0.0822 | 0.475707 | 0.7909 | 0.0643 | 0.132 | 0.62599 | 0.8596 | 0.0499 | 0.1043 | 0.632511 | 0.8621 | NaN | 0.0652 | 0.076 | 0.39128 | 0.7448 | 0.087 | 0.1157 | 0.452053 | 0.7607 | 0.0517 | 0.0978 | 0.597237 | 0.8877 | NaN | 0.0449 | 0.0579 | 0.437868 | 0.8511 | 0.0884 | 0.0919 | 0.336151 | 0.7705 | 0.0169 | 0.074 | 0.819213 | 0.9488 | NaN | 0.0231 | 0.0433 | 0.594056 | 0.8157 | -0.0238 | 0.071 | 0.73758 | 0.8684 | 0.0532 | 0.0534 | 0.31951 | 0.9622 | NaN | 0.0185 | 0.0347 | 0.594972 | 0.9708 | 0.0205 | 0.0588 | 0.7272 | 0.9977 | 0.0163 | 0.0422 | 0.698648 | 0.9967 | NaN | 0.0236 | 0.043 | 0.583216 | 0.8527 | -0.0489 | 0.0705 | 0.48759 | 0.7613 | 0.0688 | 0.0533 | 0.197187 | 0.7294 |
| possible peptide | 278.1628 | 7.824666 | Peptide | Dipeptide | 0.1459 | 0.0782 | 0.061968 | 0.2974 | 0.2287 | 0.1291 | 0.076541 | 0.313 | 0.0993 | 0.0977 | 0.309623 | 0.6892 | NaN | 0.119 | 0.0726 | 0.101208 | 0.4077 | 0.1956 | 0.1136 | 0.084977 | 0.4459 | 0.0782 | 0.092 | 0.395342 | 0.8005 | NaN | 0.1479 | 0.0545 | 0.006654 | 0.1312 | 0.235 | 0.0885 | 0.007899 | 0.2454 | 0.1104 | 0.0687 | 0.108298 | 0.4896 | NaN | 0.0507 | 0.0415 | 0.222236 | 0.538 | -0.0264 | 0.0723 | 0.71468 | 0.8608 | 0.0839 | 0.0498 | 0.092424 | 0.8712 | NaN | 0.008 | 0.0335 | 0.810694 | 0.9722 | -0.0792 | 0.06 | 0.186653 | 0.9357 | 0.0535 | 0.0394 | 0.174359 | 0.9967 | NaN | 0.0253 | 0.0414 | 0.541543 | 0.8373 | -0.0586 | 0.072 | 0.415782 | 0.7062 | 0.0634 | 0.0502 | 0.207052 | 0.7294 |
| possible peptide | 282.1234 | 8.5111 | Peptide | Dipeptide | 0.0274 | 0.0856 | 0.749063 | 0.9192 | -0.0344 | 0.152 | 0.820894 | 0.9343 | 0.0376 | 0.1036 | 0.716856 | 0.9018 | NaN | 0.0232 | 0.0792 | 0.769244 | 0.9675 | 0.0128 | 0.1337 | 0.923807 | 0.9689 | 0.024 | 0.0972 | 0.805039 | 0.9546 | NaN | 0.0971 | 0.0601 | 0.105823 | 0.5671 | -0.0426 | 0.1061 | 0.687719 | 0.8747 | 0.1638 | 0.0727 | 0.024227 | 0.3327 | NaN | -0.0166 | 0.0451 | 0.711796 | 0.8674 | -0.0441 | 0.0814 | 0.588008 | 0.7765 | -0.004 | 0.0533 | 0.94036 | 0.9994 | NaN | -0.0171 | 0.0361 | 0.636489 | 0.9708 | -0.0747 | 0.0672 | 0.266862 | 0.9821 | 0.0066 | 0.0419 | 0.875664 | 0.9967 | NaN | -0.0462 | 0.0447 | 0.301292 | 0.7695 | -0.0405 | 0.0807 | 0.616299 | 0.8191 | -0.0496 | 0.0534 | 0.352677 | 0.8297 |
