## Sheet1
| Table S4. Associations between annotated metabolites and HOMA-CP, with combined dataset of boys and girls and sex-stratified. Regression models identifying annotated metabolites (p=550) linearly associated with HOMA-CP. 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 HOMA-CP including BMIz (Model 2), MUAMA (Model 3), MUAFA (Model 4), WHtR (Model 5) and total subcutaneous adiposity (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 BMIz, 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 | NaN | 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 | -0.5841 | 0.1363 | 0.000018 | 0.0023 | -0.2982 | 0.1351 | 0.02733 | 0.2514 | -0.8848 | 0.2336 | 0.000152 | 0.0168 | NaN | -0.4536 | 0.1302 | 0.000496 | 0.0219 | -0.2255 | 0.1202 | 0.060672 | 0.4717 | -0.6984 | 0.232 | 0.002611 | 0.1201 | NaN | -0.467 | 0.1292 | 0.0003 | 0.0118 | -0.2095 | 0.1185 | 0.077115 | 0.5751 | -0.7536 | 0.2276 | 0.000927 | 0.0465 | NaN | -0.4565 | 0.1344 | 0.000685 | 0.0261 | -0.2089 | 0.1269 | 0.099642 | 0.4326 | -0.711 | 0.2374 | 0.002748 | 0.1264 | NaN | -0.4378 | 0.134 | 0.001086 | 0.04 | -0.1766 | 0.123 | 0.150977 | 0.631 | -0.726 | 0.2373 | 0.002224 | 0.1345 | NaN | -0.4529 | 0.1353 | 0.000819 | 0.0315 | -0.2061 | 0.1248 | 0.098605 | 0.4447 | -0.725 | 0.2424 | 0.002784 | 0.1675 |
| N-acetyl-L-leucine | 173.1045 | 7.169957 | Amino Acid | Acetyl Amino Acid | 0.2169 | 0.1364 | 0.111736 | 0.4781 | 0.4153 | 0.1205 | 0.000568 | 0.059 | -0.0425 | 0.2538 | 0.866949 | 0.9735 | NaN | 0.1517 | 0.1269 | 0.231974 | 0.7495 | 0.2918 | 0.1113 | 0.008759 | 0.1606 | 0 | 0.2384 | 0.999867 | 0.9999 | NaN | 0.1978 | 0.126 | 0.116307 | 0.6 | 0.341 | 0.1053 | 0.001204 | 0.0604 | 0.0034 | 0.2401 | 0.988647 | 0.9976 | NaN | 0.2118 | 0.1289 | 0.10023 | 0.5533 | 0.3437 | 0.113 | 0.002351 | 0.055 | 0.0705 | 0.2435 | 0.772046 | 0.9598 | NaN | 0.1535 | 0.1287 | 0.232946 | 0.7108 | 0.2843 | 0.1123 | 0.011364 | 0.1792 | -0.0053 | 0.2427 | 0.982519 | 0.9969 | NaN | 0.2088 | 0.1292 | 0.106031 | 0.5529 | 0.3199 | 0.1128 | 0.004554 | 0.0793 | 0.0848 | 0.247 | 0.731221 | 0.9459 |
| creatine | 131.0694 | 0.679577 | Amino Acid | Creatine Metabolism | 0.4111 | 0.144 | 0.004314 | 0.0744 | 0.1014 | 0.1806 | 0.574442 | 0.8007 | 0.5518 | 0.2134 | 0.00972 | 0.1677 | NaN | 0.4385 | 0.1324 | 0.000926 | 0.0341 | 0.068 | 0.1587 | 0.668239 | 0.9222 | 0.615 | 0.1982 | 0.001917 | 0.1176 | NaN | 0.4188 | 0.1324 | 0.001563 | 0.0431 | 0.073 | 0.1557 | 0.639076 | 0.9053 | 0.5938 | 0.2 | 0.002985 | 0.1177 | NaN | 0.4306 | 0.1356 | 0.001497 | 0.0394 | 0.0287 | 0.1663 | 0.863001 | 0.9509 | 0.6161 | 0.2013 | 0.002202 | 0.1264 | NaN | 0.4352 | 0.1343 | 0.001193 | 0.0412 | 0.0589 | 0.1591 | 0.711086 | 0.8841 | 0.6115 | 0.2023 | 0.002508 | 0.1345 | NaN | 0.4297 | 0.1359 | 0.001572 | 0.0413 | 0.0039 | 0.1643 | 0.981058 | 0.9946 | 0.6271 | 0.2035 | 0.002056 | 0.1419 |
| lysine | 146.1055 | 0.511165 | Amino Acid | Lysine Metabolism | 0.4362 | 0.1317 | 0.000924 | 0.0296 | 0.2753 | 0.1553 | 0.076306 | 0.357 | 0.5171 | 0.1978 | 0.008939 | 0.1629 | NaN | 0.3173 | 0.125 | 0.011132 | 0.1674 | 0.1409 | 0.1403 | 0.315344 | 0.8095 | 0.4024 | 0.1903 | 0.034477 | 0.5144 | NaN | 0.3219 | 0.1245 | 0.009759 | 0.1347 | 0.1054 | 0.139 | 0.448169 | 0.8947 | 0.4368 | 0.1895 | 0.021157 | 0.3073 | NaN | 0.3303 | 0.128 | 0.009872 | 0.1362 | 0.1655 | 0.1459 | 0.256538 | 0.5881 | 0.3988 | 0.1943 | 0.040141 | 0.5138 | NaN | 0.3224 | 0.1269 | 0.011071 | 0.1927 | 0.1588 | 0.1397 | 0.255746 | 0.7315 | 0.4054 | 0.1951 | 0.037703 | 0.4772 | NaN | 0.342 | 0.1277 | 0.007408 | 0.1168 | 0.1861 | 0.1423 | 0.19075 | 0.5692 | 0.4131 | 0.1959 | 0.034956 | 0.4663 |
| 3,4-hydroxyphenyl-lactate | 182.0573 | 3.796673 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.1682 | 0.1428 | 0.238806 | 0.6075 | 0.4918 | 0.1302 | 0.000159 | 0.0292 | -0.1826 | 0.2508 | 0.466522 | 0.8207 | NaN | 0.0913 | 0.133 | 0.492585 | 0.8632 | 0.4115 | 0.1162 | 0.000398 | 0.0277 | -0.2311 | 0.2351 | 0.325488 | 0.9223 | NaN | 0.0728 | 0.1332 | 0.584789 | 0.9125 | 0.3582 | 0.1176 | 0.002315 | 0.0804 | -0.2052 | 0.2366 | 0.385814 | 0.9814 | NaN | 0.1286 | 0.1354 | 0.342333 | 0.741 | 0.4718 | 0.1183 | 0.000067 | 0.0118 | -0.2313 | 0.2383 | 0.331767 | 0.9044 | NaN | 0.1269 | 0.1342 | 0.344268 | 0.7757 | 0.4579 | 0.1136 | 0.000056 | 0.0154 | -0.2224 | 0.2394 | 0.352885 | 0.9106 | NaN | 0.1315 | 0.1357 | 0.332225 | 0.7485 | 0.4565 | 0.117 | 0.000096 | 0.014 | -0.2046 | 0.2405 | 0.39501 | 0.8887 |
| tyrosine | 181.0741 | 1.297716 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.476 | 0.1352 | 0.00043 | 0.017 | 0.7383 | 0.1475 | 0.000001 | 0.0003 | 0.3363 | 0.2047 | 0.100443 | 0.5278 | NaN | 0.2707 | 0.1339 | 0.043109 | 0.4204 | 0.5546 | 0.1415 | 0.000088 | 0.0215 | 0.1164 | 0.2041 | 0.568433 | 0.954 | NaN | 0.3315 | 0.1294 | 0.010416 | 0.1402 | 0.5724 | 0.1349 | 0.000022 | 0.0061 | 0.2087 | 0.1983 | 0.292648 | 0.9294 | NaN | 0.3194 | 0.1353 | 0.018247 | 0.2168 | 0.5977 | 0.1461 | 0.000043 | 0.0118 | 0.1665 | 0.2041 | 0.414674 | 0.9375 | NaN | 0.2882 | 0.1358 | 0.0338 | 0.3392 | 0.5495 | 0.1428 | 0.000119 | 0.0219 | 0.1531 | 0.2075 | 0.460711 | 0.9359 | NaN | 0.3084 | 0.1371 | 0.024455 | 0.2755 | 0.5754 | 0.1455 | 0.000076 | 0.014 | 0.1635 | 0.2087 | 0.433355 | 0.8887 |
| proline | 115.0634 | 0.68809 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.4877 | 0.1358 | 0.000328 | 0.0165 | 0.3841 | 0.1345 | 0.004281 | 0.1153 | 0.6061 | 0.2297 | 0.008322 | 0.1612 | NaN | 0.4092 | 0.1271 | 0.001283 | 0.0416 | 0.3251 | 0.1189 | 0.006255 | 0.1439 | 0.5081 | 0.2186 | 0.0201 | 0.4623 | NaN | 0.3938 | 0.1275 | 0.002003 | 0.0481 | 0.3208 | 0.1167 | 0.005974 | 0.1538 | 0.4786 | 0.2226 | 0.031553 | 0.3706 | NaN | 0.4115 | 0.1303 | 0.001589 | 0.0399 | 0.3149 | 0.1252 | 0.011919 | 0.1382 | 0.5261 | 0.221 | 0.017288 | 0.4372 | NaN | 0.406 | 0.1292 | 0.001668 | 0.0504 | 0.3234 | 0.1193 | 0.006695 | 0.1424 | 0.5061 | 0.2237 | 0.023702 | 0.4673 | NaN | 0.41 | 0.1307 | 0.001713 | 0.043 | 0.314 | 0.1231 | 0.010733 | 0.1267 | 0.5222 | 0.2239 | 0.019715 | 0.4132 |
| glucose | 180.0636 | 0.649866 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | 0.4791 | 0.1556 | 0.002073 | 0.0458 | 0.4463 | 0.1531 | 0.003556 | 0.1044 | 0.5391 | 0.2662 | 0.042848 | 0.3491 | NaN | 0.4819 | 0.1432 | 0.000769 | 0.0303 | 0.3823 | 0.1352 | 0.004699 | 0.1179 | 0.6071 | 0.2481 | 0.01442 | 0.4257 | NaN | 0.4466 | 0.1437 | 0.001882 | 0.0481 | 0.3297 | 0.1352 | 0.014714 | 0.2463 | 0.5716 | 0.2503 | 0.022373 | 0.3167 | NaN | 0.5212 | 0.1462 | 0.000363 | 0.0167 | 0.4548 | 0.1385 | 0.001027 | 0.0436 | 0.6044 | 0.2518 | 0.016379 | 0.4372 | NaN | 0.4793 | 0.1453 | 0.000971 | 0.0383 | 0.3798 | 0.1356 | 0.005104 | 0.1424 | 0.5938 | 0.2531 | 0.01896 | 0.423 | NaN | 0.5037 | 0.1467 | 0.000595 | 0.0252 | 0.4366 | 0.1368 | 0.001417 | 0.0437 | 0.5832 | 0.2545 | 0.021925 | 0.4132 |
| raffinose | 504.1699 | 0.718023 | Exogenous | Food Component/Plant | 0.2699 | 0.1369 | 0.048655 | 0.316 | 0.4855 | 0.144 | 0.000745 | 0.059 | 0.1016 | 0.216 | 0.638033 | 0.9104 | NaN | 0.1875 | 0.128 | 0.142739 | 0.6828 | 0.3368 | 0.1331 | 0.011357 | 0.1836 | 0.0893 | 0.2026 | 0.659252 | 0.954 | NaN | 0.1779 | 0.128 | 0.164684 | 0.6736 | 0.3251 | 0.1308 | 0.012941 | 0.2304 | 0.0813 | 0.2041 | 0.690164 | 0.9894 | NaN | 0.2441 | 0.1296 | 0.059704 | 0.4583 | 0.4177 | 0.1337 | 0.001777 | 0.0516 | 0.1142 | 0.2052 | 0.578071 | 0.9375 | NaN | 0.1892 | 0.1298 | 0.144989 | 0.6708 | 0.3551 | 0.1319 | 0.007083 | 0.1424 | 0.065 | 0.2066 | 0.752953 | 0.9621 | NaN | 0.2506 | 0.1298 | 0.053559 | 0.4413 | 0.4088 | 0.1319 | 0.001934 | 0.0531 | 0.129 | 0.2073 | 0.533762 | 0.8971 |
| DG 32:0 | 568.5067 | 26.219461 | Lipid | Diacylglycerol | 0.5326 | 0.1251 | 0.000021 | 0.0023 | 0.3424 | 0.1388 | 0.013618 | 0.1879 | 0.6923 | 0.1947 | 0.000376 | 0.0279 | NaN | 0.3392 | 0.1253 | 0.006797 | 0.1217 | 0.1936 | 0.1278 | 0.129834 | 0.6118 | 0.4767 | 0.2041 | 0.019533 | 0.4623 | NaN | 0.3978 | 0.1202 | 0.000939 | 0.0273 | 0.2529 | 0.1217 | 0.037617 | 0.3993 | 0.534 | 0.1962 | 0.006496 | 0.1494 | NaN | 0.3707 | 0.1284 | 0.003892 | 0.0716 | 0.1899 | 0.1358 | 0.161906 | 0.5021 | 0.5236 | 0.2027 | 0.009794 | 0.318 | NaN | 0.3637 | 0.1264 | 0.003999 | 0.0849 | 0.1736 | 0.1296 | 0.180472 | 0.6534 | 0.5368 | 0.2029 | 0.008149 | 0.2999 | NaN | 0.3784 | 0.1281 | 0.003143 | 0.0642 | 0.1755 | 0.134 | 0.190253 | 0.5692 | 0.5524 | 0.2028 | 0.006451 | 0.2374 |
| DG 34:0 | 618.5204 | 27.634111 | Lipid | Diacylglycerol | 0.4707 | 0.1283 | 0.000245 | 0.015 | 0.3365 | 0.1604 | 0.03591 | 0.2877 | 0.548 | 0.1876 | 0.003487 | 0.1069 | NaN | 0.2793 | 0.127 | 0.027827 | 0.3293 | 0.222 | 0.144 | 0.123 | 0.6118 | 0.3236 | 0.196 | 0.098697 | 0.7567 | NaN | 0.3489 | 0.122 | 0.004247 | 0.0738 | 0.2546 | 0.1397 | 0.068338 | 0.5719 | 0.4185 | 0.1846 | 0.023386 | 0.3227 | NaN | 0.3097 | 0.1299 | 0.017106 | 0.2098 | 0.2225 | 0.151 | 0.140786 | 0.4798 | 0.3629 | 0.1968 | 0.065228 | 0.6103 | NaN | 0.2985 | 0.1285 | 0.020215 | 0.2722 | 0.1904 | 0.146 | 0.192227 | 0.6684 | 0.3814 | 0.1959 | 0.051533 | 0.5267 | NaN | 0.3179 | 0.1297 | 0.014246 | 0.1805 | 0.2113 | 0.149 | 0.15609 | 0.5288 | 0.3944 | 0.1967 | 0.04499 | 0.4743 |
| DG 30:1 | 560.4423 | 24.64577 | Lipid | Diacylglycerol | 0.4249 | 0.1299 | 0.001067 | 0.0301 | 0.2333 | 0.1463 | 0.110923 | 0.3939 | 0.5519 | 0.1995 | 0.005654 | 0.1486 | NaN | 0.2459 | 0.1269 | 0.052574 | 0.4443 | 0.1157 | 0.1316 | 0.379294 | 0.8308 | 0.3277 | 0.2049 | 0.109759 | 0.7818 | NaN | 0.3201 | 0.1224 | 0.008936 | 0.1265 | 0.1888 | 0.1265 | 0.135561 | 0.6741 | 0.4095 | 0.1965 | 0.037178 | 0.3872 | NaN | 0.2809 | 0.1291 | 0.029507 | 0.3194 | 0.1138 | 0.1383 | 0.410512 | 0.6997 | 0.3791 | 0.2036 | 0.062592 | 0.5957 | NaN | 0.2916 | 0.1264 | 0.021066 | 0.2769 | 0.1237 | 0.1315 | 0.346805 | 0.7839 | 0.4082 | 0.2011 | 0.04236 | 0.4772 | NaN | 0.2866 | 0.1291 | 0.026423 | 0.286 | 0.1013 | 0.1364 | 0.457523 | 0.7516 | 0.4065 | 0.2041 | 0.046402 | 0.4743 |
| DG 32:1 | 588.4736 | 25.42276 | Lipid | Diacylglycerol | 0.4471 | 0.1289 | 0.000526 | 0.0193 | 0.1854 | 0.138 | 0.179 | 0.4964 | 0.6784 | 0.2048 | 0.000924 | 0.051 | NaN | 0.2503 | 0.1276 | 0.04985 | 0.4443 | 0.064 | 0.1243 | 0.606789 | 0.9043 | 0.4345 | 0.2168 | 0.04508 | 0.5871 | NaN | 0.3378 | 0.1219 | 0.005584 | 0.0931 | 0.1585 | 0.119 | 0.182643 | 0.7308 | 0.5123 | 0.2056 | 0.012718 | 0.234 | NaN | 0.2768 | 0.1311 | 0.03469 | 0.3473 | 0.0372 | 0.1324 | 0.778685 | 0.9085 | 0.4916 | 0.214 | 0.021637 | 0.4551 | NaN | 0.2877 | 0.1277 | 0.024224 | 0.2903 | 0.0662 | 0.1245 | 0.594723 | 0.8623 | 0.5089 | 0.2134 | 0.017074 | 0.423 | NaN | 0.2844 | 0.1309 | 0.029825 | 0.3025 | 0.0282 | 0.1302 | 0.828558 | 0.9397 | 0.5212 | 0.2148 | 0.015231 | 0.4004 |
| DG 34:1 | 616.5049 | 26.494192 | Lipid | Diacylglycerol | 0.4186 | 0.1289 | 0.001166 | 0.0305 | 0.1793 | 0.1446 | 0.214844 | 0.5076 | 0.6164 | 0.1987 | 0.001921 | 0.0964 | NaN | 0.2149 | 0.1278 | 0.092769 | 0.622 | 0.0257 | 0.1313 | 0.844757 | 0.9729 | 0.3836 | 0.2079 | 0.065018 | 0.6334 | NaN | 0.2829 | 0.1231 | 0.021537 | 0.2499 | 0.0974 | 0.126 | 0.439464 | 0.8947 | 0.4436 | 0.2008 | 0.027145 | 0.3487 | NaN | 0.243 | 0.1312 | 0.063965 | 0.4708 | -0.0025 | 0.1404 | 0.985592 | 0.9926 | 0.4414 | 0.2049 | 0.031224 | 0.4788 | NaN | 0.2547 | 0.1278 | 0.046206 | 0.4114 | 0.0469 | 0.1306 | 0.719628 | 0.887 | 0.4475 | 0.2068 | 0.030459 | 0.4772 | NaN | 0.2528 | 0.1309 | 0.05344 | 0.4413 | -0.0083 | 0.1377 | 0.952177 | 0.9834 | 0.4674 | 0.2059 | 0.0232 | 0.4132 |
| DG 36:1 | 644.5369 | 28.001514 | Lipid | Diacylglycerol | 0.4301 | 0.1303 | 0.000964 | 0.0296 | 0.2458 | 0.1568 | 0.116835 | 0.3987 | 0.5463 | 0.1927 | 0.004591 | 0.1334 | NaN | 0.2385 | 0.1282 | 0.062842 | 0.5027 | 0.0949 | 0.1421 | 0.504156 | 0.8931 | 0.3343 | 0.1975 | 0.090609 | 0.7567 | NaN | 0.2686 | 0.1259 | 0.032855 | 0.2852 | 0.1156 | 0.1382 | 0.402879 | 0.8818 | 0.3724 | 0.1948 | 0.055925 | 0.477 | NaN | 0.2736 | 0.1306 | 0.036251 | 0.3473 | 0.0897 | 0.15 | 0.549892 | 0.7845 | 0.386 | 0.1958 | 0.0487 | 0.559 | NaN | 0.2654 | 0.1291 | 0.0398 | 0.3788 | 0.1015 | 0.1421 | 0.474961 | 0.8272 | 0.3841 | 0.1987 | 0.053239 | 0.5267 | NaN | 0.2827 | 0.1304 | 0.030139 | 0.3025 | 0.0818 | 0.1475 | 0.579064 | 0.8092 | 0.4109 | 0.1964 | 0.03645 | 0.4663 |