| possible peptide | 409.138 | 8.470251 | Peptide | Dipeptide | -0.0221 | 0.0997 | 0.824664 | 0.9405 | -0.0107 | 0.1392 | 0.938728 | 0.9682 | -0.021 | 0.1415 | 0.881798 | 0.9697 | NaN | -0.0071 | 0.0923 | 0.938572 | 0.9933 | -0.0723 | 0.1225 | 0.555267 | 0.7941 | 0.0297 | 0.1334 | 0.823674 | 0.9616 | NaN | 0.0326 | 0.0702 | 0.643005 | 0.9288 | 0.0219 | 0.0973 | 0.821507 | 0.9229 | 0.0488 | 0.1004 | 0.627039 | 0.8697 | NaN | 0.0496 | 0.0524 | 0.343979 | 0.6525 | 0.0552 | 0.0746 | 0.458891 | 0.7135 | 0.0417 | 0.0727 | 0.566588 | 0.9885 | NaN | 0.0313 | 0.042 | 0.4571 | 0.9708 | 0.0374 | 0.0619 | 0.545138 | 0.9977 | 0.0274 | 0.0572 | 0.631785 | 0.9967 | NaN | 0.0373 | 0.052 | 0.473766 | 0.8239 | -0.0083 | 0.074 | 0.910575 | 0.9654 | 0.0831 | 0.0727 | 0.25302 | 0.7533 |
| possible peptide | 414.2051 | 18.41231 | Peptide | Dipeptide | 0.0775 | 0.0864 | 0.36928 | 0.7078 | 0.1267 | 0.1595 | 0.426956 | 0.7255 | 0.0828 | 0.1032 | 0.422291 | 0.7447 | NaN | 0.0496 | 0.0801 | 0.535756 | 0.8366 | 0.036 | 0.1414 | 0.798924 | 0.9315 | 0.0635 | 0.097 | 0.512904 | 0.8742 | NaN | 0.0359 | 0.0609 | 0.55577 | 0.9023 | 0.0826 | 0.1115 | 0.458814 | 0.7964 | 0.0058 | 0.0737 | 0.937379 | 0.9766 | NaN | 0.0268 | 0.0455 | 0.555594 | 0.7987 | -0.0012 | 0.0862 | 0.989327 | 0.9914 | 0.0509 | 0.053 | 0.336989 | 0.9622 | NaN | 0.0077 | 0.0366 | 0.834134 | 0.9722 | 0.0068 | 0.0715 | 0.923826 | 0.9977 | 0.0099 | 0.0419 | 0.812803 | 0.9967 | NaN | 0.0458 | 0.0451 | 0.309487 | 0.7695 | 0.0338 | 0.0852 | 0.691581 | 0.8461 | 0.0605 | 0.053 | 0.253844 | 0.7533 |
| possible peptide | 445.2502 | 18.402573 | Peptide | Dipeptide | -0.0817 | 0.0881 | 0.353411 | 0.7019 | 0.0535 | 0.1406 | 0.703589 | 0.8949 | -0.1579 | 0.1115 | 0.156587 | 0.5166 | NaN | -0.0838 | 0.0814 | 0.303028 | 0.6692 | 0.0288 | 0.1235 | 0.815455 | 0.9349 | -0.1533 | 0.1045 | 0.142268 | 0.6249 | NaN | -0.0439 | 0.0621 | 0.479351 | 0.882 | 0.0388 | 0.0982 | 0.692545 | 0.8788 | -0.094 | 0.0794 | 0.23678 | 0.6205 | NaN | 0.0649 | 0.0466 | 0.164005 | 0.5058 | 0.1467 | 0.0742 | 0.047922 | 0.2516 | 0.011 | 0.0587 | 0.850703 | 0.9994 | NaN | 0.0728 | 0.0372 | 0.050328 | 0.9656 | 0.0871 | 0.062 | 0.160136 | 0.8793 | 0.0644 | 0.046 | 0.161925 | 0.9967 | NaN | 0.0507 | 0.0463 | 0.27283 | 0.7695 | 0.1062 | 0.0741 | 0.151998 | 0.5225 | 0.0138 | 0.0588 | 0.814701 | 0.9748 |