| DG 32:2 | 586.4577 | 24.862595 | Lipid | Diacylglycerol | 0.381 | 0.1296 | 0.003274 | 0.0645 | 0.2063 | 0.1454 | 0.156005 | 0.4721 | 0.5027 | 0.1995 | 0.011765 | 0.1921 | NaN | 0.1706 | 0.1284 | 0.183941 | 0.7251 | 0.114 | 0.1296 | 0.379148 | 0.8308 | 0.2098 | 0.2152 | 0.329581 | 0.9223 | NaN | 0.2602 | 0.1228 | 0.034098 | 0.2852 | 0.1781 | 0.1253 | 0.155252 | 0.7183 | 0.3295 | 0.1997 | 0.099011 | 0.6246 | NaN | 0.1935 | 0.1323 | 0.143707 | 0.6149 | 0.0625 | 0.1388 | 0.652447 | 0.8434 | 0.2799 | 0.2118 | 0.186335 | 0.8705 | NaN | 0.2197 | 0.1278 | 0.085568 | 0.5831 | 0.1152 | 0.1299 | 0.375196 | 0.7999 | 0.313 | 0.2084 | 0.133113 | 0.7817 | NaN | 0.2049 | 0.1319 | 0.12033 | 0.5827 | 0.0559 | 0.1364 | 0.682172 | 0.8747 | 0.3176 | 0.2116 | 0.133349 | 0.7588 |
| DG 34:3 | 612.4738 | 25.196987 | Lipid | Diacylglycerol | 0.3544 | 0.1287 | 0.005885 | 0.0902 | 0.1076 | 0.1361 | 0.429328 | 0.6991 | 0.5746 | 0.2064 | 0.005384 | 0.1486 | NaN | 0.1642 | 0.126 | 0.192277 | 0.7307 | 0.0152 | 0.1211 | 0.899953 | 0.9729 | 0.3129 | 0.2173 | 0.149998 | 0.879 | NaN | 0.2489 | 0.1213 | 0.040086 | 0.316 | 0.1 | 0.1172 | 0.393247 | 0.8818 | 0.3996 | 0.2069 | 0.053389 | 0.477 | NaN | 0.1613 | 0.1317 | 0.220739 | 0.7062 | -0.0483 | 0.13 | 0.710382 | 0.8729 | 0.3545 | 0.2192 | 0.105868 | 0.7792 | NaN | 0.2056 | 0.1259 | 0.102519 | 0.6358 | 0.0205 | 0.1212 | 0.865592 | 0.9614 | 0.3973 | 0.2133 | 0.062541 | 0.5568 | NaN | 0.1783 | 0.1307 | 0.17257 | 0.6392 | -0.0394 | 0.1269 | 0.755953 | 0.9096 | 0.3912 | 0.2192 | 0.074385 | 0.6024 |
| FA 12:2 | 196.1463 | 20.184414 | Lipid | Fatty Acid | -0.4197 | 0.1334 | 0.001655 | 0.0381 | -0.1445 | 0.1344 | 0.28245 | 0.5724 | -0.6929 | 0.2256 | 0.002125 | 0.0977 | NaN | -0.3597 | 0.1243 | 0.003794 | 0.0806 | -0.0861 | 0.1189 | 0.46909 | 0.8671 | -0.6261 | 0.213 | 0.003291 | 0.1398 | NaN | -0.3755 | 0.1236 | 0.002385 | 0.0549 | -0.016 | 0.1187 | 0.892525 | 0.973 | -0.7506 | 0.2105 | 0.000364 | 0.0287 | NaN | -0.411 | 0.1259 | 0.0011 | 0.0341 | -0.1707 | 0.1226 | 0.163972 | 0.5057 | -0.6277 | 0.2163 | 0.003706 | 0.1461 | NaN | -0.3884 | 0.1252 | 0.001928 | 0.0507 | -0.1227 | 0.1183 | 0.299723 | 0.7544 | -0.6491 | 0.2162 | 0.00268 | 0.1345 | NaN | -0.4105 | 0.1262 | 0.001146 | 0.0351 | -0.1912 | 0.1207 | 0.112956 | 0.4653 | -0.619 | 0.2194 | 0.004782 | 0.1886 |
| FA 14:2 | 224.1775 | 21.617804 | Lipid | Fatty Acid | -0.4426 | 0.1355 | 0.001091 | 0.0301 | -0.2807 | 0.1435 | 0.050474 | 0.2996 | -0.5821 | 0.2197 | 0.008076 | 0.1612 | NaN | -0.4579 | 0.1245 | 0.000236 | 0.0145 | -0.2633 | 0.1257 | 0.036109 | 0.3378 | -0.6161 | 0.2044 | 0.00258 | 0.1201 | NaN | -0.4798 | 0.124 | 0.00011 | 0.0067 | -0.1697 | 0.1265 | 0.179742 | 0.7308 | -0.7734 | 0.2057 | 0.00017 | 0.0188 | NaN | -0.5153 | 0.1271 | 0.00005 | 0.0046 | -0.3651 | 0.1298 | 0.004923 | 0.0822 | -0.6228 | 0.2074 | 0.00267 | 0.1264 | NaN | -0.4739 | 0.1261 | 0.000171 | 0.0144 | -0.2992 | 0.1251 | 0.016773 | 0.2258 | -0.6126 | 0.2085 | 0.003307 | 0.1404 | NaN | -0.499 | 0.1275 | 0.000091 | 0.0083 | -0.3697 | 0.1276 | 0.003749 | 0.0766 | -0.5945 | 0.21 | 0.004637 | 0.1886 |
| FA 14:3 | 222.1618 | 20.25606 | Lipid | Fatty Acid | 0.3069 | 0.1273 | 0.015944 | 0.163 | 0.3856 | 0.1309 | 0.003219 | 0.1044 | 0.2493 | 0.206 | 0.226296 | 0.7263 | NaN | 0.2644 | 0.1182 | 0.025273 | 0.3185 | 0.3942 | 0.113 | 0.000486 | 0.0277 | 0.1582 | 0.1955 | 0.418484 | 0.9419 | NaN | 0.2365 | 0.1187 | 0.046298 | 0.3501 | 0.346 | 0.1125 | 0.002109 | 0.0804 | 0.1496 | 0.1974 | 0.448465 | 0.9816 | NaN | 0.2958 | 0.1203 | 0.013954 | 0.1791 | 0.4413 | 0.1172 | 0.000167 | 0.0153 | 0.1775 | 0.1976 | 0.369009 | 0.9223 | NaN | 0.2822 | 0.1195 | 0.018157 | 0.257 | 0.4229 | 0.1124 | 0.000168 | 0.0232 | 0.1774 | 0.1987 | 0.371891 | 0.9106 | NaN | 0.2951 | 0.1206 | 0.014388 | 0.1805 | 0.4412 | 0.1151 | 0.000127 | 0.014 | 0.1857 | 0.1994 | 0.351795 | 0.8785 |
| FA 16:3 | 250.1933 | 22.076328 | Lipid | Fatty Acid | -0.3824 | 0.1338 | 0.004256 | 0.0744 | -0.1969 | 0.1392 | 0.157266 | 0.4721 | -0.5469 | 0.2192 | 0.012583 | 0.1929 | NaN | -0.4752 | 0.1226 | 0.000106 | 0.0117 | -0.2978 | 0.121 | 0.013848 | 0.1911 | -0.6168 | 0.2036 | 0.002454 | 0.1201 | NaN | -0.4516 | 0.1224 | 0.000226 | 0.0096 | -0.14 | 0.1208 | 0.2463 | 0.8037 | -0.7632 | 0.2059 | 0.00021 | 0.0194 | NaN | -0.536 | 0.1264 | 0.000022 | 0.0034 | -0.4129 | 0.1288 | 0.001349 | 0.0459 | -0.6213 | 0.2068 | 0.002657 | 0.1264 | NaN | -0.4694 | 0.1245 | 0.000163 | 0.0144 | -0.2932 | 0.1213 | 0.015636 | 0.2158 | -0.6157 | 0.2078 | 0.003053 | 0.1404 | NaN | -0.5229 | 0.1266 | 0.000036 | 0.0047 | -0.4333 | 0.1263 | 0.0006 | 0.0301 | -0.5945 | 0.2091 | 0.004467 | 0.1886 |
| AC 2:0 | 203.116 | 0.914417 | Lipid | Fatty Acid Metabolism (also BCAA Metabolism) | -0.4066 | 0.1347 | 0.002537 | 0.0539 | -0.2764 | 0.1427 | 0.052769 | 0.3003 | -0.4848 | 0.2236 | 0.03017 | 0.3084 | NaN | -0.3824 | 0.1245 | 0.002134 | 0.0607 | -0.3398 | 0.1234 | 0.005891 | 0.1414 | -0.3898 | 0.2126 | 0.066719 | 0.635 | NaN | -0.3661 | 0.1247 | 0.003324 | 0.0633 | -0.2856 | 0.1219 | 0.019108 | 0.2637 | -0.4416 | 0.2118 | 0.037108 | 0.3872 | NaN | -0.4268 | 0.1267 | 0.000757 | 0.0261 | -0.3922 | 0.1292 | 0.002392 | 0.055 | -0.4139 | 0.2146 | 0.05377 | 0.5708 | NaN | -0.3972 | 0.126 | 0.001617 | 0.0504 | -0.3438 | 0.1236 | 0.005409 | 0.1424 | -0.4284 | 0.215 | 0.046301 | 0.5011 | NaN | -0.4193 | 0.1271 | 0.000971 | 0.0315 | -0.3867 | 0.1268 | 0.002287 | 0.0553 | -0.4228 | 0.2165 | 0.05083 | 0.5102 |
| AC 6:0 | 259.1784 | 7.03923 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.3812 | 0.1402 | 0.006549 | 0.0931 | -0.2553 | 0.1471 | 0.082699 | 0.3594 | -0.4726 | 0.2288 | 0.038921 | 0.3491 | NaN | -0.4653 | 0.1286 | 0.000297 | 0.0164 | -0.4295 | 0.1271 | 0.000725 | 0.0333 | -0.4687 | 0.2141 | 0.028594 | 0.5113 | NaN | -0.4785 | 0.1284 | 0.000194 | 0.0092 | -0.3622 | 0.1245 | 0.003634 | 0.1056 | -0.568 | 0.2148 | 0.008198 | 0.174 | NaN | -0.4795 | 0.132 | 0.00028 | 0.014 | -0.4447 | 0.1343 | 0.000933 | 0.0436 | -0.4759 | 0.217 | 0.028316 | 0.4788 | NaN | -0.4516 | 0.1306 | 0.000541 | 0.0249 | -0.3898 | 0.1274 | 0.00222 | 0.0875 | -0.4883 | 0.2178 | 0.024962 | 0.4751 | NaN | -0.4747 | 0.1323 | 0.000333 | 0.0167 | -0.4654 | 0.1317 | 0.00041 | 0.0251 | -0.4684 | 0.2193 | 0.032701 | 0.4663 |
| AC 8:0 | 287.21 | 11.700219 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.393 | 0.1382 | 0.004451 | 0.0744 | -0.4041 | 0.157 | 0.010071 | 0.1685 | -0.3726 | 0.2112 | 0.077683 | 0.4717 | NaN | -0.3736 | 0.1277 | 0.003427 | 0.0791 | -0.4089 | 0.1363 | 0.002692 | 0.0908 | -0.3329 | 0.1986 | 0.093789 | 0.7567 | NaN | -0.4253 | 0.1267 | 0.000792 | 0.0255 | -0.4234 | 0.1331 | 0.001461 | 0.0672 | -0.4208 | 0.1986 | 0.034121 | 0.3815 | NaN | -0.3942 | 0.1303 | 0.002482 | 0.0548 | -0.4322 | 0.1419 | 0.002327 | 0.055 | -0.3451 | 0.2011 | 0.08609 | 0.7393 | NaN | -0.3752 | 0.1294 | 0.003741 | 0.0826 | -0.4016 | 0.1368 | 0.003318 | 0.1082 | -0.3446 | 0.202 | 0.088098 | 0.6316 | NaN | -0.3941 | 0.1306 | 0.002544 | 0.0585 | -0.4443 | 0.1393 | 0.001424 | 0.0437 | -0.3437 | 0.2031 | 0.090643 | 0.6639 |
| AC 10:0 | 315.2413 | 15.299243 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.461 | 0.1384 | 0.000867 | 0.0296 | -0.4648 | 0.1528 | 0.002353 | 0.0999 | -0.4478 | 0.2144 | 0.036739 | 0.3491 | NaN | -0.4031 | 0.1288 | 0.001749 | 0.0536 | -0.4249 | 0.1338 | 0.001494 | 0.0568 | -0.375 | 0.2029 | 0.064577 | 0.6334 | NaN | -0.4725 | 0.127 | 0.000199 | 0.0092 | -0.4747 | 0.129 | 0.000234 | 0.0129 | -0.4673 | 0.2016 | 0.020463 | 0.3053 | NaN | -0.4232 | 0.1313 | 0.001269 | 0.035 | -0.4444 | 0.1392 | 0.001414 | 0.0459 | -0.3898 | 0.2053 | 0.057547 | 0.5776 | NaN | -0.4087 | 0.1305 | 0.001733 | 0.0504 | -0.4192 | 0.1343 | 0.001807 | 0.0831 | -0.392 | 0.2062 | 0.057251 | 0.5267 | NaN | -0.4245 | 0.1316 | 0.001252 | 0.0364 | -0.4493 | 0.1367 | 0.001012 | 0.0399 | -0.3937 | 0.2073 | 0.05751 | 0.5263 |
| AC 12:0 | 343.2717 | 17.918053 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.3707 | 0.1334 | 0.005458 | 0.0886 | -0.3901 | 0.1369 | 0.004388 | 0.1153 | -0.3368 | 0.2187 | 0.123502 | 0.598 | NaN | -0.3465 | 0.1234 | 0.004987 | 0.0949 | -0.4087 | 0.118 | 0.000536 | 0.0277 | -0.2793 | 0.2062 | 0.175519 | 0.879 | NaN | -0.4089 | 0.1223 | 0.000831 | 0.0255 | -0.4545 | 0.1142 | 0.000069 | 0.009 | -0.3755 | 0.2059 | 0.068141 | 0.5233 | NaN | -0.3658 | 0.1259 | 0.003667 | 0.0698 | -0.4258 | 0.1232 | 0.00055 | 0.0337 | -0.2939 | 0.2086 | 0.15897 | 0.8688 | NaN | -0.3405 | 0.1252 | 0.006559 | 0.1299 | -0.3931 | 0.1188 | 0.000936 | 0.0574 | -0.2871 | 0.2099 | 0.171354 | 0.8386 | NaN | -0.3589 | 0.1263 | 0.0045 | 0.0828 | -0.4246 | 0.1211 | 0.000455 | 0.0251 | -0.2897 | 0.2109 | 0.169642 | 0.8194 |
| AC 10:1 | 313.2253 | 13.943843 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.393 | 0.1373 | 0.00419 | 0.0744 | -0.3668 | 0.1458 | 0.011862 | 0.177 | -0.3984 | 0.2208 | 0.07117 | 0.4554 | NaN | -0.3712 | 0.1269 | 0.003438 | 0.0791 | -0.3605 | 0.1269 | 0.004484 | 0.1179 | -0.3557 | 0.2077 | 0.08677 | 0.7567 | NaN | -0.4286 | 0.1259 | 0.000661 | 0.0228 | -0.3739 | 0.1239 | 0.002545 | 0.0804 | -0.4644 | 0.2076 | 0.025272 | 0.3402 | NaN | -0.3884 | 0.1295 | 0.002708 | 0.0554 | -0.3892 | 0.1319 | 0.003169 | 0.0673 | -0.3537 | 0.2107 | 0.093296 | 0.7393 | NaN | -0.3739 | 0.1286 | 0.003641 | 0.0826 | -0.3585 | 0.1272 | 0.004829 | 0.1424 | -0.3672 | 0.2113 | 0.082181 | 0.6055 | NaN | -0.3848 | 0.1299 | 0.003049 | 0.0642 | -0.3997 | 0.1295 | 0.002019 | 0.0531 | -0.3474 | 0.2132 | 0.103105 | 0.6941 |
| AC 12:1 | 341.2561 | 16.741268 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.4827 | 0.1357 | 0.000373 | 0.017 | -0.421 | 0.1432 | 0.003282 | 0.1044 | -0.5177 | 0.2176 | 0.017353 | 0.2228 | NaN | -0.5026 | 0.1244 | 0.000054 | 0.0074 | -0.4637 | 0.1226 | 0.000156 | 0.0215 | -0.5181 | 0.2034 | 0.010842 | 0.399 | NaN | -0.5148 | 0.1241 | 0.000033 | 0.0027 | -0.4486 | 0.1204 | 0.000196 | 0.0129 | -0.5639 | 0.2041 | 0.005718 | 0.1494 | NaN | -0.5256 | 0.1272 | 0.000036 | 0.004 | -0.5026 | 0.1279 | 0.000085 | 0.0118 | -0.5232 | 0.2061 | 0.011151 | 0.342 | NaN | -0.5026 | 0.1262 | 0.000068 | 0.0094 | -0.4507 | 0.1233 | 0.000256 | 0.0279 | -0.532 | 0.207 | 0.010158 | 0.3298 | NaN | -0.522 | 0.1276 | 0.000043 | 0.0047 | -0.4964 | 0.1256 | 0.000078 | 0.014 | -0.5278 | 0.2081 | 0.011222 | 0.3442 |
| AC 14:1 | 369.2874 | 18.959509 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.4714 | 0.1336 | 0.000418 | 0.017 | -0.4575 | 0.1427 | 0.001344 | 0.0675 | -0.465 | 0.2123 | 0.028482 | 0.3083 | NaN | -0.4302 | 0.1239 | 0.000515 | 0.0219 | -0.4665 | 0.1229 | 0.000146 | 0.0215 | -0.386 | 0.2012 | 0.055073 | 0.608 | NaN | -0.4856 | 0.1225 | 0.000073 | 0.0051 | -0.4874 | 0.1195 | 0.000045 | 0.0083 | -0.4844 | 0.1996 | 0.015217 | 0.2532 | NaN | -0.4638 | 0.126 | 0.000233 | 0.0128 | -0.5102 | 0.1276 | 0.000063 | 0.0118 | -0.4059 | 0.2033 | 0.04588 | 0.5506 | NaN | -0.4375 | 0.1254 | 0.000487 | 0.0244 | -0.4475 | 0.1239 | 0.000303 | 0.0279 | -0.4191 | 0.2037 | 0.03967 | 0.4772 | NaN | -0.4541 | 0.1265 | 0.000332 | 0.0167 | -0.4883 | 0.1259 | 0.000105 | 0.014 | -0.4135 | 0.2051 | 0.043823 | 0.4743 |
| AC 10:2 | 311.2083 | 12.303444 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.3995 | 0.1371 | 0.003571 | 0.068 | -0.3609 | 0.1513 | 0.017019 | 0.2037 | -0.4191 | 0.2139 | 0.050123 | 0.3843 | NaN | -0.3643 | 0.127 | 0.00413 | 0.0844 | -0.3738 | 0.1312 | 0.004395 | 0.1179 | -0.3384 | 0.2028 | 0.095189 | 0.7567 | NaN | -0.3911 | 0.1263 | 0.001955 | 0.0481 | -0.354 | 0.1291 | 0.006129 | 0.1538 | -0.4069 | 0.2018 | 0.043772 | 0.438 | NaN | -0.4044 | 0.1292 | 0.00175 | 0.042 | -0.4386 | 0.1362 | 0.001281 | 0.0459 | -0.3566 | 0.205 | 0.081944 | 0.7393 | NaN | -0.3735 | 0.1286 | 0.003675 | 0.0826 | -0.3598 | 0.1319 | 0.006374 | 0.1424 | -0.3718 | 0.2053 | 0.070176 | 0.6053 | NaN | -0.4035 | 0.1295 | 0.001837 | 0.0441 | -0.4333 | 0.1339 | 0.00121 | 0.0423 | -0.3693 | 0.2066 | 0.073834 | 0.6024 |