| dipeptide (serine isoleucine/leucine) | 218.1243 | 2.663722 | Peptide | Dipeptide | 0.1789 | 0.0877 | 0.041381 | 0.2354 | 0.3476 | 0.1215 | 0.004231 | 0.1112 | 0.0315 | 0.1233 | 0.798594 | 0.948 | NaN | 0.1271 | 0.082 | 0.121049 | 0.4437 | 0.2509 | 0.1099 | 0.022447 | 0.3387 | -0.0105 | 0.1162 | 0.928066 | 0.9876 | NaN | 0.0683 | 0.0626 | 0.275739 | 0.7604 | 0.2002 | 0.0874 | 0.022058 | 0.3282 | -0.0703 | 0.0876 | 0.422167 | 0.7865 | NaN | 0.0487 | 0.0468 | 0.298448 | 0.6019 | 0.0591 | 0.0705 | 0.401344 | 0.6775 | 0.056 | 0.0632 | 0.375633 | 0.9689 | NaN | -0.0214 | 0.0379 | 0.571638 | 0.9708 | 0.0989 | 0.057 | 0.082716 | 0.7247 | -0.133 | 0.0486 | 0.006264 | 0.4891 | NaN | 0.0265 | 0.0467 | 0.570205 | 0.8527 | 0.0546 | 0.07 | 0.435391 | 0.7217 | 0.0121 | 0.0635 | 0.848796 | 0.9809 |
| dipeptide (tyrosine histidine) | 279.132 | 1.012568 | Peptide | Dipeptide | 0.1351 | 0.0816 | 0.097815 | 0.3673 | 0.2227 | 0.1181 | 0.059245 | 0.2819 | 0.0596 | 0.1125 | 0.596062 | 0.8415 | NaN | 0.0894 | 0.0761 | 0.240572 | 0.6038 | 0.0512 | 0.111 | 0.644267 | 0.8459 | 0.0528 | 0.1055 | 0.617068 | 0.8939 | NaN | 0.0756 | 0.0577 | 0.190241 | 0.6946 | 0.1224 | 0.0837 | 0.143723 | 0.5917 | 0.0168 | 0.0799 | 0.833085 | 0.9506 | NaN | 0.0279 | 0.0434 | 0.520584 | 0.7773 | 0.0042 | 0.0661 | 0.949683 | 0.9654 | 0.0651 | 0.0576 | 0.258135 | 0.9622 | NaN | 0.0318 | 0.0347 | 0.36011 | 0.9708 | 0.0046 | 0.0547 | 0.93244 | 0.9977 | 0.0508 | 0.0452 | 0.26117 | 0.9967 | NaN | 0.035 | 0.043 | 0.41635 | 0.8132 | 0.0107 | 0.0654 | 0.870201 | 0.9452 | 0.0674 | 0.0576 | 0.242273 | 0.7389 |
| dipeptide (methionine isoleucine/leucine) | 262.1418 | 8.063479 | Peptide | Dipeptide | -0.1236 | 0.0835 | 0.138823 | 0.4388 | -0.0076 | 0.1273 | 0.952581 | 0.974 | -0.2118 | 0.1168 | 0.069703 | 0.3664 | NaN | -0.1004 | 0.0774 | 0.194755 | 0.5485 | 0.0001 | 0.1117 | 0.999107 | 0.9991 | -0.1696 | 0.1106 | 0.125027 | 0.6104 | NaN | -0.0387 | 0.0593 | 0.513654 | 0.8944 | -0.0007 | 0.0889 | 0.993877 | 0.9998 | -0.0378 | 0.0857 | 0.659325 | 0.8899 | NaN | 0.0251 | 0.0446 | 0.573589 | 0.8059 | 0.0561 | 0.0681 | 0.41063 | 0.6798 | -0.0319 | 0.0618 | 0.605883 | 0.9994 | NaN | 0.0071 | 0.0357 | 0.842182 | 0.9722 | 0.0051 | 0.0566 | 0.92842 | 0.9977 | 0.0184 | 0.0489 | 0.707342 | 0.9967 | NaN | 0.0069 | 0.0442 | 0.876668 | 0.9668 | -0.0068 | 0.0677 | 0.919947 | 0.9654 | -0.0029 | 0.0623 | 0.962616 | 0.996 |
| n-gamma-L-glutamyl-L-methionine | 278.0956 | 2.337805 | Peptide | Gamma-glutamyl Amino Acid | 0.1761 | 0.0913 | 0.053606 | 0.2666 | 0.2737 | 0.1457 | 0.060296 | 0.2836 | 0.1139 | 0.1163 | 0.327197 | 0.6994 | NaN | 0.1127 | 0.0855 | 0.187777 | 0.5455 | 0.1181 | 0.1333 | 0.375527 | 0.7136 | 0.0801 | 0.1096 | 0.464937 | 0.8416 | NaN | 0.0247 | 0.0656 | 0.707211 | 0.9414 | 0.1086 | 0.1044 | 0.298429 | 0.7488 | -0.0194 | 0.0837 | 0.816867 | 0.9488 | NaN | 0.0885 | 0.0482 | 0.066038 | 0.3995 | 0.0756 | 0.0803 | 0.346272 | 0.6506 | 0.0882 | 0.0594 | 0.137792 | 0.9514 | NaN | 0.0437 | 0.039 | 0.262429 | 0.9708 | 0.1229 | 0.0653 | 0.059658 | 0.6733 | -0.0033 | 0.0474 | 0.945137 | 0.9967 | NaN | 0.1003 | 0.0476 | 0.035218 | 0.7271 | 0.108 | 0.0789 | 0.171021 | 0.5384 | 0.0904 | 0.0595 | 0.128814 | 0.7232 |
| tripeptide (cysteine histidine lysine) | 386.1737 | 16.45213 | Peptide | Tripeptide | 0.1198 | 0.0856 | 0.161333 | 0.4783 | 0.1895 | 0.1346 | 0.159166 | 0.4348 | 0.0981 | 0.1111 | 0.377042 | 0.7082 | NaN | 0.1221 | 0.079 | 0.122497 | 0.4437 | 0.0909 | 0.1205 | 0.450695 | 0.7607 | 0.124 | 0.1041 | 0.233553 | 0.6818 | NaN | 0.086 | 0.0602 | 0.153217 | 0.6546 | 0.1217 | 0.0944 | 0.197387 | 0.6538 | 0.0477 | 0.079 | 0.545794 | 0.8359 | NaN | 0.0217 | 0.0454 | 0.632611 | 0.8435 | -0.0409 | 0.0744 | 0.582671 | 0.7765 | 0.0788 | 0.0568 | 0.1655 | 0.9514 | NaN | 0.0037 | 0.0364 | 0.919314 | 0.9722 | -0.0533 | 0.0615 | 0.386298 | 0.9977 | 0.0398 | 0.0449 | 0.37605 | 0.9967 | NaN | 0.0233 | 0.045 | 0.604364 | 0.8583 | -0.0413 | 0.0738 | 0.575169 | 0.8075 | 0.0768 | 0.0569 | 0.177434 | 0.7294 |