| AC 12:2 | 339.2397 | 15.794398 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.5864 | 0.1267 | 0.000004 | 0.0007 | -0.2957 | 0.1418 | 0.037024 | 0.2877 | -0.7907 | 0.1953 | 0.000051 | 0.0094 | NaN | -0.5209 | 0.1183 | 0.000011 | 0.002 | -0.2516 | 0.1249 | 0.044012 | 0.3796 | -0.7095 | 0.1859 | 0.000135 | 0.0188 | NaN | -0.57 | 0.1164 | 0.000001 | 0.0002 | -0.311 | 0.1208 | 0.010053 | 0.2019 | -0.7565 | 0.1843 | 0.00004 | 0.0061 | NaN | -0.5142 | 0.1218 | 0.000024 | 0.0034 | -0.2609 | 0.1302 | 0.045022 | 0.2792 | -0.6873 | 0.1918 | 0.000339 | 0.0374 | NaN | -0.5289 | 0.1198 | 0.00001 | 0.0019 | -0.2303 | 0.126 | 0.06749 | 0.4198 | -0.7399 | 0.1878 | 0.000082 | 0.015 | NaN | -0.5231 | 0.1217 | 0.000017 | 0.0032 | -0.2697 | 0.1278 | 0.034822 | 0.2595 | -0.7049 | 0.1927 | 0.000253 | 0.0283 |
| AC 14:2 | 367.2715 | 17.837961 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.4589 | 0.1267 | 0.000293 | 0.0162 | -0.3378 | 0.1309 | 0.009832 | 0.1685 | -0.5483 | 0.2083 | 0.008471 | 0.1612 | NaN | -0.4356 | 0.1171 | 0.000198 | 0.0145 | -0.358 | 0.1131 | 0.001542 | 0.0568 | -0.4857 | 0.1968 | 0.01356 | 0.4257 | NaN | -0.4808 | 0.116 | 0.000034 | 0.0027 | -0.4036 | 0.1096 | 0.00023 | 0.0129 | -0.547 | 0.1959 | 0.005238 | 0.1494 | NaN | -0.4694 | 0.1192 | 0.000082 | 0.0064 | -0.3888 | 0.1178 | 0.00096 | 0.0436 | -0.5154 | 0.1984 | 0.009372 | 0.318 | NaN | -0.4436 | 0.1185 | 0.000182 | 0.0144 | -0.3478 | 0.1136 | 0.002203 | 0.0875 | -0.5161 | 0.1993 | 0.009618 | 0.3298 | NaN | -0.4572 | 0.1197 | 0.000133 | 0.0105 | -0.375 | 0.116 | 0.001226 | 0.0423 | -0.5126 | 0.2006 | 0.010588 | 0.3438 |
| AC 11:3 | 323.2119 | 20.819927 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.234 | 0.1247 | 0.060469 | 0.3473 | -0.5279 | 0.1228 | 0.000017 | 0.0047 | 0.0029 | 0.2013 | 0.988563 | 0.9935 | NaN | -0.1659 | 0.1163 | 0.153736 | 0.7013 | -0.4373 | 0.1106 | 0.000077 | 0.0215 | 0.0338 | 0.189 | 0.857937 | 0.9765 | NaN | -0.2435 | 0.1149 | 0.034027 | 0.2852 | -0.4645 | 0.106 | 0.000012 | 0.0061 | -0.0862 | 0.1915 | 0.652675 | 0.9894 | NaN | -0.1497 | 0.1198 | 0.211458 | 0.6949 | -0.4444 | 0.1163 | 0.000133 | 0.0146 | 0.0769 | 0.1925 | 0.689616 | 0.9476 | NaN | -0.1917 | 0.1173 | 0.102357 | 0.6358 | -0.4583 | 0.1092 | 0.000027 | 0.0149 | 0.0132 | 0.1923 | 0.945358 | 0.9854 | NaN | -0.1363 | 0.1207 | 0.25868 | 0.7205 | -0.4194 | 0.1164 | 0.000315 | 0.0249 | 0.0794 | 0.1946 | 0.683238 | 0.9459 |
| AC 6:0 (OH) | 275.1739 | 3.553601 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.361 | 0.1336 | 0.006912 | 0.0954 | -0.1804 | 0.143 | 0.207164 | 0.506 | -0.4879 | 0.2149 | 0.023187 | 0.2723 | NaN | -0.3586 | 0.1232 | 0.003613 | 0.0798 | -0.2766 | 0.1245 | 0.02632 | 0.2806 | -0.3969 | 0.2043 | 0.05205 | 0.5991 | NaN | -0.3701 | 0.1229 | 0.002598 | 0.0574 | -0.2641 | 0.122 | 0.030463 | 0.3503 | -0.4475 | 0.2035 | 0.027892 | 0.3487 | NaN | -0.4077 | 0.1257 | 0.00118 | 0.0343 | -0.349 | 0.1317 | 0.008029 | 0.1108 | -0.422 | 0.2062 | 0.040668 | 0.5138 | NaN | -0.3637 | 0.1249 | 0.003586 | 0.0826 | -0.2524 | 0.1248 | 0.043158 | 0.3563 | -0.4386 | 0.2064 | 0.033564 | 0.4772 | NaN | -0.4036 | 0.126 | 0.001362 | 0.0376 | -0.3396 | 0.1289 | 0.00841 | 0.1222 | -0.4383 | 0.2075 | 0.034712 | 0.4663 |
| AC 8:0 (OH) | 303.2045 | 7.959024 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.5435 | 0.1346 | 0.000054 | 0.0049 | -0.5216 | 0.1547 | 0.000748 | 0.059 | -0.5417 | 0.2042 | 0.007981 | 0.1612 | NaN | -0.4658 | 0.126 | 0.000217 | 0.0145 | -0.4715 | 0.1356 | 0.000509 | 0.0277 | -0.4491 | 0.1947 | 0.021069 | 0.4652 | NaN | -0.5285 | 0.1237 | 0.000019 | 0.0021 | -0.5013 | 0.1314 | 0.000135 | 0.0124 | -0.5472 | 0.1919 | 0.004352 | 0.1413 | NaN | -0.48 | 0.1286 | 0.00019 | 0.0128 | -0.4951 | 0.141 | 0.000446 | 0.0308 | -0.4491 | 0.198 | 0.023322 | 0.4551 | NaN | -0.4706 | 0.1277 | 0.000229 | 0.0155 | -0.4586 | 0.1366 | 0.00079 | 0.0574 | -0.4688 | 0.1977 | 0.017713 | 0.423 | NaN | -0.4829 | 0.1288 | 0.000178 | 0.0123 | -0.5015 | 0.1383 | 0.000287 | 0.0249 | -0.4586 | 0.1998 | 0.021703 | 0.4132 |
| AC 10:0 (OH) | 331.2357 | 12.493725 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.5451 | 0.1373 | 0.000072 | 0.0057 | -0.5052 | 0.1553 | 0.001141 | 0.0675 | -0.5646 | 0.2098 | 0.007128 | 0.1612 | NaN | -0.474 | 0.1282 | 0.000218 | 0.0145 | -0.4684 | 0.1356 | 0.000552 | 0.0277 | -0.4745 | 0.1997 | 0.017525 | 0.4591 | NaN | -0.5547 | 0.1257 | 0.00001 | 0.0014 | -0.5151 | 0.1308 | 0.000082 | 0.009 | -0.5872 | 0.1968 | 0.002851 | 0.1177 | NaN | -0.4843 | 0.1311 | 0.00022 | 0.0128 | -0.4811 | 0.1415 | 0.000673 | 0.0372 | -0.4784 | 0.2028 | 0.018341 | 0.4372 | NaN | -0.4761 | 0.1301 | 0.000252 | 0.0155 | -0.4472 | 0.1369 | 0.001093 | 0.0603 | -0.4951 | 0.2028 | 0.014635 | 0.423 | NaN | -0.4852 | 0.1314 | 0.000222 | 0.0136 | -0.4867 | 0.1388 | 0.000455 | 0.0251 | -0.4834 | 0.205 | 0.018354 | 0.4132 |
| FA 8:0 (DiC) | 174.0893 | 8.243132 | Lipid | Fatty Acid, Dicarboxylate | 0.2938 | 0.135 | 0.029562 | 0.2368 | 0.418 | 0.1427 | 0.00339 | 0.1044 | 0.2066 | 0.2135 | 0.333285 | 0.7534 | NaN | 0.1972 | 0.1267 | 0.119677 | 0.6749 | 0.2429 | 0.1337 | 0.069288 | 0.4801 | 0.188 | 0.2004 | 0.348006 | 0.9223 | NaN | 0.1123 | 0.1301 | 0.387664 | 0.8424 | 0.2189 | 0.1323 | 0.09803 | 0.6366 | 0.0396 | 0.2081 | 0.849221 | 0.9935 | NaN | 0.2657 | 0.1279 | 0.037748 | 0.3473 | 0.3389 | 0.1333 | 0.010987 | 0.1343 | 0.2311 | 0.2028 | 0.25442 | 0.8705 | NaN | 0.215 | 0.128 | 0.093153 | 0.6195 | 0.267 | 0.1321 | 0.043252 | 0.3563 | 0.186 | 0.2041 | 0.362029 | 0.9106 | NaN | 0.2676 | 0.1281 | 0.036779 | 0.346 | 0.3203 | 0.1321 | 0.015323 | 0.1579 | 0.2423 | 0.2048 | 0.236657 | 0.8424 |
| FA 10:1 (DiC) | 200.1056 | 10.504287 | Lipid | Fatty Acid, Dicarboxylate | -0.0749 | 0.133 | 0.573429 | 0.8418 | -0.3826 | 0.131 | 0.003501 | 0.1044 | 0.1834 | 0.2274 | 0.420056 | 0.7762 | NaN | 0 | 0.1238 | 0.999893 | 0.9999 | -0.3028 | 0.1171 | 0.009696 | 0.1622 | 0.2302 | 0.2131 | 0.28008 | 0.9223 | NaN | 0.0013 | 0.1236 | 0.991677 | 0.9939 | -0.2771 | 0.116 | 0.016966 | 0.2556 | 0.222 | 0.2146 | 0.30098 | 0.944 | NaN | -0.0031 | 0.1267 | 0.980653 | 0.9932 | -0.3373 | 0.1207 | 0.005212 | 0.0822 | 0.2583 | 0.2165 | 0.232769 | 0.8705 | NaN | 0.0097 | 0.1258 | 0.938322 | 0.9796 | -0.2765 | 0.119 | 0.020118 | 0.2314 | 0.2307 | 0.2171 | 0.288071 | 0.9039 | NaN | -0.0118 | 0.1268 | 0.926137 | 0.9775 | -0.3553 | 0.1179 | 0.002577 | 0.0593 | 0.2657 | 0.2189 | 0.224857 | 0.8424 |
| Keto 14:0 | 242.1884 | 20.796713 | Lipid | Fatty Acid, Keto | -0.4328 | 0.1338 | 0.001217 | 0.0305 | -0.2845 | 0.14 | 0.042099 | 0.2929 | -0.5488 | 0.218 | 0.01183 | 0.1921 | NaN | -0.3808 | 0.1244 | 0.002198 | 0.0607 | -0.2734 | 0.1223 | 0.025428 | 0.2806 | -0.4671 | 0.2068 | 0.02391 | 0.4888 | NaN | -0.4338 | 0.123 | 0.000419 | 0.0154 | -0.2349 | 0.1211 | 0.052344 | 0.4874 | -0.6231 | 0.2041 | 0.002264 | 0.1042 | NaN | -0.4273 | 0.1262 | 0.000709 | 0.0261 | -0.3405 | 0.1266 | 0.007173 | 0.1015 | -0.4897 | 0.2088 | 0.019009 | 0.4372 | NaN | -0.391 | 0.1259 | 0.001892 | 0.0507 | -0.2729 | 0.1226 | 0.026007 | 0.2579 | -0.4914 | 0.2098 | 0.019159 | 0.423 | NaN | -0.4219 | 0.1266 | 0.000862 | 0.0315 | -0.354 | 0.1244 | 0.004421 | 0.0793 | -0.4805 | 0.2117 | 0.023204 | 0.4132 |
| PA 22:3 | 488.2996 | 19.989008 | Lipid | Phosphatidic Acid | -0.3523 | 0.1277 | 0.005791 | 0.0902 | -0.2523 | 0.1482 | 0.088804 | 0.3714 | -0.4697 | 0.1968 | 0.017008 | 0.2228 | NaN | -0.3199 | 0.1183 | 0.006832 | 0.1217 | -0.2229 | 0.1302 | 0.086852 | 0.5387 | -0.4428 | 0.1847 | 0.0165 | 0.4554 | NaN | -0.2692 | 0.1195 | 0.024262 | 0.2679 | -0.1487 | 0.1301 | 0.252744 | 0.8037 | -0.3897 | 0.1885 | 0.038693 | 0.3955 | NaN | -0.3274 | 0.1209 | 0.006749 | 0.1035 | -0.2588 | 0.1351 | 0.055353 | 0.3183 | -0.4409 | 0.1874 | 0.018662 | 0.4372 | NaN | -0.3024 | 0.1204 | 0.012008 | 0.195 | -0.2295 | 0.1303 | 0.078153 | 0.4639 | -0.4078 | 0.1899 | 0.031772 | 0.4772 | NaN | -0.3327 | 0.121 | 0.005973 | 0.103 | -0.2741 | 0.1327 | 0.038849 | 0.2714 | -0.4392 | 0.1894 | 0.020411 | 0.4132 |
| PC 33:3/PE 36:3 | 741.568 | 25.137949 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.4657 | 0.1229 | 0.000151 | 0.0104 | -0.1924 | 0.1421 | 0.175832 | 0.4964 | -0.6254 | 0.1885 | 0.000907 | 0.051 | NaN | -0.374 | 0.1159 | 0.001254 | 0.0416 | -0.0507 | 0.1288 | 0.693574 | 0.9315 | -0.5684 | 0.1781 | 0.001415 | 0.1116 | NaN | -0.3463 | 0.1171 | 0.003094 | 0.0615 | -0.0566 | 0.1258 | 0.652749 | 0.9053 | -0.5312 | 0.1822 | 0.003556 | 0.1309 | NaN | -0.4094 | 0.1174 | 0.000488 | 0.0207 | -0.0918 | 0.1331 | 0.490413 | 0.7494 | -0.5932 | 0.1795 | 0.000951 | 0.075 | NaN | -0.3902 | 0.117 | 0.000855 | 0.0363 | -0.0836 | 0.1276 | 0.512328 | 0.8496 | -0.5727 | 0.1816 | 0.001616 | 0.1274 | NaN | -0.418 | 0.1173 | 0.000368 | 0.0169 | -0.0756 | 0.1316 | 0.565691 | 0.8092 | -0.6194 | 0.1803 | 0.000592 | 0.0467 |
| PC 38:6/PE 41:6 | 805.5625 | 24.26375 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2292 | 0.1402 | 0.102078 | 0.4619 | -0.4542 | 0.1404 | 0.001217 | 0.0675 | -0.0244 | 0.2298 | 0.915527 | 0.9838 | NaN | -0.1777 | 0.1302 | 0.172156 | 0.7251 | -0.3415 | 0.1272 | 0.007255 | 0.154 | -0.0399 | 0.2156 | 0.853136 | 0.9765 | NaN | -0.1706 | 0.1301 | 0.189723 | 0.7173 | -0.3354 | 0.1248 | 0.007177 | 0.1723 | -0.0302 | 0.217 | 0.88949 | 0.9935 | NaN | -0.1988 | 0.1328 | 0.134396 | 0.5986 | -0.3575 | 0.1327 | 0.007068 | 0.1015 | -0.0648 | 0.2187 | 0.766892 | 0.9598 | NaN | -0.1834 | 0.1319 | 0.16435 | 0.6753 | -0.3411 | 0.1275 | 0.007476 | 0.1424 | -0.0401 | 0.2195 | 0.854889 | 0.9621 | NaN | -0.1968 | 0.1331 | 0.139381 | 0.605 | -0.3471 | 0.131 | 0.008058 | 0.1202 | -0.0599 | 0.2208 | 0.78597 | 0.9525 |
| myo-inositol | 180.0635 | 0.624334 | Lipid | Inositol Metabolism | 0.4666 | 0.1458 | 0.001376 | 0.033 | 0.1016 | 0.146 | 0.486618 | 0.7524 | 0.8641 | 0.2443 | 0.000405 | 0.0279 | NaN | 0.4768 | 0.1341 | 0.000377 | 0.0189 | 0.1201 | 0.1279 | 0.347838 | 0.8132 | 0.8667 | 0.2272 | 0.000136 | 0.0188 | NaN | 0.5007 | 0.1336 | 0.000178 | 0.0092 | 0.104 | 0.1257 | 0.408088 | 0.8818 | 0.9425 | 0.227 | 0.000033 | 0.0061 | NaN | 0.4493 | 0.1378 | 0.001111 | 0.0341 | 0.0691 | 0.1339 | 0.606067 | 0.8188 | 0.8729 | 0.2305 | 0.000152 | 0.028 | NaN | 0.4886 | 0.1358 | 0.000322 | 0.0178 | 0.1459 | 0.1281 | 0.254934 | 0.7315 | 0.8642 | 0.2319 | 0.000194 | 0.0268 | NaN | 0.4563 | 0.1379 | 0.00094 | 0.0315 | 0.0945 | 0.1315 | 0.47246 | 0.7643 | 0.854 | 0.2336 | 0.000257 | 0.0283 |
| LysoPC 14:0 | 467.3013 | 21.544027 | Lipid | Lysolipid, PC | 0.3609 | 0.132 | 0.006265 | 0.0931 | 0.0296 | 0.1545 | 0.84792 | 0.932 | 0.5803 | 0.1967 | 0.003175 | 0.1069 | NaN | 0.2423 | 0.1251 | 0.052726 | 0.4443 | -0.0175 | 0.1359 | 0.897784 | 0.9729 | 0.4149 | 0.1947 | 0.0331 | 0.5144 | NaN | 0.283 | 0.1233 | 0.021729 | 0.2499 | 0.0794 | 0.1331 | 0.550727 | 0.9053 | 0.4263 | 0.1958 | 0.029445 | 0.3533 | NaN | 0.2485 | 0.1284 | 0.052926 | 0.436 | -0.057 | 0.1426 | 0.689166 | 0.8587 | 0.4465 | 0.1957 | 0.02247 | 0.4551 | NaN | 0.2807 | 0.1255 | 0.025244 | 0.2903 | 0.0022 | 0.136 | 0.98687 | 0.9923 | 0.473 | 0.194 | 0.014735 | 0.423 | NaN | 0.2663 | 0.1278 | 0.03719 | 0.346 | -0.0604 | 0.1404 | 0.666795 | 0.8681 | 0.4811 | 0.1947 | 0.013461 | 0.3715 |
| glycochenodeoxycholate | 449.315 | 20.243961 | Lipid | Primary Bile Acid Metabolism | 0.677 | 0.1241 | 0.0 | <.0001 | 0.2999 | 0.1289 | 0.019975 | 0.208 | 1.0568 | 0.2013 | 0.0 | <.0001 | NaN | 0.6703 | 0.1136 | 0.0 | <.0001 | 0.3624 | 0.1108 | 0.001069 | 0.0454 | 0.9764 | 0.1911 | 0.0 | 0.0002 | NaN | 0.6437 | 0.1143 | 0.0 | <.0001 | 0.3288 | 0.1092 | 0.002597 | 0.0804 | 0.9682 | 0.1938 | 0.000001 | 0.0003 | NaN | 0.6975 | 0.1158 | 0.0 | <.0001 | 0.3568 | 0.1162 | 0.002139 | 0.055 | 1.0281 | 0.1904 | 0.0 | <.0001 | NaN | 0.6614 | 0.1156 | 0.0 | <.0001 | 0.3357 | 0.1115 | 0.002609 | 0.096 | 0.9957 | 0.1941 | 0.0 | 0.0002 | NaN | 0.6896 | 0.1163 | 0.0 | <.0001 | 0.3212 | 0.1148 | 0.005142 | 0.0852 | 1.0545 | 0.1912 | 0.0 | <.0001 |
| glycocholate | 465.309 | 18.850445 | Lipid | Primary Bile Acid Metabolism | 0.6307 | 0.1261 | 0.000001 | 0.0002 | 0.365 | 0.1334 | 0.006232 | 0.1405 | 0.8732 | 0.2028 | 0.000017 | 0.0046 | NaN | 0.6136 | 0.1159 | 0.0 | <.0001 | 0.4169 | 0.1143 | 0.000264 | 0.0277 | 0.7845 | 0.1934 | 0.00005 | 0.0138 | NaN | 0.5882 | 0.1165 | 0.0 | 0.0001 | 0.3532 | 0.1138 | 0.001911 | 0.0804 | 0.7939 | 0.1944 | 0.000044 | 0.0061 | NaN | 0.6603 | 0.1177 | 0.0 | <.0001 | 0.4312 | 0.1197 | 0.000314 | 0.0247 | 0.8528 | 0.192 | 0.000009 | 0.0025 | NaN | 0.6199 | 0.1174 | 0.0 | <.0001 | 0.3705 | 0.1158 | 0.001381 | 0.0693 | 0.84 | 0.1937 | 0.000015 | 0.004 | NaN | 0.644 | 0.1183 | 0.0 | <.0001 | 0.3972 | 0.1182 | 0.000779 | 0.0358 | 0.8582 | 0.1939 | 0.00001 | 0.0026 |
| taurocholate | 515.2836 | 24.507624 | Lipid | Primary Bile Acid Metabolism | -0.2432 | 0.1327 | 0.066932 | 0.3704 | 0.1881 | 0.1245 | 0.130876 | 0.424 | -0.8494 | 0.2319 | 0.000249 | 0.023 | NaN | -0.285 | 0.1223 | 0.019826 | 0.2736 | 0.069 | 0.1128 | 0.540749 | 0.8967 | -0.7462 | 0.2212 | 0.000744 | 0.0685 | NaN | -0.2724 | 0.1222 | 0.025746 | 0.27 | 0.0995 | 0.1092 | 0.362172 | 0.873 | -0.7618 | 0.222 | 0.0006 | 0.0368 | NaN | -0.2708 | 0.1252 | 0.030541 | 0.3242 | 0.0947 | 0.1171 | 0.418566 | 0.7106 | -0.7536 | 0.2246 | 0.000793 | 0.073 | NaN | -0.2817 | 0.124 | 0.023115 | 0.2887 | 0.0659 | 0.1132 | 0.560471 | 0.8618 | -0.7637 | 0.2251 | 0.000691 | 0.0636 | NaN | -0.2936 | 0.1255 | 0.019329 | 0.2319 | 0.0736 | 0.1161 | 0.525966 | 0.7998 | -0.7897 | 0.2244 | 0.000434 | 0.0399 |
| norhyodeoxycholic acid | 378.2799 | 22.721872 | Lipid | Secondary Bile Acid Metabolism | 0.1939 | 0.1313 | 0.139696 | 0.5159 | 0.4594 | 0.1322 | 0.00051 | 0.059 | -0.0185 | 0.2127 | 0.930507 | 0.9887 | NaN | 0.105 | 0.1228 | 0.39266 | 0.8498 | 0.2931 | 0.1251 | 0.019146 | 0.2349 | 0.0007 | 0.1995 | 0.997089 | 0.9999 | NaN | 0.1613 | 0.1215 | 0.184378 | 0.7111 | 0.308 | 0.1205 | 0.010608 | 0.2019 | 0.0814 | 0.2026 | 0.687657 | 0.9894 | NaN | 0.1315 | 0.1251 | 0.29322 | 0.7388 | 0.3247 | 0.13 | 0.012496 | 0.14 | 0.0301 | 0.2027 | 0.881806 | 0.99 | NaN | 0.1324 | 0.1239 | 0.285243 | 0.7504 | 0.2953 | 0.1252 | 0.018374 | 0.2263 | 0.0299 | 0.2036 | 0.883278 | 0.9633 | NaN | 0.1029 | 0.1264 | 0.41557 | 0.791 | 0.2953 | 0.1303 | 0.023459 | 0.1992 | -0.0157 | 0.2041 | 0.938661 | 0.9869 |
| DHEA sulfate | 368.1666 | 15.235868 | Lipid | Steroid | 0.4953 | 0.1674 | 0.003094 | 0.0632 | 0.3231 | 0.17 | 0.057322 | 0.3054 | 0.6673 | 0.2799 | 0.017125 | 0.2228 | NaN | 0.3226 | 0.1598 | 0.043439 | 0.4204 | 0.1158 | 0.1572 | 0.461103 | 0.8628 | 0.5156 | 0.2683 | 0.05463 | 0.608 | NaN | 0.3308 | 0.159 | 0.037565 | 0.3049 | 0.2107 | 0.149 | 0.157202 | 0.7183 | 0.4393 | 0.2779 | 0.113879 | 0.6617 | NaN | 0.3439 | 0.1635 | 0.035446 | 0.3473 | 0.1487 | 0.1638 | 0.364047 | 0.6762 | 0.5186 | 0.2729 | 0.05738 | 0.5776 | NaN | 0.3528 | 0.161 | 0.028411 | 0.3137 | 0.1331 | 0.1565 | 0.394844 | 0.8162 | 0.5529 | 0.2718 | 0.041951 | 0.4772 | NaN | 0.3553 | 0.1633 | 0.029629 | 0.3025 | 0.1244 | 0.1621 | 0.44295 | 0.7458 | 0.5594 | 0.2731 | 0.04055 | 0.4663 |
| cycloheptanecarboxylic acid | 142.0996 | 10.720997 | Organic acids and derivatives | Carboxylic Acid | 0.2935 | 0.1349 | 0.029602 | 0.2368 | 0.4161 | 0.1429 | 0.003594 | 0.1044 | 0.2088 | 0.2132 | 0.327393 | 0.7534 | NaN | 0.2084 | 0.1263 | 0.098823 | 0.6343 | 0.2629 | 0.1321 | 0.046544 | 0.3924 | 0.1889 | 0.2001 | 0.345082 | 0.9223 | NaN | 0.1279 | 0.1292 | 0.322387 | 0.8008 | 0.2428 | 0.1305 | 0.062696 | 0.5493 | 0.0461 | 0.2075 | 0.824148 | 0.9935 | NaN | 0.267 | 0.1278 | 0.03665 | 0.3473 | 0.3454 | 0.1329 | 0.009345 | 0.12 | 0.2253 | 0.2024 | 0.265634 | 0.8705 | NaN | 0.2244 | 0.1277 | 0.07883 | 0.5579 | 0.2863 | 0.1307 | 0.028427 | 0.266 | 0.1864 | 0.2038 | 0.360188 | 0.9106 | NaN | 0.2714 | 0.128 | 0.033973 | 0.329 | 0.3285 | 0.1316 | 0.012552 | 0.1359 | 0.241 | 0.2044 | 0.238295 | 0.8424 |
| dipeptide (tyrosine proline) | 279.132 | 1.012568 | Peptide | Dipeptide | 0.193 | 0.1284 | 0.132832 | 0.5022 | 0.4117 | 0.1277 | 0.001264 | 0.0675 | 0.0374 | 0.2126 | 0.860322 | 0.9732 | NaN | 0.1137 | 0.1199 | 0.343135 | 0.8307 | 0.3032 | 0.1161 | 0.00902 | 0.1606 | -0.0016 | 0.1997 | 0.993419 | 0.9999 | NaN | 0.1428 | 0.1191 | 0.230362 | 0.7361 | 0.3355 | 0.1115 | 0.002623 | 0.0804 | -0.0003 | 0.2011 | 0.998778 | 0.9988 | NaN | 0.1297 | 0.1224 | 0.289356 | 0.7388 | 0.3095 | 0.122 | 0.011194 | 0.1343 | 0.0412 | 0.2021 | 0.838673 | 0.9726 | NaN | 0.1315 | 0.1212 | 0.27791 | 0.7462 | 0.2946 | 0.117 | 0.011844 | 0.1816 | 0.032 | 0.2031 | 0.874683 | 0.9621 | NaN | 0.1351 | 0.1226 | 0.270325 | 0.7315 | 0.3036 | 0.12 | 0.011401 | 0.1311 | 0.0422 | 0.204 | 0.836071 | 0.9641 |
| 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 | 0.0234 | 0.1271 | 0.853792 | 0.9778 | 0.1331 | 0.1361 | 0.328188 | 0.6183 | -0.0668 | 0.202 | 0.740913 | 0.9647 | NaN | -0.0641 | 0.1184 | 0.588499 | 0.9079 | -0.044 | 0.1247 | 0.72423 | 0.9386 | -0.0782 | 0.1894 | 0.679771 | 0.954 | NaN | -0.0518 | 0.118 | 0.660687 | 0.935 | -0.0204 | 0.1209 | 0.866314 | 0.9581 | -0.0814 | 0.1907 | 0.669507 | 0.9894 | NaN | -0.018 | 0.1205 | 0.881254 | 0.9749 | 0.0349 | 0.1273 | 0.784151 | 0.9094 | -0.0618 | 0.192 | 0.747532 | 0.9572 | NaN | 0.001 | 0.1192 | 0.993412 | 0.9988 | 0.0545 | 0.1211 | 0.652969 | 0.8623 | -0.0495 | 0.193 | 0.797639 | 0.9621 | NaN | -0.0113 | 0.1206 | 0.925209 | 0.9775 | 0.0094 | 0.1261 | 0.940735 | 0.9823 | -0.0365 | 0.1941 | 0.851049 | 0.9641 |
| N-acetyl-L-aspartic acid | 175.0479 | 0.965545 | Amino Acid | Acetyl Amino Acid | -0.1792 | 0.1468 | 0.222105 | 0.601 | -0.1381 | 0.1653 | 0.403443 | 0.6737 | -0.1951 | 0.2277 | 0.39161 | 0.7585 | NaN | -0.0678 | 0.1375 | 0.622084 | 0.9079 | -0.035 | 0.1469 | 0.811862 | 0.965 | -0.0905 | 0.2159 | 0.675283 | 0.954 | NaN | -0.0904 | 0.1367 | 0.508192 | 0.9053 | -0.0095 | 0.1447 | 0.94747 | 0.9765 | -0.1573 | 0.2155 | 0.465325 | 0.9816 | NaN | -0.0715 | 0.141 | 0.611936 | 0.8573 | -0.0328 | 0.1537 | 0.830793 | 0.9302 | -0.0916 | 0.2193 | 0.676047 | 0.9476 | NaN | -0.0874 | 0.139 | 0.529712 | 0.8625 | 0.0264 | 0.1492 | 0.85976 | 0.9614 | -0.1619 | 0.2179 | 0.457513 | 0.9359 | NaN | -0.0678 | 0.1415 | 0.631763 | 0.8817 | -0.0373 | 0.151 | 0.804852 | 0.9294 | -0.0838 | 0.2224 | 0.706104 | 0.9459 |
| N-acetyl-DL-serine | 147.0529 | 0.853391 | Amino Acid | Acetyl Amino Acid | -0.0064 | 0.1431 | 0.96418 | 0.9911 | 0.3082 | 0.1259 | 0.01434 | 0.1931 | -0.4719 | 0.2711 | 0.081756 | 0.4769 | NaN | -0.0612 | 0.1326 | 0.644071 | 0.9179 | 0.2104 | 0.1136 | 0.063852 | 0.4801 | -0.4225 | 0.2549 | 0.097463 | 0.7567 | NaN | -0.0624 | 0.1324 | 0.637263 | 0.9282 | 0.2265 | 0.1104 | 0.040174 | 0.4184 | -0.4837 | 0.2554 | 0.058225 | 0.4797 | NaN | -0.0249 | 0.1353 | 0.85419 | 0.9662 | 0.2548 | 0.1165 | 0.028758 | 0.2205 | -0.3991 | 0.2594 | 0.12398 | 0.8047 | NaN | -0.0097 | 0.1341 | 0.942433 | 0.9796 | 0.2705 | 0.111 | 0.01478 | 0.2092 | -0.4176 | 0.26 | 0.108219 | 0.6946 | NaN | -0.0334 | 0.1357 | 0.80531 | 0.9477 | 0.2293 | 0.1159 | 0.047944 | 0.2877 | -0.3949 | 0.2624 | 0.132299 | 0.7588 |
| N-alpha-acetyl-L-lysine | 188.1158 | 0.893928 | Amino Acid | Acetyl Amino Acid | -0.2171 | 0.1249 | 0.082014 | 0.4079 | -0.2235 | 0.1252 | 0.074203 | 0.3531 | -0.2044 | 0.2102 | 0.330794 | 0.7534 | NaN | -0.1694 | 0.116 | 0.144074 | 0.6828 | -0.1407 | 0.1119 | 0.208707 | 0.7304 | -0.2114 | 0.1969 | 0.283152 | 0.9223 | NaN | -0.1583 | 0.116 | 0.172426 | 0.6847 | -0.2039 | 0.1077 | 0.058227 | 0.5223 | -0.1209 | 0.2004 | 0.546446 | 0.9894 | NaN | -0.1415 | 0.1196 | 0.236637 | 0.7062 | -0.1275 | 0.1181 | 0.28013 | 0.6088 | -0.1636 | 0.2004 | 0.414271 | 0.9375 | NaN | -0.1607 | 0.1178 | 0.172473 | 0.6753 | -0.1543 | 0.1116 | 0.166897 | 0.631 | -0.1693 | 0.2012 | 0.400042 | 0.9295 | NaN | -0.1515 | 0.1195 | 0.204915 | 0.6633 | -0.1198 | 0.1164 | 0.3031 | 0.6619 | -0.1859 | 0.2019 | 0.357063 | 0.8785 |
| trans-4-hydroxyproline | 131.0586 | 0.616758 | Amino Acid | Arginine and Proline Metabolism | 0.1376 | 0.1326 | 0.299712 | 0.6742 | 0.0826 | 0.128 | 0.518933 | 0.7731 | 0.2028 | 0.2332 | 0.384526 | 0.7534 | NaN | 0.1909 | 0.1226 | 0.119466 | 0.6749 | 0.1262 | 0.1122 | 0.260522 | 0.7828 | 0.2751 | 0.2186 | 0.208252 | 0.9223 | NaN | 0.1279 | 0.1225 | 0.296199 | 0.7865 | 0.1049 | 0.1101 | 0.340689 | 0.8587 | 0.1616 | 0.2207 | 0.464022 | 0.9816 | NaN | 0.1685 | 0.1253 | 0.17891 | 0.6547 | 0.1053 | 0.117 | 0.368248 | 0.6762 | 0.2546 | 0.2216 | 0.250545 | 0.8705 | NaN | 0.189 | 0.1243 | 0.128395 | 0.6708 | 0.1454 | 0.1125 | 0.196054 | 0.6722 | 0.2467 | 0.2225 | 0.267675 | 0.9039 | NaN | 0.1755 | 0.1256 | 0.1625 | 0.6278 | 0.1141 | 0.1152 | 0.321973 | 0.6724 | 0.2577 | 0.2238 | 0.249642 | 0.8424 |
| m-hydroxymandelic acid | 168.0402 | 2.245258 | Amino Acid | catecholamine | -0.0164 | 0.1336 | 0.902187 | 0.9809 | 0.0199 | 0.1568 | 0.899001 | 0.953 | -0.022 | 0.2023 | 0.913236 | 0.9838 | NaN | -0.0267 | 0.1236 | 0.828873 | 0.967 | -0.0149 | 0.1377 | 0.914059 | 0.9729 | -0.0064 | 0.1898 | 0.973109 | 0.9911 | NaN | -0.0356 | 0.1234 | 0.772708 | 0.9628 | -0.026 | 0.1353 | 0.847775 | 0.95 | -0.0235 | 0.191 | 0.901906 | 0.9935 | NaN | -0.0447 | 0.1264 | 0.72393 | 0.9 | -0.0741 | 0.1448 | 0.608622 | 0.8188 | 0.0115 | 0.1925 | 0.952418 | 0.99 | NaN | -0.0358 | 0.1253 | 0.775143 | 0.938 | 0.0052 | 0.1379 | 0.970162 | 0.9923 | -0.0383 | 0.1932 | 0.842942 | 0.9621 | NaN | -0.0491 | 0.1268 | 0.698456 | 0.9035 | -0.0694 | 0.1423 | 0.625656 | 0.8423 | -0.0092 | 0.1941 | 0.962081 | 0.9892 |
| phosphocreatine | 211.0126 | 13.180015 | Amino Acid | Creatine Metabolism | -0.0407 | 0.1313 | 0.756406 | 0.9343 | -0.1021 | 0.1227 | 0.405224 | 0.6737 | 0.054 | 0.2398 | 0.821709 | 0.9713 | NaN | -0.0747 | 0.1214 | 0.538499 | 0.8926 | -0.096 | 0.1076 | 0.372628 | 0.824 | -0.0356 | 0.2261 | 0.874819 | 0.977 | NaN | -0.0407 | 0.1212 | 0.736882 | 0.9571 | -0.0627 | 0.1061 | 0.55428 | 0.9053 | -0.0017 | 0.227 | 0.994001 | 0.9976 | NaN | -0.1326 | 0.1251 | 0.289368 | 0.7388 | -0.1837 | 0.1125 | 0.102517 | 0.4326 | -0.0399 | 0.2296 | 0.861975 | 0.9831 | NaN | -0.0897 | 0.1232 | 0.466546 | 0.8625 | -0.1135 | 0.1077 | 0.291733 | 0.7544 | -0.0401 | 0.2308 | 0.862059 | 0.9621 | NaN | -0.1278 | 0.1253 | 0.307873 | 0.7485 | -0.1774 | 0.1105 | 0.108428 | 0.4629 | -0.0414 | 0.2323 | 0.858397 | 0.9641 |
| 5-oxoproline | 129.0429 | 1.13778 | Amino Acid | Creatine Metabolism | 0.0203 | 0.1423 | 0.886659 | 0.9809 | 0.0257 | 0.1671 | 0.877839 | 0.9409 | 0.0041 | 0.2138 | 0.984596 | 0.9935 | NaN | 0.0717 | 0.1318 | 0.586312 | 0.9079 | -0.0421 | 0.1471 | 0.774703 | 0.9615 | 0.1535 | 0.2036 | 0.450905 | 0.9478 | NaN | 0.0586 | 0.1315 | 0.655764 | 0.9331 | -0.1486 | 0.1462 | 0.309434 | 0.8373 | 0.1977 | 0.2075 | 0.340659 | 0.957 | NaN | 0.0988 | 0.1353 | 0.465235 | 0.7864 | 0.042 | 0.1528 | 0.783468 | 0.9094 | 0.1418 | 0.2066 | 0.492421 | 0.9375 | NaN | 0.0582 | 0.1335 | 0.662567 | 0.9055 | -0.0641 | 0.1477 | 0.664634 | 0.8623 | 0.1266 | 0.2071 | 0.541075 | 0.9621 | NaN | 0.0813 | 0.1353 | 0.547765 | 0.8553 | 0.0353 | 0.1505 | 0.814525 | 0.9294 | 0.1068 | 0.2076 | 0.606897 | 0.9384 |
| glutamate | 147.0536 | 0.611569 | Amino Acid | Creatine Metabolism | -0.1431 | 0.1397 | 0.305459 | 0.6742 | -0.1853 | 0.1421 | 0.192355 | 0.4993 | -0.1101 | 0.2311 | 0.633724 | 0.9104 | NaN | -0.1617 | 0.129 | 0.210006 | 0.7479 | -0.1625 | 0.1248 | 0.193093 | 0.7154 | -0.1733 | 0.2169 | 0.424413 | 0.9419 | NaN | -0.1481 | 0.1289 | 0.250418 | 0.7434 | -0.1509 | 0.1227 | 0.218696 | 0.7942 | -0.1493 | 0.2182 | 0.493863 | 0.9848 | NaN | -0.1734 | 0.132 | 0.188831 | 0.6616 | -0.1932 | 0.1297 | 0.136235 | 0.4784 | -0.1667 | 0.2199 | 0.448587 | 0.9375 | NaN | -0.1735 | 0.1308 | 0.184655 | 0.6753 | -0.1553 | 0.1252 | 0.21502 | 0.6963 | -0.1961 | 0.2216 | 0.376097 | 0.9106 | NaN | -0.1633 | 0.1322 | 0.216759 | 0.676 | -0.1518 | 0.1284 | 0.237283 | 0.6121 | -0.185 | 0.2226 | 0.405992 | 0.8887 |
| isovalerylcarnitine | 245.1626 | 4.58061 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.2855 | 0.1309 | 0.029128 | 0.2368 | 0.2946 | 0.1351 | 0.029193 | 0.2636 | 0.3052 | 0.2159 | 0.157527 | 0.6354 | NaN | 0.1014 | 0.1268 | 0.423625 | 0.8498 | 0.1169 | 0.1263 | 0.354882 | 0.8148 | 0.126 | 0.21 | 0.548527 | 0.954 | NaN | 0.1728 | 0.1233 | 0.161012 | 0.6683 | 0.1869 | 0.1193 | 0.117328 | 0.6704 | 0.1887 | 0.2078 | 0.363625 | 0.9578 | NaN | 0.1273 | 0.1297 | 0.326319 | 0.741 | 0.135 | 0.1327 | 0.309186 | 0.6362 | 0.1632 | 0.2114 | 0.440126 | 0.9375 | NaN | 0.1308 | 0.1277 | 0.305539 | 0.7529 | 0.1485 | 0.1244 | 0.232615 | 0.7214 | 0.1489 | 0.2142 | 0.486817 | 0.9403 | NaN | 0.1227 | 0.1306 | 0.347464 | 0.7531 | 0.1111 | 0.1317 | 0.399024 | 0.7198 | 0.1688 | 0.2141 | 0.430607 | 0.8887 |