| Tripeptide (glycine proline valine) | 271.1541 | 2.897597 | Peptide | Tripeptide | 0.1308 | 0.0886 | 0.139908 | 0.4388 | 0.2977 | 0.1444 | 0.039162 | 0.2428 | 0.0602 | 0.1121 | 0.591333 | 0.8413 | NaN | 0.0963 | 0.0823 | 0.241969 | 0.6038 | 0.2279 | 0.1281 | 0.075247 | 0.4408 | 0.0375 | 0.1053 | 0.721733 | 0.9342 | NaN | 0.0683 | 0.0626 | 0.275515 | 0.7604 | 0.1913 | 0.1018 | 0.060075 | 0.4995 | 0.0084 | 0.0796 | 0.915864 | 0.9752 | NaN | 0.0912 | 0.0464 | 0.049349 | 0.3914 | 0.1035 | 0.0795 | 0.1926 | 0.4899 | 0.0811 | 0.0572 | 0.155837 | 0.9514 | NaN | -0.0019 | 0.0378 | 0.959215 | 0.9897 | 0.0038 | 0.0674 | 0.955371 | 0.9977 | -0.0017 | 0.0454 | 0.97039 | 0.9967 | NaN | 0.0536 | 0.0464 | 0.248235 | 0.7516 | 0.0657 | 0.0797 | 0.409634 | 0.7022 | 0.0443 | 0.0576 | 0.44157 | 0.8627 |
| tripeptide (tryptophan tyrosine isoleucine/leucine) | 457.2177 | 4.079669 | Peptide | Tripeptide | 0.143 | 0.0885 | 0.106003 | 0.3775 | 0.2609 | 0.1445 | 0.071024 | 0.3039 | 0.0916 | 0.1122 | 0.414191 | 0.7446 | NaN | 0.1217 | 0.082 | 0.137835 | 0.4502 | 0.1909 | 0.1282 | 0.136419 | 0.4744 | 0.0877 | 0.1052 | 0.40481 | 0.8023 | NaN | 0.1073 | 0.0623 | 0.084906 | 0.5364 | 0.1849 | 0.1012 | 0.06758 | 0.5245 | 0.0806 | 0.0794 | 0.309855 | 0.6892 | NaN | 0.1 | 0.0463 | 0.030939 | 0.3584 | 0.0685 | 0.0795 | 0.388833 | 0.6687 | 0.1087 | 0.0569 | 0.056267 | 0.8712 | NaN | -0.0235 | 0.0379 | 0.534938 | 0.9708 | -0.0118 | 0.0669 | 0.859628 | 0.9977 | -0.0269 | 0.0457 | 0.556509 | 0.9967 | NaN | 0.0353 | 0.0466 | 0.449601 | 0.8178 | -0.0081 | 0.0801 | 0.919696 | 0.9654 | 0.0516 | 0.0578 | 0.372289 | 0.8297 |
| diethylstilbestrol | 268.1314 | 18.64137 | Phenylpropanoids and polyketides | Stilbenes | 0.1745 | 0.09 | 0.052593 | 0.2644 | 0.3705 | 0.1351 | 0.006087 | 0.1275 | 0.0451 | 0.1195 | 0.705677 | 0.8959 | NaN | 0.1779 | 0.0831 | 0.0323 | 0.2661 | 0.2451 | 0.1233 | 0.046802 | 0.4173 | 0.0854 | 0.1124 | 0.447012 | 0.8364 | NaN | 0.089 | 0.0639 | 0.163652 | 0.6546 | 0.2731 | 0.0945 | 0.003839 | 0.1766 | -0.0644 | 0.0852 | 0.449753 | 0.7881 | NaN | 0.0017 | 0.0484 | 0.971876 | 0.9898 | 0.0255 | 0.0788 | 0.74645 | 0.873 | 0.0051 | 0.0615 | 0.933731 | 0.9994 | NaN | 0.0485 | 0.0384 | 0.206045 | 0.9708 | 0.0817 | 0.0637 | 0.19995 | 0.9357 | 0.0241 | 0.0483 | 0.616974 | 0.9967 | NaN | 0.0247 | 0.0478 | 0.60487 | 0.8583 | -0.0155 | 0.079 | 0.84495 | 0.9254 | 0.0651 | 0.0613 | 0.287626 | 0.8005 |