| betaine | 117.0793 | 0.650488 | Amino Acid | Glycine, Serine and Threonine Metabolism | -0.1341 | 0.1338 | 0.316011 | 0.6805 | 0.0056 | 0.1317 | 0.966241 | 0.987 | -0.2797 | 0.2299 | 0.223658 | 0.7251 | NaN | -0.1118 | 0.1238 | 0.366434 | 0.8459 | 0.0235 | 0.1156 | 0.839281 | 0.9729 | -0.2456 | 0.216 | 0.255351 | 0.9223 | NaN | -0.0836 | 0.124 | 0.500117 | 0.9053 | 0.0538 | 0.1136 | 0.6357 | 0.9053 | -0.2218 | 0.2181 | 0.309143 | 0.9479 | NaN | -0.1329 | 0.1264 | 0.293103 | 0.7388 | -0.0094 | 0.1205 | 0.938133 | 0.9799 | -0.2469 | 0.2189 | 0.25948 | 0.8705 | NaN | -0.1125 | 0.1255 | 0.369967 | 0.7978 | 0.0202 | 0.1158 | 0.861823 | 0.9614 | -0.2457 | 0.22 | 0.264043 | 0.9039 | NaN | -0.1346 | 0.1267 | 0.288031 | 0.743 | 0.0102 | 0.1187 | 0.931327 | 0.9823 | -0.2782 | 0.2205 | 0.206999 | 0.8424 |
| homoserine | 119.0581 | 0.684298 | Amino Acid | Glycine, Serine and Threonine Metabolism | 0.1104 | 0.1317 | 0.401918 | 0.7322 | -0.2678 | 0.1331 | 0.044195 | 0.2929 | 0.4341 | 0.2138 | 0.042329 | 0.3491 | NaN | 0.1638 | 0.1218 | 0.178766 | 0.7251 | -0.2176 | 0.1175 | 0.064057 | 0.4801 | 0.4865 | 0.1993 | 0.014654 | 0.4257 | NaN | 0.1777 | 0.1217 | 0.144347 | 0.6585 | -0.1901 | 0.1162 | 0.102024 | 0.6422 | 0.4947 | 0.2008 | 0.013739 | 0.2416 | NaN | 0.1241 | 0.1245 | 0.318763 | 0.741 | -0.2402 | 0.122 | 0.048889 | 0.2946 | 0.4227 | 0.2031 | 0.037421 | 0.5138 | NaN | 0.1713 | 0.1236 | 0.165693 | 0.6753 | -0.2052 | 0.1182 | 0.082685 | 0.4705 | 0.4911 | 0.2033 | 0.015699 | 0.423 | NaN | 0.1248 | 0.1248 | 0.317069 | 0.7485 | -0.2463 | 0.1198 | 0.039862 | 0.2717 | 0.4356 | 0.2048 | 0.033433 | 0.4663 |
| sarcosine | 89.0478 | 0.671801 | Amino Acid | Glycine, Serine and Threonine Metabolism | 0.2834 | 0.1205 | 0.018654 | 0.1745 | 0.119 | 0.1318 | 0.366539 | 0.6407 | 0.3862 | 0.1912 | 0.043361 | 0.3491 | NaN | 0.2968 | 0.111 | 0.007513 | 0.1296 | 0.1102 | 0.1156 | 0.340609 | 0.8095 | 0.4208 | 0.1783 | 0.018298 | 0.4591 | NaN | 0.306 | 0.1108 | 0.005733 | 0.0931 | 0.1356 | 0.1132 | 0.230828 | 0.8003 | 0.4291 | 0.1796 | 0.016856 | 0.2658 | NaN | 0.2959 | 0.1136 | 0.009181 | 0.1299 | 0.0714 | 0.1213 | 0.556004 | 0.787 | 0.4524 | 0.1809 | 0.012379 | 0.3596 | NaN | 0.269 | 0.1129 | 0.017194 | 0.2552 | 0.0847 | 0.1162 | 0.466188 | 0.8272 | 0.3878 | 0.1822 | 0.033274 | 0.4772 | NaN | 0.2968 | 0.1138 | 0.009131 | 0.1362 | 0.0664 | 0.1195 | 0.578317 | 0.8092 | 0.4532 | 0.1829 | 0.013187 | 0.3715 |
| serine | 105.0421 | 0.978105 | Amino Acid | Glycine, Serine and Threonine Metabolism | 0.2714 | 0.1397 | 0.052012 | 0.3263 | 0.2802 | 0.1761 | 0.111597 | 0.3939 | 0.2583 | 0.2023 | 0.201699 | 0.7107 | NaN | 0.2339 | 0.1295 | 0.07082 | 0.5283 | 0.3106 | 0.1534 | 0.042942 | 0.3763 | 0.179 | 0.1916 | 0.35015 | 0.9223 | NaN | 0.2275 | 0.1294 | 0.078689 | 0.5097 | 0.3029 | 0.1506 | 0.044301 | 0.446 | 0.1833 | 0.1928 | 0.341936 | 0.957 | NaN | 0.2709 | 0.1319 | 0.039984 | 0.356 | 0.292 | 0.1605 | 0.068819 | 0.3688 | 0.2424 | 0.1924 | 0.207652 | 0.8705 | NaN | 0.2427 | 0.1311 | 0.064036 | 0.4979 | 0.3297 | 0.1535 | 0.031757 | 0.2922 | 0.1933 | 0.1948 | 0.321139 | 0.9106 | NaN | 0.2555 | 0.1324 | 0.053561 | 0.4413 | 0.3121 | 0.1577 | 0.047729 | 0.2877 | 0.2133 | 0.1951 | 0.274308 | 0.8424 |
| 3-hydroxypyruvic acid | 104.0115 | 0.910453 | Amino Acid | Glycine, serine, and threonine metabolism | -0.2364 | 0.1338 | 0.07735 | 0.3936 | -0.0459 | 0.1445 | 0.750686 | 0.9087 | -0.3574 | 0.2187 | 0.102301 | 0.5278 | NaN | -0.1349 | 0.1256 | 0.282953 | 0.7683 | 0.0651 | 0.1284 | 0.612103 | 0.9043 | -0.2802 | 0.207 | 0.17585 | 0.879 | NaN | -0.1451 | 0.1251 | 0.245991 | 0.7434 | 0.0226 | 0.1251 | 0.856408 | 0.9531 | -0.2912 | 0.2081 | 0.161706 | 0.7677 | NaN | -0.1239 | 0.1294 | 0.338372 | 0.741 | 0.055 | 0.1342 | 0.68205 | 0.853 | -0.2301 | 0.2132 | 0.280468 | 0.8705 | NaN | -0.1502 | 0.127 | 0.237146 | 0.7114 | 0.0637 | 0.1287 | 0.620442 | 0.8623 | -0.3036 | 0.2101 | 0.148471 | 0.8056 | NaN | -0.1501 | 0.1287 | 0.243503 | 0.7034 | 0.0291 | 0.1312 | 0.824225 | 0.9381 | -0.2665 | 0.2134 | 0.211629 | 0.8424 |
| L-histidine | 155.0693 | 0.637818 | Amino Acid | Histidine Metabolism | 0.2596 | 0.1418 | 0.067108 | 0.3704 | 0.2945 | 0.1427 | 0.039094 | 0.2877 | 0.2259 | 0.2361 | 0.338799 | 0.7534 | NaN | 0.2288 | 0.1313 | 0.081415 | 0.5913 | 0.3084 | 0.1241 | 0.012978 | 0.1892 | 0.1522 | 0.2228 | 0.494512 | 0.954 | NaN | 0.2247 | 0.1312 | 0.08668 | 0.5342 | 0.3196 | 0.1214 | 0.008473 | 0.1839 | 0.1406 | 0.2248 | 0.531796 | 0.9894 | NaN | 0.2232 | 0.1344 | 0.096827 | 0.5399 | 0.325 | 0.1294 | 0.012019 | 0.1382 | 0.1179 | 0.2275 | 0.604404 | 0.9375 | NaN | 0.2006 | 0.1337 | 0.133565 | 0.6708 | 0.2783 | 0.1251 | 0.026162 | 0.2579 | 0.1317 | 0.2281 | 0.563516 | 0.9621 | NaN | 0.2236 | 0.1347 | 0.097047 | 0.55 | 0.3061 | 0.1277 | 0.016481 | 0.1596 | 0.1477 | 0.2287 | 0.518355 | 0.8946 |
| isoleucine | 131.0954 | 1.502874 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.1783 | 0.1328 | 0.179187 | 0.5465 | 0.2766 | 0.1203 | 0.021486 | 0.2196 | 0.0745 | 0.2505 | 0.766059 | 0.9647 | NaN | -0.0096 | 0.1276 | 0.940127 | 0.9885 | 0.0609 | 0.1175 | 0.604084 | 0.9043 | -0.0266 | 0.2365 | 0.910387 | 0.9793 | NaN | 0.0757 | 0.1243 | 0.542283 | 0.9125 | 0.1247 | 0.1095 | 0.254669 | 0.8037 | 0.0522 | 0.2367 | 0.825414 | 0.9935 | NaN | 0.0086 | 0.1311 | 0.947478 | 0.9828 | 0.0821 | 0.1248 | 0.510613 | 0.7647 | 0.0049 | 0.2391 | 0.983779 | 0.9923 | NaN | -0.0097 | 0.1302 | 0.940315 | 0.9796 | 0.051 | 0.1188 | 0.667916 | 0.8623 | -0.0438 | 0.2421 | 0.856563 | 0.9621 | NaN | 0.0251 | 0.1306 | 0.847656 | 0.9532 | 0.0735 | 0.1218 | 0.546229 | 0.8009 | 0.0244 | 0.241 | 0.919392 | 0.9807 |
| leucine | 131.0951 | 1.596301 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.161 | 0.13 | 0.215397 | 0.5857 | 0.2999 | 0.1171 | 0.010413 | 0.1691 | -0.0445 | 0.241 | 0.853348 | 0.9732 | NaN | 0.0512 | 0.1221 | 0.675065 | 0.9208 | 0.1272 | 0.1117 | 0.254659 | 0.7821 | -0.0173 | 0.2262 | 0.939166 | 0.9911 | NaN | 0.0691 | 0.1214 | 0.569164 | 0.9125 | 0.1806 | 0.105 | 0.08551 | 0.613 | -0.0753 | 0.2276 | 0.740688 | 0.9935 | NaN | 0.0966 | 0.1239 | 0.435584 | 0.7844 | 0.1544 | 0.1167 | 0.18576 | 0.5328 | 0.0671 | 0.2314 | 0.771762 | 0.9598 | NaN | 0.0959 | 0.1227 | 0.434453 | 0.8472 | 0.1679 | 0.1086 | 0.122208 | 0.588 | -0.0005 | 0.2305 | 0.998318 | 0.9999 | NaN | 0.0879 | 0.1244 | 0.479693 | 0.8278 | 0.1453 | 0.1146 | 0.204899 | 0.5756 | 0.0233 | 0.2323 | 0.920256 | 0.9807 |
| valine | 117.0793 | 0.870426 | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.2225 | 0.1341 | 0.097039 | 0.4501 | 0.3797 | 0.1383 | 0.006023 | 0.1405 | 0.1083 | 0.2159 | 0.615971 | 0.8995 | NaN | 0.0695 | 0.1277 | 0.586349 | 0.9079 | 0.2018 | 0.13 | 0.120616 | 0.6118 | -0.0118 | 0.2052 | 0.954113 | 0.9911 | NaN | 0.1229 | 0.1256 | 0.327748 | 0.8017 | 0.2778 | 0.1219 | 0.022622 | 0.3046 | 0.0049 | 0.2061 | 0.981229 | 0.9976 | NaN | 0.0903 | 0.1306 | 0.489405 | 0.8037 | 0.2192 | 0.1369 | 0.109269 | 0.4435 | 0.0171 | 0.2073 | 0.934146 | 0.99 | NaN | 0.0966 | 0.1287 | 0.453155 | 0.8543 | 0.241 | 0.1272 | 0.058186 | 0.4149 | -0.0056 | 0.2095 | 0.978612 | 0.9969 | NaN | 0.0908 | 0.131 | 0.488316 | 0.8278 | 0.1992 | 0.1356 | 0.141711 | 0.5193 | 0.0255 | 0.2092 | 0.903018 | 0.9769 |
| 5-aminopentanoate | 117.079 | 0.650918 | Amino Acid | Lysine Metabolism | -0.1571 | 0.1622 | 0.33284 | 0.6942 | 0.0122 | 0.1595 | 0.938903 | 0.9724 | -0.3351 | 0.2791 | 0.230034 | 0.7298 | NaN | -0.1302 | 0.1502 | 0.386092 | 0.8498 | 0.0347 | 0.14 | 0.804083 | 0.965 | -0.2948 | 0.2622 | 0.260936 | 0.9223 | NaN | -0.0981 | 0.1503 | 0.514024 | 0.9068 | 0.0694 | 0.1376 | 0.613847 | 0.9053 | -0.2677 | 0.2648 | 0.312047 | 0.9479 | NaN | -0.1548 | 0.1534 | 0.312913 | 0.741 | -0.0045 | 0.146 | 0.975284 | 0.9926 | -0.2948 | 0.2659 | 0.267498 | 0.8705 | NaN | -0.1334 | 0.1522 | 0.380814 | 0.7993 | 0.0295 | 0.1403 | 0.833217 | 0.9444 | -0.2982 | 0.267 | 0.264028 | 0.9039 | NaN | -0.1572 | 0.1537 | 0.306281 | 0.7481 | 0.0189 | 0.1437 | 0.895527 | 0.9683 | -0.3333 | 0.2677 | 0.213168 | 0.8424 |
| glutarylcarnitine | 275.1374 | 1.605139 | Amino Acid | Lysine Metabolism | 0.0934 | 0.1375 | 0.497137 | 0.8054 | 0.1364 | 0.1523 | 0.370262 | 0.6407 | 0.0892 | 0.2146 | 0.677516 | 0.935 | NaN | 0.1067 | 0.1271 | 0.400972 | 0.8498 | 0.0019 | 0.1366 | 0.989158 | 0.9953 | 0.2339 | 0.2034 | 0.250132 | 0.9223 | NaN | 0.0912 | 0.1269 | 0.47236 | 0.8967 | 0.0282 | 0.1331 | 0.832272 | 0.9472 | 0.1539 | 0.203 | 0.448373 | 0.9816 | NaN | 0.1094 | 0.1299 | 0.399825 | 0.7795 | 0.0266 | 0.1422 | 0.851617 | 0.9459 | 0.2355 | 0.207 | 0.255162 | 0.8705 | NaN | 0.1465 | 0.1289 | 0.255919 | 0.7358 | 0.0653 | 0.135 | 0.628618 | 0.8623 | 0.2366 | 0.2083 | 0.256164 | 0.9039 | NaN | 0.1039 | 0.1302 | 0.425079 | 0.795 | 0.0196 | 0.14 | 0.888406 | 0.9667 | 0.2063 | 0.2084 | 0.322101 | 0.8727 |
| N6,N6,N6-trimethyl-L-lysine | 188.1515 | 0.598599 | Amino Acid | Lysine Metabolism | -0.282 | 0.1325 | 0.033305 | 0.2621 | -0.1412 | 0.1362 | 0.300112 | 0.5924 | -0.4498 | 0.2198 | 0.040714 | 0.3491 | NaN | -0.193 | 0.1242 | 0.120009 | 0.6749 | -0.0161 | 0.1226 | 0.895496 | 0.9729 | -0.3846 | 0.2076 | 0.06389 | 0.6334 | NaN | -0.1925 | 0.124 | 0.120551 | 0.6049 | -0.0088 | 0.1203 | 0.941389 | 0.9765 | -0.3689 | 0.2099 | 0.078733 | 0.5795 | NaN | -0.1908 | 0.1275 | 0.13446 | 0.5986 | -0.0432 | 0.1274 | 0.734386 | 0.8813 | -0.3568 | 0.2122 | 0.092686 | 0.7393 | NaN | -0.2084 | 0.1255 | 0.096881 | 0.6292 | -0.0289 | 0.1224 | 0.81341 | 0.9396 | -0.3968 | 0.2111 | 0.060215 | 0.5449 | NaN | -0.204 | 0.1273 | 0.109086 | 0.554 | -0.0418 | 0.1252 | 0.738399 | 0.9018 | -0.3807 | 0.2132 | 0.07415 | 0.6024 |
| pipecolate | 129.079 | 0.940523 | Amino Acid | Lysine Metabolism | -0.1443 | 0.1337 | 0.280512 | 0.6589 | 0.0388 | 0.1464 | 0.790954 | 0.932 | -0.2678 | 0.2088 | 0.199591 | 0.7107 | NaN | -0.1295 | 0.1237 | 0.294879 | 0.7802 | 0.0347 | 0.1285 | 0.786931 | 0.9616 | -0.2406 | 0.1961 | 0.219758 | 0.9223 | NaN | -0.1669 | 0.1233 | 0.175715 | 0.6928 | -0.0334 | 0.1268 | 0.792429 | 0.9363 | -0.261 | 0.1971 | 0.18536 | 0.8252 | NaN | -0.1335 | 0.1264 | 0.290936 | 0.7388 | 0.0021 | 0.1343 | 0.987295 | 0.9926 | -0.2155 | 0.1995 | 0.280145 | 0.8705 | NaN | -0.1394 | 0.1252 | 0.265779 | 0.7442 | 0.0244 | 0.1288 | 0.849748 | 0.9534 | -0.2525 | 0.1994 | 0.205455 | 0.8792 | NaN | -0.1255 | 0.1268 | 0.32207 | 0.7485 | 0.0101 | 0.1321 | 0.939352 | 0.9823 | -0.2151 | 0.2016 | 0.286021 | 0.8424 |
| N-(tert-Butoxycarbonyl)-L-methionine | 249.1031 | 13.127769 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.0243 | 0.128 | 0.849417 | 0.9778 | 0.0342 | 0.1341 | 0.798524 | 0.932 | 0.0217 | 0.2074 | 0.916611 | 0.9838 | NaN | 0.0547 | 0.1184 | 0.644104 | 0.9179 | 0.0967 | 0.1179 | 0.411788 | 0.847 | 0.0197 | 0.1945 | 0.919299 | 0.9835 | NaN | 0.0261 | 0.1182 | 0.825188 | 0.9714 | 0.0766 | 0.1155 | 0.507362 | 0.9053 | -0.0156 | 0.1961 | 0.936666 | 0.9935 | NaN | 0.0719 | 0.1213 | 0.553478 | 0.8434 | 0.1035 | 0.1232 | 0.400958 | 0.6937 | 0.0499 | 0.1972 | 0.800211 | 0.9662 | NaN | 0.0703 | 0.1202 | 0.558266 | 0.8722 | 0.1174 | 0.1184 | 0.321296 | 0.7579 | 0.037 | 0.198 | 0.851921 | 0.9621 | NaN | 0.0678 | 0.1215 | 0.57683 | 0.8765 | 0.0816 | 0.1209 | 0.49993 | 0.7818 | 0.0642 | 0.1994 | 0.747501 | 0.9486 |
| hypotaurine | 109.0016 | 0.502127 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.0933 | 0.1294 | 0.470909 | 0.7972 | -0.0046 | 0.1269 | 0.970859 | 0.987 | 0.24 | 0.2267 | 0.289752 | 0.7534 | NaN | 0.0693 | 0.1198 | 0.563171 | 0.9079 | -0.0171 | 0.1114 | 0.87796 | 0.9729 | 0.1791 | 0.2137 | 0.401891 | 0.94 | NaN | 0.0994 | 0.1195 | 0.405128 | 0.8502 | -0.0359 | 0.1094 | 0.742623 | 0.9241 | 0.2505 | 0.2139 | 0.241386 | 0.8883 | NaN | 0.0837 | 0.1224 | 0.494219 | 0.8047 | 0.0112 | 0.1161 | 0.922931 | 0.9748 | 0.1811 | 0.2167 | 0.403228 | 0.9375 | NaN | 0.1031 | 0.1212 | 0.39489 | 0.8103 | 0.0294 | 0.1117 | 0.792704 | 0.929 | 0.2045 | 0.217 | 0.346024 | 0.9106 | NaN | 0.0944 | 0.1226 | 0.441175 | 0.801 | 0.0417 | 0.1146 | 0.716312 | 0.8905 | 0.174 | 0.2192 | 0.427253 | 0.8887 |
| methionine | 149.0516 | 0.977423 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.243 | 0.1358 | 0.073405 | 0.3859 | 0.3651 | 0.1751 | 0.03708 | 0.2877 | 0.1879 | 0.1941 | 0.333053 | 0.7534 | NaN | 0.2046 | 0.1259 | 0.104148 | 0.6608 | 0.3288 | 0.1537 | 0.032351 | 0.3133 | 0.1413 | 0.1827 | 0.439439 | 0.9478 | NaN | 0.1776 | 0.1262 | 0.159356 | 0.6683 | 0.2996 | 0.1516 | 0.048135 | 0.4581 | 0.1183 | 0.1848 | 0.521998 | 0.9894 | NaN | 0.2616 | 0.1281 | 0.041139 | 0.3605 | 0.331 | 0.1604 | 0.039121 | 0.2571 | 0.229 | 0.1844 | 0.214118 | 0.8705 | NaN | 0.2196 | 0.1274 | 0.084592 | 0.5831 | 0.3579 | 0.1532 | 0.019447 | 0.2314 | 0.154 | 0.1858 | 0.407179 | 0.9359 | NaN | 0.2514 | 0.1284 | 0.050342 | 0.4342 | 0.3572 | 0.1571 | 0.022982 | 0.1982 | 0.1973 | 0.1861 | 0.289012 | 0.8424 |
| S-adenosyl-L-homocysteine | 384.121 | 1.490665 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.0368 | 0.1252 | 0.768691 | 0.9439 | 0.1562 | 0.1392 | 0.261804 | 0.5505 | -0.0157 | 0.1963 | 0.936285 | 0.9887 | NaN | -0.049 | 0.1166 | 0.674201 | 0.9208 | 0.0681 | 0.1239 | 0.582871 | 0.904 | -0.0958 | 0.1851 | 0.604551 | 0.954 | NaN | -0.0153 | 0.1159 | 0.894968 | 0.9714 | 0.1201 | 0.1202 | 0.318022 | 0.844 | -0.0897 | 0.1863 | 0.63014 | 0.9894 | NaN | -0.0691 | 0.1202 | 0.565366 | 0.846 | 0.0408 | 0.1311 | 0.755767 | 0.8953 | -0.1007 | 0.188 | 0.592245 | 0.9375 | NaN | -0.0177 | 0.1178 | 0.880325 | 0.9672 | 0.1274 | 0.1227 | 0.298997 | 0.7544 | -0.087 | 0.1886 | 0.644443 | 0.9621 | NaN | -0.0447 | 0.1198 | 0.708772 | 0.9078 | 0.0551 | 0.128 | 0.666782 | 0.8681 | -0.0739 | 0.1892 | 0.696073 | 0.9459 |
| S-Allyl-L-cysteine | 161.0512 | 1.868486 | Amino Acid | Methionine, Cysteine, SAM and Taurine Metabolism | 0.1488 | 0.1402 | 0.288772 | 0.6698 | 0.2372 | 0.2079 | 0.253885 | 0.5474 | 0.1299 | 0.1908 | 0.496172 | 0.8401 | NaN | 0.086 | 0.1304 | 0.509323 | 0.8786 | -0.0035 | 0.1894 | 0.985371 | 0.9953 | 0.125 | 0.179 | 0.484735 | 0.954 | NaN | 0.0738 | 0.1304 | 0.571471 | 0.9125 | 0.0915 | 0.1819 | 0.614966 | 0.9053 | 0.0712 | 0.1812 | 0.694513 | 0.9894 | NaN | 0.0997 | 0.1331 | 0.454025 | 0.7844 | 0.0324 | 0.1976 | 0.869793 | 0.9545 | 0.1356 | 0.1813 | 0.454552 | 0.9375 | NaN | 0.0577 | 0.1329 | 0.664273 | 0.9055 | 0.0016 | 0.1897 | 0.993399 | 0.9941 | 0.0795 | 0.1831 | 0.664059 | 0.9621 | NaN | 0.088 | 0.1337 | 0.510324 | 0.8285 | -0.0142 | 0.1964 | 0.942419 | 0.9823 | 0.1256 | 0.1831 | 0.492636 | 0.8887 |
| 3-methoxytyrosine | 211.0857 | 1.982335 | Amino Acid | Phenylalanine and Tyrosine Metabolism | -0.3357 | 0.1269 | 0.00814 | 0.107 | -0.1886 | 0.1515 | 0.212948 | 0.5076 | -0.4142 | 0.1902 | 0.029418 | 0.3084 | NaN | -0.2386 | 0.1195 | 0.045783 | 0.4283 | -0.1254 | 0.1339 | 0.349147 | 0.8132 | -0.2826 | 0.1842 | 0.125034 | 0.8417 | NaN | -0.2621 | 0.1184 | 0.026905 | 0.27 | -0.2054 | 0.1299 | 0.11375 | 0.661 | -0.2857 | 0.1858 | 0.124124 | 0.6991 | NaN | -0.2486 | 0.1222 | 0.041971 | 0.362 | -0.1223 | 0.14 | 0.382085 | 0.6816 | -0.2925 | 0.1871 | 0.117974 | 0.7964 | NaN | -0.2584 | 0.1205 | 0.032054 | 0.332 | -0.1531 | 0.1335 | 0.251589 | 0.7309 | -0.3095 | 0.1868 | 0.09754 | 0.673 | NaN | -0.2659 | 0.1218 | 0.029028 | 0.3025 | -0.1338 | 0.1374 | 0.330222 | 0.6739 | -0.3225 | 0.187 | 0.084577 | 0.6395 |
| phenylacetic acid | 136.0526 | 4.193451 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.105 | 0.1219 | 0.388948 | 0.726 | 0.165 | 0.1524 | 0.278828 | 0.5701 | 0.0625 | 0.1797 | 0.727893 | 0.9635 | NaN | 0.1503 | 0.1127 | 0.182331 | 0.7251 | 0.056 | 0.136 | 0.680547 | 0.9267 | 0.1975 | 0.171 | 0.24802 | 0.9223 | NaN | 0.1341 | 0.1124 | 0.232833 | 0.7361 | 0.1128 | 0.1319 | 0.392482 | 0.8818 | 0.1334 | 0.1704 | 0.43384 | 0.9816 | NaN | 0.1558 | 0.1153 | 0.17677 | 0.6547 | 0.0727 | 0.1417 | 0.60793 | 0.8188 | 0.1967 | 0.174 | 0.258439 | 0.8705 | NaN | 0.1572 | 0.1143 | 0.168931 | 0.6753 | 0.0695 | 0.1359 | 0.60925 | 0.8623 | 0.1876 | 0.1747 | 0.283016 | 0.9039 | NaN | 0.1529 | 0.1156 | 0.186009 | 0.6463 | 0.0339 | 0.141 | 0.810116 | 0.9294 | 0.2029 | 0.1769 | 0.251205 | 0.8424 |
| phenylalanine | 165.0792 | 2.503736 | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.2542 | 0.1356 | 0.06077 | 0.3473 | 0.3178 | 0.1931 | 0.099815 | 0.3816 | 0.246 | 0.1869 | 0.188194 | 0.6943 | NaN | 0.1135 | 0.1287 | 0.377961 | 0.8465 | 0.0941 | 0.1772 | 0.59553 | 0.904 | 0.1301 | 0.1791 | 0.467561 | 0.9478 | NaN | 0.1525 | 0.1271 | 0.229905 | 0.7361 | 0.1899 | 0.1691 | 0.26158 | 0.8057 | 0.1463 | 0.1797 | 0.415743 | 0.9816 | NaN | 0.1412 | 0.1312 | 0.281602 | 0.7388 | 0.0671 | 0.1898 | 0.723665 | 0.876 | 0.1811 | 0.1794 | 0.312695 | 0.8963 | NaN | 0.1264 | 0.1303 | 0.33202 | 0.7669 | 0.1035 | 0.1771 | 0.558847 | 0.8618 | 0.1459 | 0.1824 | 0.423828 | 0.9359 | NaN | 0.1429 | 0.1315 | 0.276987 | 0.7337 | 0.0561 | 0.1862 | 0.762985 | 0.9096 | 0.1824 | 0.1813 | 0.314361 | 0.8727 |
| 5-methylthioadenosine | 297.0898 | 4.448414 | Amino Acid | Polyamine Metabolism | 0.3375 | 0.1358 | 0.012956 | 0.149 | 0.4452 | 0.1632 | 0.006364 | 0.1405 | 0.2933 | 0.1998 | 0.142035 | 0.6043 | NaN | 0.1664 | 0.1309 | 0.203644 | 0.7395 | 0.1749 | 0.159 | 0.271335 | 0.7967 | 0.1773 | 0.1911 | 0.3535 | 0.9223 | NaN | 0.1948 | 0.1292 | 0.131476 | 0.6366 | 0.2886 | 0.1459 | 0.047948 | 0.4581 | 0.15 | 0.1947 | 0.441028 | 0.9816 | NaN | 0.1924 | 0.1337 | 0.150234 | 0.6283 | 0.212 | 0.1674 | 0.205315 | 0.5478 | 0.2 | 0.193 | 0.300022 | 0.8823 | NaN | 0.174 | 0.133 | 0.190844 | 0.6753 | 0.1785 | 0.1592 | 0.261925 | 0.7339 | 0.1808 | 0.1955 | 0.354986 | 0.9106 | NaN | 0.2001 | 0.1337 | 0.134466 | 0.605 | 0.1831 | 0.1659 | 0.269681 | 0.6417 | 0.2189 | 0.1942 | 0.259501 | 0.8424 |
| hypaphorine | 246.137 | 4.095109 | Amino Acid | Tryptophan Metabolism | -0.0849 | 0.1322 | 0.520914 | 0.8173 | -0.1241 | 0.1349 | 0.357695 | 0.6361 | -0.0412 | 0.2191 | 0.850861 | 0.9732 | NaN | -0.0968 | 0.1222 | 0.428218 | 0.8498 | -0.0737 | 0.1191 | 0.535756 | 0.8967 | -0.1201 | 0.2062 | 0.560416 | 0.954 | NaN | -0.0944 | 0.1221 | 0.439459 | 0.8792 | -0.0902 | 0.1165 | 0.43889 | 0.8947 | -0.0938 | 0.2072 | 0.650908 | 0.9894 | NaN | -0.1451 | 0.1253 | 0.247022 | 0.7139 | -0.143 | 0.1232 | 0.24555 | 0.5817 | -0.1436 | 0.21 | 0.494105 | 0.9375 | NaN | -0.1072 | 0.1239 | 0.386703 | 0.8025 | -0.1081 | 0.1187 | 0.36231 | 0.7936 | -0.0967 | 0.2097 | 0.644804 | 0.9621 | NaN | -0.1388 | 0.1255 | 0.268719 | 0.7315 | -0.135 | 0.1213 | 0.265877 | 0.6386 | -0.1341 | 0.212 | 0.527002 | 0.8971 |
| 5-hydroxytryptophan | 220.0946 | 2.440203 | Amino acid | Tryptophan Metabolism | 0.1182 | 0.1379 | 0.391392 | 0.726 | 0.1613 | 0.149 | 0.279091 | 0.5701 | 0.0769 | 0.2178 | 0.723924 | 0.9629 | NaN | 0.0941 | 0.1277 | 0.460989 | 0.8498 | 0.1286 | 0.1311 | 0.326457 | 0.8095 | 0.0649 | 0.2044 | 0.750777 | 0.954 | NaN | 0.0329 | 0.1284 | 0.797471 | 0.9641 | 0.0978 | 0.1292 | 0.449186 | 0.8947 | -0.017 | 0.2075 | 0.934536 | 0.9935 | NaN | 0.1243 | 0.1303 | 0.340282 | 0.741 | 0.1631 | 0.1361 | 0.230681 | 0.571 | 0.0888 | 0.207 | 0.668098 | 0.9432 | NaN | 0.1142 | 0.1292 | 0.376627 | 0.7993 | 0.1401 | 0.1311 | 0.285324 | 0.7544 | 0.0898 | 0.208 | 0.665743 | 0.9621 | NaN | 0.1246 | 0.1306 | 0.340261 | 0.7513 | 0.1288 | 0.1346 | 0.338493 | 0.6758 | 0.1173 | 0.2093 | 0.5751 | 0.9205 |
| indole-3-acetate | 175.064 | 8.37482 | Amino Acid | Tryptophan Metabolism | -0.1542 | 0.1306 | 0.237646 | 0.6073 | -0.2958 | 0.1196 | 0.013392 | 0.1879 | 0.054 | 0.2387 | 0.820922 | 0.9713 | NaN | -0.0916 | 0.1215 | 0.450534 | 0.8498 | -0.25 | 0.1056 | 0.017922 | 0.2248 | 0.1264 | 0.2243 | 0.573032 | 0.954 | NaN | -0.1113 | 0.1209 | 0.357309 | 0.8251 | -0.2321 | 0.1042 | 0.025967 | 0.3319 | 0.0371 | 0.2254 | 0.869369 | 0.9935 | NaN | -0.1032 | 0.1241 | 0.405617 | 0.7795 | -0.2597 | 0.11 | 0.018227 | 0.1649 | 0.1229 | 0.2275 | 0.58892 | 0.9375 | NaN | -0.1065 | 0.1229 | 0.386219 | 0.8025 | -0.2264 | 0.1069 | 0.034228 | 0.3097 | 0.0582 | 0.2279 | 0.798494 | 0.9621 | NaN | -0.1208 | 0.124 | 0.330015 | 0.7485 | -0.2796 | 0.1075 | 0.009265 | 0.1247 | 0.1061 | 0.2295 | 0.643764 | 0.9459 |
| indolelactic acid | 205.1461 | 5.755592 | Amino Acid | Tryptophan Metabolism | 0.2593 | 0.1295 | 0.045161 | 0.3113 | 0.1187 | 0.1571 | 0.449995 | 0.72 | 0.3558 | 0.1923 | 0.064299 | 0.4426 | NaN | 0.1399 | 0.1224 | 0.252905 | 0.7495 | 0.0483 | 0.1388 | 0.727896 | 0.9386 | 0.2115 | 0.1867 | 0.257215 | 0.9223 | NaN | 0.1444 | 0.122 | 0.236566 | 0.7361 | 0.0715 | 0.1358 | 0.598531 | 0.9053 | 0.2069 | 0.189 | 0.273661 | 0.91 | NaN | 0.1437 | 0.1257 | 0.252936 | 0.714 | -0.0149 | 0.1475 | 0.91953 | 0.9748 | 0.2557 | 0.1868 | 0.17121 | 0.8705 | NaN | 0.1625 | 0.1235 | 0.188219 | 0.6753 | 0.0585 | 0.1389 | 0.673591 | 0.8623 | 0.2477 | 0.1887 | 0.189178 | 0.8608 | NaN | 0.1591 | 0.1253 | 0.204336 | 0.6633 | -0.0093 | 0.1446 | 0.948908 | 0.9834 | 0.2767 | 0.1877 | 0.140412 | 0.7588 |
| kynurenine | 208.0858 | 2.196904 | Amino Acid | Tryptophan Metabolism | 0.0649 | 0.1367 | 0.635111 | 0.8678 | -0.0483 | 0.1516 | 0.750121 | 0.9087 | 0.132 | 0.2123 | 0.534035 | 0.8655 | NaN | 0.0053 | 0.1269 | 0.966506 | 0.9952 | -0.0546 | 0.133 | 0.681269 | 0.9267 | 0.0255 | 0.2014 | 0.899167 | 0.977 | NaN | -0.0179 | 0.1271 | 0.888048 | 0.9714 | -0.0754 | 0.1305 | 0.563196 | 0.9053 | 0.0111 | 0.2037 | 0.956707 | 0.9976 | NaN | 0.0204 | 0.1296 | 0.874675 | 0.9749 | -0.0829 | 0.1387 | 0.550018 | 0.7845 | 0.0707 | 0.2029 | 0.727482 | 0.9551 | NaN | 0.0391 | 0.1282 | 0.760216 | 0.938 | -0.0449 | 0.1333 | 0.736314 | 0.9032 | 0.0854 | 0.2034 | 0.674603 | 0.9621 | NaN | 0.0363 | 0.1297 | 0.779496 | 0.9414 | -0.0767 | 0.1365 | 0.57419 | 0.8092 | 0.098 | 0.2042 | 0.631288 | 0.9459 |
| tryptophan | 204.0898 | 3.571538 | Amino Acid | Tryptophan Metabolism | 0.1103 | 0.1253 | 0.378599 | 0.7219 | 0.0203 | 0.1229 | 0.868852 | 0.9386 | 0.1912 | 0.2168 | 0.377959 | 0.7534 | NaN | 0.052 | 0.1164 | 0.655227 | 0.918 | -0.0032 | 0.108 | 0.976644 | 0.9947 | 0.0874 | 0.2058 | 0.670886 | 0.954 | NaN | 0.0737 | 0.1159 | 0.524722 | 0.9101 | 0.0297 | 0.1059 | 0.779368 | 0.9312 | 0.1093 | 0.2065 | 0.596609 | 0.9894 | NaN | 0.0554 | 0.1191 | 0.641823 | 0.8652 | -0.0133 | 0.1127 | 0.906295 | 0.9695 | 0.0986 | 0.2085 | 0.636167 | 0.9375 | NaN | 0.0492 | 0.1181 | 0.677061 | 0.9097 | -0.0146 | 0.1083 | 0.892814 | 0.9727 | 0.1016 | 0.2095 | 0.627738 | 0.9621 | NaN | 0.0463 | 0.1196 | 0.698951 | 0.9035 | -0.032 | 0.1113 | 0.773387 | 0.9173 | 0.1061 | 0.2106 | 0.614282 | 0.9445 |
| 4-hydroxyphenylethanol | 138.0682 | 6.78909 | Amino Acid | Tyrosine Metabolism | 0.1016 | 0.1329 | 0.44488 | 0.7722 | -0.0198 | 0.1472 | 0.893254 | 0.9519 | 0.1609 | 0.208 | 0.439136 | 0.7974 | NaN | 0.0453 | 0.1234 | 0.713589 | 0.9325 | -0.0755 | 0.1294 | 0.55951 | 0.9009 | 0.1053 | 0.1959 | 0.590977 | 0.954 | NaN | 0.0434 | 0.1233 | 0.725068 | 0.9552 | 0.0113 | 0.1269 | 0.929172 | 0.9733 | 0.0519 | 0.1993 | 0.794691 | 0.9935 | NaN | 0.0557 | 0.1261 | 0.658942 | 0.8697 | -0.0975 | 0.1355 | 0.471526 | 0.7332 | 0.1326 | 0.1981 | 0.503203 | 0.9375 | NaN | 0.0543 | 0.125 | 0.663709 | 0.9055 | -0.0926 | 0.1298 | 0.475837 | 0.8272 | 0.1339 | 0.1989 | 0.501059 | 0.9436 | NaN | 0.0598 | 0.1264 | 0.635861 | 0.8819 | -0.117 | 0.1336 | 0.381183 | 0.6983 | 0.1534 | 0.1996 | 0.442193 | 0.8887 |
| D-ornithine | 132.0897 | 0.510411 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.0883 | 0.128 | 0.490478 | 0.8041 | 0.061 | 0.13 | 0.638695 | 0.8434 | 0.1005 | 0.2148 | 0.63988 | 0.9104 | NaN | -0.0404 | 0.1205 | 0.737619 | 0.9401 | -0.0575 | 0.1162 | 0.620523 | 0.9073 | -0.0243 | 0.2043 | 0.905239 | 0.9779 | NaN | -0.0148 | 0.1196 | 0.901722 | 0.9717 | 0.0138 | 0.1124 | 0.902074 | 0.973 | -0.038 | 0.2066 | 0.854 | 0.9935 | NaN | 0.0147 | 0.1221 | 0.904421 | 0.9828 | 0.0036 | 0.1198 | 0.975838 | 0.9926 | 0.0164 | 0.2059 | 0.936481 | 0.99 | NaN | -0.0321 | 0.1222 | 0.792657 | 0.9477 | -0.0495 | 0.1162 | 0.669841 | 0.8623 | -0.0184 | 0.2086 | 0.92982 | 0.9795 | NaN | 0.0283 | 0.122 | 0.816689 | 0.9491 | 0.0211 | 0.1175 | 0.857503 | 0.9524 | 0.0285 | 0.2077 | 0.890833 | 0.9702 |
| L-ornithine | 132.0897 | 0.510411 | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.0986 | 0.1283 | 0.441951 | 0.772 | 0.0279 | 0.1316 | 0.832021 | 0.932 | 0.1451 | 0.213 | 0.495656 | 0.8401 | NaN | -0.0314 | 0.1208 | 0.794721 | 0.9571 | -0.0948 | 0.1173 | 0.418996 | 0.847 | 0.0184 | 0.203 | 0.927958 | 0.9908 | NaN | -0.014 | 0.1201 | 0.906924 | 0.9717 | -0.0224 | 0.1137 | 0.843947 | 0.95 | -0.0073 | 0.2061 | 0.971833 | 0.9976 | NaN | 0.0244 | 0.1224 | 0.842205 | 0.962 | -0.0324 | 0.1211 | 0.788932 | 0.913 | 0.0586 | 0.2045 | 0.774386 | 0.9606 | NaN | -0.0213 | 0.1225 | 0.861807 | 0.962 | -0.0884 | 0.1174 | 0.451594 | 0.8246 | 0.0306 | 0.207 | 0.882483 | 0.9633 | NaN | 0.0421 | 0.1222 | 0.730639 | 0.9166 | -0.0128 | 0.1188 | 0.914379 | 0.979 | 0.0781 | 0.2059 | 0.704375 | 0.9459 |
| N-acetyl-DL-methionine | 191.0621 | 1.239334 | Amino Acid | Acetyl Amino Acid | -0.2401 | 0.132 | 0.06899 | 0.3759 | -0.0293 | 0.1284 | 0.819324 | 0.932 | -0.4921 | 0.2321 | 0.034002 | 0.3293 | NaN | -0.1917 | 0.1226 | 0.117982 | 0.6749 | 0.0064 | 0.1129 | 0.955088 | 0.9836 | -0.4093 | 0.2199 | 0.062648 | 0.6334 | NaN | -0.2416 | 0.1217 | 0.047083 | 0.3512 | -0.0701 | 0.1106 | 0.52634 | 0.9053 | -0.4286 | 0.2206 | 0.052092 | 0.477 | NaN | -0.239 | 0.1247 | 0.055273 | 0.445 | -0.0504 | 0.1175 | 0.667896 | 0.8438 | -0.4363 | 0.2219 | 0.049305 | 0.559 | NaN | -0.1696 | 0.1249 | 0.174325 | 0.6753 | 0.0355 | 0.1136 | 0.754279 | 0.9131 | -0.401 | 0.225 | 0.074667 | 0.6055 | NaN | -0.2351 | 0.125 | 0.060059 | 0.4541 | -0.0316 | 0.1157 | 0.784438 | 0.9203 | -0.4586 | 0.2233 | 0.040012 | 0.4663 |
| 4-acetamidobutanoate | 145.0737 | 1.814703 | Amino Acid | Arginine and proline metabolism | 0.0936 | 0.138 | 0.497549 | 0.8054 | 0.2496 | 0.1556 | 0.108717 | 0.3922 | 0.0269 | 0.2139 | 0.899875 | 0.9836 | NaN | 0.1017 | 0.1275 | 0.425107 | 0.8498 | 0.2778 | 0.1356 | 0.040461 | 0.3602 | 0.0274 | 0.2006 | 0.89119 | 0.977 | NaN | 0.1046 | 0.1273 | 0.411617 | 0.8542 | 0.2923 | 0.1327 | 0.027629 | 0.3319 | 0.0098 | 0.202 | 0.961338 | 0.9976 | NaN | 0.0852 | 0.1305 | 0.513712 | 0.8197 | 0.2285 | 0.1424 | 0.108685 | 0.4435 | 0.0477 | 0.2034 | 0.814722 | 0.9674 | NaN | 0.1241 | 0.1293 | 0.33707 | 0.7711 | 0.3062 | 0.1355 | 0.02386 | 0.2532 | 0.0464 | 0.2043 | 0.820504 | 0.9621 | NaN | 0.0892 | 0.1307 | 0.494892 | 0.8278 | 0.2269 | 0.1403 | 0.105715 | 0.4566 | 0.0491 | 0.2053 | 0.8112 | 0.9641 |
| 4-hydroxy-L-proline | 131.0579 | 0.616786 | Amino Acid | Arginine and proline metabolism | 0.0785 | 0.1308 | 0.548376 | 0.8252 | 0.1108 | 0.129 | 0.390245 | 0.6593 | 0.0335 | 0.2245 | 0.881372 | 0.9789 | NaN | 0.1262 | 0.1211 | 0.297131 | 0.781 | 0.1401 | 0.1129 | 0.214365 | 0.7304 | 0.1126 | 0.2113 | 0.594157 | 0.954 | NaN | 0.0548 | 0.1209 | 0.650356 | 0.9331 | 0.0865 | 0.1113 | 0.436904 | 0.8947 | 0.0264 | 0.212 | 0.901033 | 0.9935 | NaN | 0.1273 | 0.1239 | 0.304211 | 0.741 | 0.1612 | 0.1178 | 0.171135 | 0.5146 | 0.0869 | 0.2138 | 0.684601 | 0.9476 | NaN | 0.1423 | 0.1229 | 0.246889 | 0.7211 | 0.1906 | 0.1131 | 0.092061 | 0.5082 | 0.0892 | 0.2149 | 0.677932 | 0.9621 | NaN | 0.131 | 0.1242 | 0.29166 | 0.7478 | 0.1686 | 0.116 | 0.145878 | 0.5201 | 0.0884 | 0.216 | 0.682486 | 0.9459 |
| S-3-methyl-2-oxopentanoate | 130.0634 | 4.355281 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.0373 | 0.1402 | 0.790037 | 0.9564 | 0.2442 | 0.1338 | 0.068027 | 0.3294 | -0.1909 | 0.2439 | 0.433818 | 0.7903 | NaN | -0.0048 | 0.1299 | 0.970522 | 0.9952 | 0.1454 | 0.1201 | 0.226158 | 0.7475 | -0.1499 | 0.2292 | 0.51298 | 0.954 | NaN | -0.0227 | 0.1299 | 0.861491 | 0.9714 | 0.1948 | 0.1159 | 0.092791 | 0.6246 | -0.2676 | 0.2304 | 0.245427 | 0.8972 | NaN | 0.0328 | 0.1326 | 0.804633 | 0.9433 | 0.1523 | 0.1256 | 0.225499 | 0.5613 | -0.0636 | 0.2356 | 0.787287 | 0.9657 | NaN | 0.0181 | 0.1315 | 0.890741 | 0.9674 | 0.1808 | 0.1189 | 0.128449 | 0.5958 | -0.1595 | 0.2332 | 0.493926 | 0.9434 | NaN | 0.0247 | 0.1329 | 0.852537 | 0.9543 | 0.1306 | 0.1246 | 0.294635 | 0.6559 | -0.077 | 0.2377 | 0.745959 | 0.9486 |
| 4-methyl-2-oxopentanoate | 130.0634 | 4.760282 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.0445 | 0.1349 | 0.741515 | 0.9321 | 0.2525 | 0.1303 | 0.05267 | 0.3003 | -0.1825 | 0.2312 | 0.429868 | 0.7857 | NaN | 0.0217 | 0.1249 | 0.861931 | 0.9705 | 0.1639 | 0.1167 | 0.160225 | 0.66 | -0.1145 | 0.218 | 0.599405 | 0.954 | NaN | -0.0103 | 0.125 | 0.934565 | 0.9728 | 0.2175 | 0.1124 | 0.052979 | 0.4874 | -0.2569 | 0.2185 | 0.239702 | 0.888 | NaN | 0.0461 | 0.1276 | 0.71767 | 0.8983 | 0.1563 | 0.1228 | 0.202991 | 0.5466 | -0.0421 | 0.2245 | 0.851334 | 0.9772 | NaN | 0.0381 | 0.1265 | 0.763047 | 0.938 | 0.196 | 0.1156 | 0.090074 | 0.5022 | -0.133 | 0.2216 | 0.548335 | 0.9621 | NaN | 0.0383 | 0.1279 | 0.764243 | 0.9333 | 0.1382 | 0.1217 | 0.256101 | 0.6316 | -0.0602 | 0.2263 | 0.790304 | 0.9525 |
| methyl-acetoacetate | 116.0478 | 2.239242 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.1392 | 0.135 | 0.302548 | 0.6742 | 0.2381 | 0.1253 | 0.057436 | 0.3054 | -0.0059 | 0.2451 | 0.980864 | 0.9935 | NaN | 0.0639 | 0.1258 | 0.611411 | 0.9079 | 0.1152 | 0.1141 | 0.312829 | 0.8095 | 0.0102 | 0.2299 | 0.964614 | 0.9911 | NaN | 0.0427 | 0.1261 | 0.735119 | 0.957 | 0.1676 | 0.1094 | 0.125395 | 0.6704 | -0.123 | 0.2333 | 0.598122 | 0.9894 | NaN | 0.0827 | 0.1284 | 0.519551 | 0.8227 | 0.114 | 0.1204 | 0.343481 | 0.67 | 0.0623 | 0.2338 | 0.789833 | 0.9662 | NaN | 0.0897 | 0.1271 | 0.480378 | 0.8625 | 0.1526 | 0.1125 | 0.174762 | 0.6515 | -0.0002 | 0.234 | 0.999324 | 0.9999 | NaN | 0.078 | 0.1288 | 0.544729 | 0.8553 | 0.0922 | 0.1195 | 0.440496 | 0.7458 | 0.0592 | 0.2361 | 0.801952 | 0.9623 |
| methyl-malonate | 118.027 | 1.412051 | Amino Acid | Branched Chain Amino Acid Metabolism | 0.128 | 0.135 | 0.343097 | 0.7042 | 0.0546 | 0.1385 | 0.693557 | 0.8728 | 0.2224 | 0.224 | 0.320902 | 0.7534 | NaN | 0.0965 | 0.125 | 0.440286 | 0.8498 | -0.0611 | 0.1234 | 0.620483 | 0.9073 | 0.272 | 0.2098 | 0.194793 | 0.919 | NaN | 0.2124 | 0.1248 | 0.088623 | 0.5342 | 0.0703 | 0.1192 | 0.555123 | 0.9053 | 0.354 | 0.2125 | 0.095802 | 0.6246 | NaN | 0.0492 | 0.1289 | 0.702348 | 0.8872 | -0.0659 | 0.1296 | 0.611162 | 0.8188 | 0.1813 | 0.2135 | 0.395964 | 0.9375 | NaN | 0.1037 | 0.1266 | 0.412924 | 0.8289 | -0.0739 | 0.124 | 0.551355 | 0.8618 | 0.2829 | 0.2139 | 0.185934 | 0.8608 | NaN | 0.0584 | 0.1289 | 0.650293 | 0.8907 | -0.0709 | 0.1274 | 0.577947 | 0.8092 | 0.1948 | 0.2153 | 0.36558 | 0.8851 |
| 3-amino-5-hydroxybenzoic acid | 153.0414 | 1.468679 | Benzenoids | Benzoic acid and derivatives | -0.2015 | 0.1286 | 0.117245 | 0.4809 | -0.2354 | 0.1174 | 0.045002 | 0.2929 | -0.126 | 0.2446 | 0.606455 | 0.8951 | NaN | -0.1609 | 0.1193 | 0.177601 | 0.7251 | -0.1849 | 0.1039 | 0.075292 | 0.4865 | -0.0929 | 0.2296 | 0.685724 | 0.954 | NaN | -0.1417 | 0.1195 | 0.235754 | 0.7361 | -0.1145 | 0.105 | 0.275374 | 0.806 | -0.1697 | 0.231 | 0.462483 | 0.9816 | NaN | -0.2075 | 0.1215 | 0.087505 | 0.5308 | -0.2525 | 0.1066 | 0.017837 | 0.1641 | -0.0843 | 0.233 | 0.717421 | 0.9477 | NaN | -0.1734 | 0.1208 | 0.15105 | 0.6753 | -0.2076 | 0.1034 | 0.04462 | 0.357 | -0.0884 | 0.2339 | 0.70565 | 0.9621 | NaN | -0.1928 | 0.1219 | 0.113528 | 0.5578 | -0.2479 | 0.105 | 0.018216 | 0.1704 | -0.0635 | 0.2358 | 0.787638 | 0.9525 |
| bis(2-ethylhexyl)phthalate | 390.2777 | 23.077421 | Benzenoids | Benzoic acids and derivatives | -0.143 | 0.1294 | 0.269113 | 0.6376 | 0.0537 | 0.1176 | 0.647962 | 0.8471 | -0.4263 | 0.2484 | 0.086136 | 0.4852 | NaN | -0.1547 | 0.1196 | 0.195895 | 0.7307 | 0.0617 | 0.1031 | 0.549394 | 0.9009 | -0.5015 | 0.2319 | 0.030566 | 0.5113 | NaN | -0.1513 | 0.1194 | 0.205262 | 0.7361 | 0.0295 | 0.1014 | 0.770865 | 0.9284 | -0.4505 | 0.2338 | 0.053996 | 0.477 | NaN | -0.1643 | 0.1223 | 0.179083 | 0.6547 | 0.0533 | 0.1075 | 0.620188 | 0.8228 | -0.5071 | 0.2354 | 0.031179 | 0.4788 | NaN | -0.1593 | 0.1212 | 0.188577 | 0.6753 | 0.0334 | 0.1035 | 0.746667 | 0.9085 | -0.4567 | 0.2365 | 0.05345 | 0.5267 | NaN | -0.1696 | 0.1225 | 0.166437 | 0.6293 | 0.044 | 0.106 | 0.678172 | 0.8734 | -0.5019 | 0.2378 | 0.03485 | 0.4663 |
| monoethylhexyl phthalic acid | 278.1524 | 20.82011 | Benzenoids | Benzoic acids and derivatives | -0.0708 | 0.1297 | 0.585243 | 0.8423 | -0.0064 | 0.1637 | 0.968703 | 0.987 | -0.0938 | 0.1886 | 0.618927 | 0.9014 | NaN | 0.0353 | 0.1214 | 0.771102 | 0.9527 | 0.0589 | 0.144 | 0.682703 | 0.9267 | 0.0287 | 0.1799 | 0.873174 | 0.977 | NaN | -0.017 | 0.1202 | 0.887303 | 0.9714 | 0.1103 | 0.142 | 0.43711 | 0.8947 | -0.0856 | 0.1781 | 0.630812 | 0.9894 | NaN | -0.0075 | 0.1234 | 0.951673 | 0.9828 | 0.0081 | 0.1497 | 0.957121 | 0.9894 | -0.0064 | 0.1813 | 0.971666 | 0.99 | NaN | -0.0001 | 0.1224 | 0.999138 | 0.9991 | 0.0036 | 0.1439 | 0.979967 | 0.9923 | -0.0037 | 0.1825 | 0.983691 | 0.9969 | NaN | 0.0046 | 0.124 | 0.970562 | 0.9893 | -0.0051 | 0.1474 | 0.972311 | 0.9946 | 0.0129 | 0.1846 | 0.944463 | 0.9869 |
| 3-hydroxybenzyl alcohol | 124.0521 | 5.697804 | Benzenoids | benzyl alcohols | 0.1833 | 0.1206 | 0.128597 | 0.4964 | 0.2435 | 0.1416 | 0.08555 | 0.3625 | 0.1489 | 0.1803 | 0.408972 | 0.7758 | NaN | 0.08 | 0.1135 | 0.480864 | 0.8576 | 0.0719 | 0.1305 | 0.581606 | 0.904 | 0.0927 | 0.17 | 0.585802 | 0.954 | NaN | 0.0315 | 0.1151 | 0.784183 | 0.9641 | 0.082 | 0.127 | 0.518791 | 0.9053 | 0.0051 | 0.1756 | 0.976793 | 0.9976 | NaN | 0.0901 | 0.1162 | 0.43811 | 0.7844 | 0.0836 | 0.1373 | 0.542405 | 0.7845 | 0.1013 | 0.1722 | 0.556392 | 0.9375 | NaN | 0.0812 | 0.1153 | 0.481072 | 0.8625 | 0.0819 | 0.1302 | 0.529477 | 0.8496 | 0.0828 | 0.1738 | 0.633546 | 0.9621 | NaN | 0.1019 | 0.1161 | 0.379821 | 0.7638 | 0.0883 | 0.1339 | 0.50973 | 0.786 | 0.1117 | 0.1737 | 0.52001 | 0.8946 |
| phenylethanolamine | 137.0845 | 2.631094 | Benzenoids | Halobenzenes | 0.1131 | 0.1319 | 0.391337 | 0.726 | 0.013 | 0.1694 | 0.938765 | 0.9724 | 0.1664 | 0.1894 | 0.379618 | 0.7534 | NaN | 0.0233 | 0.1232 | 0.849747 | 0.9705 | -0.0605 | 0.1491 | 0.684943 | 0.9267 | 0.069 | 0.1801 | 0.701563 | 0.954 | NaN | 0.0104 | 0.1233 | 0.932588 | 0.9728 | -0.1283 | 0.1473 | 0.383713 | 0.8818 | 0.0796 | 0.181 | 0.66029 | 0.9894 | NaN | 0.0822 | 0.125 | 0.510565 | 0.8197 | 0.0021 | 0.1549 | 0.989037 | 0.9926 | 0.1301 | 0.1806 | 0.471305 | 0.9375 | NaN | 0.0691 | 0.124 | 0.577328 | 0.8828 | -0.0167 | 0.149 | 0.91079 | 0.9768 | 0.1194 | 0.1818 | 0.511379 | 0.9516 | NaN | 0.0869 | 0.1252 | 0.487436 | 0.8278 | 0.007 | 0.1526 | 0.963635 | 0.9924 | 0.1362 | 0.1822 | 0.454871 | 0.8887 |
| epinephrine | 183.0886 | 0.92338 | Benzenoids | phenols | 0.3273 | 0.1304 | 0.012102 | 0.1478 | 0.2161 | 0.1243 | 0.082109 | 0.3594 | 0.4461 | 0.2343 | 0.056895 | 0.4132 | NaN | 0.2072 | 0.1235 | 0.09353 | 0.622 | 0.1057 | 0.1124 | 0.347099 | 0.8132 | 0.3092 | 0.2247 | 0.168825 | 0.879 | NaN | 0.2356 | 0.1222 | 0.05389 | 0.3814 | 0.1299 | 0.109 | 0.233494 | 0.8003 | 0.352 | 0.224 | 0.116139 | 0.6678 | NaN | 0.2366 | 0.1257 | 0.059772 | 0.4583 | 0.125 | 0.1169 | 0.284929 | 0.6122 | 0.3407 | 0.2265 | 0.132553 | 0.8047 | NaN | 0.2201 | 0.125 | 0.078365 | 0.5579 | 0.1057 | 0.1126 | 0.348155 | 0.7839 | 0.3371 | 0.2281 | 0.139457 | 0.8053 | NaN | 0.2383 | 0.1259 | 0.05843 | 0.4541 | 0.1297 | 0.1146 | 0.257463 | 0.6316 | 0.3391 | 0.2295 | 0.139472 | 0.7588 |
| normethanephrine | 183.0897 | 2.503736 | Benzenoids | phenols | 0.254 | 0.1356 | 0.061022 | 0.3473 | 0.3179 | 0.1932 | 0.099815 | 0.3816 | 0.2457 | 0.1869 | 0.18869 | 0.6943 | NaN | 0.1132 | 0.1287 | 0.379132 | 0.8465 | 0.0941 | 0.1773 | 0.59553 | 0.904 | 0.1298 | 0.1791 | 0.468724 | 0.9478 | NaN | 0.1523 | 0.127 | 0.230606 | 0.7361 | 0.1899 | 0.1692 | 0.26158 | 0.8057 | 0.146 | 0.1797 | 0.416658 | 0.9816 | NaN | 0.141 | 0.1312 | 0.282365 | 0.7388 | 0.0671 | 0.1899 | 0.723665 | 0.876 | 0.1808 | 0.1794 | 0.313363 | 0.8963 | NaN | 0.1262 | 0.1303 | 0.332838 | 0.7669 | 0.1036 | 0.1772 | 0.558847 | 0.8618 | 0.1456 | 0.1823 | 0.424619 | 0.9359 | NaN | 0.1427 | 0.1315 | 0.27781 | 0.7337 | 0.0562 | 0.1862 | 0.762985 | 0.9096 | 0.1821 | 0.1813 | 0.315115 | 0.8727 |
| fluvoxamino acid | 304.1505 | 6.009206 | Benzenoids | Trifluoromethylbenzenes | 0.0176 | 0.1355 | 0.896477 | 0.9809 | 0.0364 | 0.188 | 0.846444 | 0.932 | 0.0109 | 0.1885 | 0.953889 | 0.9887 | NaN | -0.0085 | 0.1254 | 0.94573 | 0.9906 | -0.0389 | 0.1655 | 0.814235 | 0.965 | 0.0074 | 0.1768 | 0.966665 | 0.9911 | NaN | -0.0122 | 0.1252 | 0.922599 | 0.9728 | -0.1693 | 0.1648 | 0.304263 | 0.8336 | 0.0473 | 0.1782 | 0.790633 | 0.9935 | NaN | 0.0147 | 0.1281 | 0.90874 | 0.9828 | 0.0228 | 0.172 | 0.894499 | 0.9695 | 0.016 | 0.1791 | 0.92895 | 0.99 | NaN | 0.0274 | 0.127 | 0.829147 | 0.9564 | 0.0169 | 0.1653 | 0.91836 | 0.9808 | 0.0335 | 0.1801 | 0.852482 | 0.9621 | NaN | -0.0043 | 0.1285 | 0.973208 | 0.9893 | -0.0285 | 0.1699 | 0.866542 | 0.9586 | 0.0072 | 0.1809 | 0.968083 | 0.9896 |
| allose | 180.0642 | 1.594537 | Carbohydrate | Aldohexose sugar | -0.079 | 0.1562 | 0.612975 | 0.861 | 0.1454 | 0.1457 | 0.318466 | 0.6107 | -0.3516 | 0.284 | 0.215776 | 0.7178 | NaN | -0.0696 | 0.1445 | 0.629845 | 0.9079 | 0.1179 | 0.1281 | 0.357206 | 0.8148 | -0.2969 | 0.2671 | 0.266428 | 0.9223 | NaN | -0.1132 | 0.1442 | 0.432647 | 0.878 | 0.1311 | 0.1255 | 0.29614 | 0.8336 | -0.4451 | 0.2678 | 0.096541 | 0.6246 | NaN | -0.0698 | 0.1477 | 0.636458 | 0.8611 | 0.1226 | 0.1335 | 0.358313 | 0.6762 | -0.2947 | 0.2709 | 0.276718 | 0.8705 | NaN | -0.0439 | 0.1466 | 0.764792 | 0.938 | 0.1705 | 0.1277 | 0.18178 | 0.6534 | -0.3147 | 0.2717 | 0.246676 | 0.9039 | NaN | -0.0586 | 0.1481 | 0.692144 | 0.9035 | 0.1217 | 0.1315 | 0.354549 | 0.6867 | -0.2769 | 0.2743 | 0.312872 | 0.8727 |
| glucaric acid | 210.0387 | 0.884294 | Carbohydrate | Aminosugar Metabolism | -0.0631 | 0.1323 | 0.633539 | 0.8678 | -0.1147 | 0.1405 | 0.414465 | 0.6809 | 0.0027 | 0.2136 | 0.989925 | 0.9935 | NaN | -0.0789 | 0.1224 | 0.519089 | 0.8844 | -0.0745 | 0.1238 | 0.547341 | 0.9009 | -0.0661 | 0.2011 | 0.742363 | 0.954 | NaN | -0.0255 | 0.1224 | 0.83467 | 0.9714 | -0.0461 | 0.122 | 0.705519 | 0.9195 | 0.004 | 0.2017 | 0.984043 | 0.9976 | NaN | -0.081 | 0.1251 | 0.517288 | 0.8227 | -0.0833 | 0.1289 | 0.518092 | 0.7667 | -0.0552 | 0.2037 | 0.786443 | 0.9657 | NaN | -0.0591 | 0.124 | 0.633842 | 0.8971 | -0.0582 | 0.1243 | 0.639677 | 0.8623 | -0.0354 | 0.2043 | 0.862544 | 0.9621 | NaN | -0.0664 | 0.1254 | 0.596385 | 0.8765 | -0.0684 | 0.1272 | 0.590842 | 0.8199 | -0.0359 | 0.2054 | 0.861408 | 0.9641 |
| glucuronic acid | 194.042 | 0.662189 | Carbohydrate | Aminosugar Metabolism | 0.2039 | 0.1368 | 0.136112 | 0.5077 | 0.1453 | 0.1377 | 0.291075 | 0.58 | 0.237 | 0.2314 | 0.305731 | 0.7534 | NaN | 0.1395 | 0.1273 | 0.273491 | 0.7625 | 0.1031 | 0.1213 | 0.395365 | 0.8426 | 0.154 | 0.2186 | 0.481318 | 0.954 | NaN | 0.1136 | 0.1277 | 0.373856 | 0.8283 | 0.1472 | 0.1183 | 0.213634 | 0.7942 | 0.0702 | 0.2246 | 0.754475 | 0.9935 | NaN | 0.1286 | 0.1307 | 0.325181 | 0.741 | 0.0936 | 0.1269 | 0.460731 | 0.7319 | 0.129 | 0.2231 | 0.563039 | 0.9375 | NaN | 0.1269 | 0.1295 | 0.326958 | 0.7669 | 0.0775 | 0.1222 | 0.52602 | 0.8496 | 0.1571 | 0.2229 | 0.481001 | 0.9403 | NaN | 0.1475 | 0.1305 | 0.258499 | 0.7205 | 0.0863 | 0.1251 | 0.490351 | 0.7774 | 0.1821 | 0.2232 | 0.414418 | 0.8887 |
| lactose | 342.1173 | 0.670231 | Carbohydrate | Aminosugar Metabolism | 0.2645 | 0.1274 | 0.037876 | 0.2818 | 0.0336 | 0.1276 | 0.792398 | 0.932 | 0.5069 | 0.2144 | 0.018074 | 0.2268 | NaN | 0.1805 | 0.1193 | 0.130217 | 0.6772 | 0.0169 | 0.1121 | 0.880286 | 0.9729 | 0.3568 | 0.2081 | 0.08642 | 0.7567 | NaN | 0.1766 | 0.1192 | 0.138437 | 0.6531 | -0.0625 | 0.111 | 0.573144 | 0.9053 | 0.4315 | 0.2047 | 0.034995 | 0.3815 | NaN | 0.2186 | 0.1211 | 0.071053 | 0.4947 | 0.0842 | 0.117 | 0.471554 | 0.7332 | 0.3592 | 0.2123 | 0.090744 | 0.7393 | NaN | 0.2136 | 0.1201 | 0.075304 | 0.5579 | 0.0408 | 0.1122 | 0.715882 | 0.8866 | 0.4082 | 0.2091 | 0.050896 | 0.5267 | NaN | 0.2297 | 0.1211 | 0.057882 | 0.4541 | 0.0803 | 0.1151 | 0.485617 | 0.777 | 0.4004 | 0.2113 | 0.058165 | 0.5263 |
| N-acetyl-D-glucosamine | 221.0905 | 0.68895 | Carbohydrate | Aminosugar Metabolism | 0.1929 | 0.1448 | 0.182925 | 0.5518 | 0.3076 | 0.1307 | 0.018606 | 0.2054 | -0.007 | 0.2734 | 0.979683 | 0.9935 | NaN | 0.0792 | 0.1359 | 0.559817 | 0.9079 | 0.2855 | 0.1144 | 0.012566 | 0.1892 | -0.2778 | 0.2639 | 0.292437 | 0.9223 | NaN | 0.0476 | 0.1366 | 0.72734 | 0.9559 | 0.2744 | 0.1125 | 0.014723 | 0.2463 | -0.3166 | 0.2689 | 0.239109 | 0.888 | NaN | 0.1064 | 0.1385 | 0.442445 | 0.7844 | 0.2954 | 0.1192 | 0.013207 | 0.14 | -0.2399 | 0.2672 | 0.369237 | 0.9223 | NaN | 0.0965 | 0.1374 | 0.482645 | 0.8625 | 0.3038 | 0.1141 | 0.007736 | 0.1424 | -0.2435 | 0.2693 | 0.36606 | 0.9106 | NaN | 0.1137 | 0.1386 | 0.412131 | 0.791 | 0.2936 | 0.1174 | 0.01237 | 0.1359 | -0.1937 | 0.2684 | 0.470492 | 0.8887 |
| N-acetylneuraminate | 309.1045 | 0.672557 | Carbohydrate | Aminosugar Metabolism | -0.1527 | 0.1305 | 0.24206 | 0.6129 | -0.1171 | 0.1305 | 0.369712 | 0.6407 | -0.194 | 0.2232 | 0.384866 | 0.7534 | NaN | -0.1329 | 0.1208 | 0.271116 | 0.7625 | -0.0545 | 0.1155 | 0.637224 | 0.9073 | -0.2096 | 0.2092 | 0.316282 | 0.9223 | NaN | -0.093 | 0.1212 | 0.442771 | 0.8792 | 0.0212 | 0.1155 | 0.85415 | 0.9525 | -0.1956 | 0.2107 | 0.353211 | 0.9578 | NaN | -0.1282 | 0.1236 | 0.29966 | 0.741 | -0.0785 | 0.12 | 0.513069 | 0.7647 | -0.1668 | 0.2125 | 0.43256 | 0.9375 | NaN | -0.123 | 0.1225 | 0.315427 | 0.7669 | -0.0817 | 0.1152 | 0.4781 | 0.8272 | -0.1554 | 0.2137 | 0.467221 | 0.9359 | NaN | -0.1269 | 0.1239 | 0.305588 | 0.7481 | -0.0854 | 0.118 | 0.469206 | 0.7618 | -0.1556 | 0.2148 | 0.468834 | 0.8887 |
| 2-deoxy-D-glucose | 164.0684 | 0.704827 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | -0.158 | 0.131 | 0.227943 | 0.6042 | 0.2981 | 0.1257 | 0.017709 | 0.2037 | -0.6368 | 0.2179 | 0.003478 | 0.1069 | NaN | -0.2014 | 0.121 | 0.096017 | 0.6297 | 0.2229 | 0.1122 | 0.046916 | 0.3924 | -0.6373 | 0.2033 | 0.001716 | 0.1176 | NaN | -0.2567 | 0.1211 | 0.034056 | 0.2852 | 0.1556 | 0.1135 | 0.170194 | 0.7308 | -0.6795 | 0.2038 | 0.000857 | 0.0465 | NaN | -0.1641 | 0.1238 | 0.18483 | 0.6616 | 0.2834 | 0.1147 | 0.013518 | 0.14 | -0.6354 | 0.2063 | 0.002072 | 0.1264 | NaN | -0.1673 | 0.1227 | 0.172603 | 0.6753 | 0.2719 | 0.1104 | 0.013777 | 0.2001 | -0.6329 | 0.2074 | 0.002275 | 0.1345 | NaN | -0.1663 | 0.124 | 0.179965 | 0.6463 | 0.2639 | 0.1136 | 0.020141 | 0.1823 | -0.6195 | 0.209 | 0.003034 | 0.1675 |
| glyceraldehyde | 90.0314 | 1.593113 | Carbohydrate | Fructose, Mannose and Galactose Metabolism | -0.1092 | 0.1566 | 0.485638 | 0.8041 | 0.0624 | 0.1377 | 0.650662 | 0.8471 | -0.4073 | 0.3136 | 0.194014 | 0.7046 | NaN | -0.0861 | 0.1449 | 0.552575 | 0.9073 | 0.064 | 0.1208 | 0.596113 | 0.904 | -0.3549 | 0.2947 | 0.228506 | 0.9223 | NaN | -0.1304 | 0.1445 | 0.366943 | 0.8283 | 0.0702 | 0.1185 | 0.553659 | 0.9053 | -0.5145 | 0.2956 | 0.081791 | 0.5886 | NaN | -0.083 | 0.1482 | 0.575353 | 0.8473 | 0.0694 | 0.1259 | 0.581429 | 0.804 | -0.3511 | 0.299 | 0.240257 | 0.8705 | NaN | -0.0606 | 0.1471 | 0.68026 | 0.9114 | 0.1139 | 0.121 | 0.346638 | 0.7839 | -0.3756 | 0.2997 | 0.210155 | 0.8887 | NaN | -0.0794 | 0.1486 | 0.592991 | 0.8765 | 0.0639 | 0.124 | 0.60604 | 0.826 | -0.3347 | 0.3025 | 0.268638 | 0.8424 |
| D-lyxose | 150.0527 | 0.706673 | Carbohydrate | Pentose Metabolism | 0.1165 | 0.159 | 0.463794 | 0.7951 | 0.1177 | 0.1565 | 0.452211 | 0.7214 | 0.0797 | 0.2791 | 0.775241 | 0.9647 | NaN | 0.3202 | 0.1492 | 0.031851 | 0.3509 | 0.243 | 0.1374 | 0.076916 | 0.488 | 0.3756 | 0.2693 | 0.163173 | 0.879 | NaN | 0.1729 | 0.1468 | 0.238844 | 0.7365 | 0.1598 | 0.1344 | 0.234477 | 0.8003 | 0.1607 | 0.2641 | 0.542797 | 0.9894 | NaN | 0.3155 | 0.1536 | 0.039984 | 0.356 | 0.2282 | 0.1438 | 0.112496 | 0.4439 | 0.3767 | 0.2753 | 0.1711 | 0.8705 | NaN | 0.3389 | 0.1524 | 0.026139 | 0.2945 | 0.2576 | 0.1378 | 0.061632 | 0.4149 | 0.3978 | 0.2789 | 0.153815 | 0.8056 | NaN | 0.3208 | 0.1543 | 0.037604 | 0.346 | 0.2045 | 0.141 | 0.146924 | 0.5201 | 0.4278 | 0.2841 | 0.132099 | 0.7588 |
| 5-phospho-alpha-D-ribose-1-diphosphate | 389.977 | 0.999379 | Carbohydrate | Pentose Phosphate Pathway | 0.1788 | 0.1432 | 0.211892 | 0.5792 | 0.1368 | 0.1508 | 0.364479 | 0.6407 | 0.2388 | 0.2419 | 0.323538 | 0.7534 | NaN | 0.0366 | 0.1352 | 0.786345 | 0.9571 | 0.0746 | 0.1333 | 0.575741 | 0.904 | 0.0334 | 0.2345 | 0.886613 | 0.977 | NaN | 0.0513 | 0.1345 | 0.702682 | 0.9481 | 0.0875 | 0.1305 | 0.502595 | 0.9053 | 0.0618 | 0.2349 | 0.792384 | 0.9935 | NaN | 0.0592 | 0.1381 | 0.668062 | 0.8697 | 0.0202 | 0.1413 | 0.886076 | 0.9685 | 0.1435 | 0.2324 | 0.537025 | 0.9375 | NaN | 0.0694 | 0.1362 | 0.61042 | 0.8964 | 0.0614 | 0.1338 | 0.646365 | 0.8623 | 0.1175 | 0.235 | 0.616937 | 0.9621 | NaN | 0.0538 | 0.1387 | 0.698266 | 0.9035 | 0.0191 | 0.1388 | 0.890631 | 0.9667 | 0.128 | 0.2359 | 0.587526 | 0.9319 |
| ascorbate | 176.0311 | 1.087867 | Cofactors and Vitamins | Ascorbate and Aldarate Metabolism | -0.12 | 0.1329 | 0.366604 | 0.7161 | -0.0849 | 0.1545 | 0.58241 | 0.8037 | -0.1243 | 0.2011 | 0.536369 | 0.8655 | NaN | -0.1915 | 0.123 | 0.119394 | 0.6749 | -0.1689 | 0.1356 | 0.212899 | 0.7304 | -0.1879 | 0.1888 | 0.319657 | 0.9223 | NaN | -0.1231 | 0.1226 | 0.31547 | 0.7952 | -0.1525 | 0.1329 | 0.250929 | 0.8037 | -0.0953 | 0.1902 | 0.616342 | 0.9894 | NaN | -0.1482 | 0.1256 | 0.238014 | 0.7062 | -0.1446 | 0.1414 | 0.306419 | 0.6359 | -0.1236 | 0.1911 | 0.517856 | 0.9375 | NaN | -0.1497 | 0.1244 | 0.228874 | 0.7058 | -0.0653 | 0.1359 | 0.631022 | 0.8623 | -0.1851 | 0.1924 | 0.335887 | 0.9106 | NaN | -0.1481 | 0.1258 | 0.239226 | 0.7024 | -0.1231 | 0.139 | 0.375931 | 0.6983 | -0.1424 | 0.1929 | 0.460412 | 0.8887 |
| dethiobiotin | 214.1178 | 7.308711 | Cofactors and Vitamins | biotin metabolism | -0.0439 | 0.1401 | 0.753826 | 0.9343 | -0.0953 | 0.15 | 0.525161 | 0.7793 | 0.0147 | 0.2242 | 0.947714 | 0.9887 | NaN | -0.0667 | 0.1296 | 0.606856 | 0.9079 | -0.0841 | 0.1316 | 0.52294 | 0.8967 | -0.0532 | 0.211 | 0.800863 | 0.9617 | NaN | -0.0482 | 0.1294 | 0.709242 | 0.9481 | 0.0172 | 0.1309 | 0.895586 | 0.973 | -0.113 | 0.2143 | 0.597941 | 0.9894 | NaN | -0.0757 | 0.1326 | 0.567879 | 0.846 | -0.1462 | 0.1371 | 0.286415 | 0.6122 | -0.0075 | 0.2133 | 0.971991 | 0.99 | NaN | -0.0813 | 0.1314 | 0.536004 | 0.8632 | -0.1076 | 0.1317 | 0.413899 | 0.8188 | -0.0535 | 0.2151 | 0.803489 | 0.9621 | NaN | -0.0577 | 0.1328 | 0.663628 | 0.9035 | -0.1346 | 0.1349 | 0.318558 | 0.672 | 0.0132 | 0.2152 | 0.951191 | 0.9869 |
| biliverdin | 582.2489 | 18.410517 | Cofactors and Vitamins | Hemoglobin and Porphyrin Metabolism | 0.0779 | 0.1517 | 0.607375 | 0.8575 | 0.1086 | 0.178 | 0.541959 | 0.7852 | 0.072 | 0.2279 | 0.75197 | 0.9647 | NaN | 0.1694 | 0.1407 | 0.22861 | 0.7495 | 0.2247 | 0.1563 | 0.150463 | 0.634 | 0.1557 | 0.2144 | 0.467788 | 0.9478 | NaN | 0.1719 | 0.1405 | 0.221168 | 0.7361 | 0.1753 | 0.153 | 0.252023 | 0.8037 | 0.186 | 0.2167 | 0.390838 | 0.9816 | NaN | 0.135 | 0.1436 | 0.347129 | 0.7456 | 0.1899 | 0.163 | 0.243992 | 0.5817 | 0.1266 | 0.217 | 0.559675 | 0.9375 | NaN | 0.1911 | 0.1431 | 0.181818 | 0.6753 | 0.2787 | 0.1573 | 0.076341 | 0.4631 | 0.1586 | 0.2187 | 0.468289 | 0.9359 | NaN | 0.155 | 0.1443 | 0.282545 | 0.7342 | 0.2144 | 0.1606 | 0.181967 | 0.5692 | 0.1437 | 0.2196 | 0.512863 | 0.8946 |
| bilirubin | 584.265 | 12.192934 | Cofactors and Vitamins | Hemoglobin and Porphyrin Metabolism | 0.1828 | 0.141 | 0.194751 | 0.5541 | 0.3538 | 0.1475 | 0.016453 | 0.2018 | 0.0625 | 0.2252 | 0.781421 | 0.9647 | NaN | 0.1089 | 0.1313 | 0.407147 | 0.8498 | 0.2043 | 0.1351 | 0.130532 | 0.6118 | 0.0656 | 0.2111 | 0.75593 | 0.954 | NaN | 0.0841 | 0.1317 | 0.523135 | 0.9101 | 0.2315 | 0.1306 | 0.076366 | 0.5751 | -0.0214 | 0.2139 | 0.920258 | 0.9935 | NaN | 0.1684 | 0.1334 | 0.20675 | 0.6875 | 0.2952 | 0.1363 | 0.030349 | 0.2264 | 0.0965 | 0.2141 | 0.652108 | 0.9375 | NaN | 0.1303 | 0.1327 | 0.326326 | 0.7669 | 0.245 | 0.133 | 0.065516 | 0.4198 | 0.0558 | 0.215 | 0.795129 | 0.9621 | NaN | 0.1669 | 0.1337 | 0.211751 | 0.6756 | 0.2733 | 0.1352 | 0.043186 | 0.2805 | 0.1049 | 0.2163 | 0.627801 | 0.9459 |
| nicotinamide | 122.0481 | 1.119239 | Cofactors and Vitamins | Nicotinate and Nicotinamide Metabolism | 0.0111 | 0.1326 | 0.933492 | 0.9834 | 0.077 | 0.1721 | 0.654744 | 0.8482 | -0.0062 | 0.1894 | 0.973928 | 0.9935 | NaN | -0.0715 | 0.1234 | 0.56228 | 0.9079 | 0.0261 | 0.1515 | 0.863373 | 0.9729 | -0.1111 | 0.1793 | 0.535559 | 0.954 | NaN | -0.0234 | 0.1226 | 0.84878 | 0.9714 | 0.0803 | 0.1482 | 0.587768 | 0.9053 | -0.0657 | 0.1794 | 0.714296 | 0.99 | NaN | -0.0417 | 0.1258 | 0.740257 | 0.9111 | 0.0718 | 0.1574 | 0.648335 | 0.8421 | -0.0882 | 0.1814 | 0.626738 | 0.9375 | NaN | -0.0529 | 0.1248 | 0.67174 | 0.9077 | 0.0952 | 0.1512 | 0.529058 | 0.8496 | -0.1093 | 0.1832 | 0.550772 | 0.9621 | NaN | -0.0427 | 0.1261 | 0.734751 | 0.918 | 0.0664 | 0.1551 | 0.668466 | 0.8682 | -0.082 | 0.1832 | 0.654303 | 0.9459 |
| pantothenate | 219.1106 | 3.27496 | Cofactors and Vitamins | Pantothenate and CoA Metabolism | 0.1517 | 0.1301 | 0.243573 | 0.6139 | -0.0284 | 0.1491 | 0.849207 | 0.932 | 0.255 | 0.2044 | 0.21211 | 0.7154 | NaN | 0.1089 | 0.1207 | 0.366787 | 0.8459 | -0.0531 | 0.1309 | 0.685132 | 0.9267 | 0.2236 | 0.192 | 0.244224 | 0.9223 | NaN | 0.0617 | 0.1214 | 0.611636 | 0.9125 | -0.0485 | 0.1285 | 0.705472 | 0.9195 | 0.156 | 0.1959 | 0.425934 | 0.9816 | NaN | 0.1308 | 0.1231 | 0.288004 | 0.7388 | -0.0252 | 0.1364 | 0.853597 | 0.9462 | 0.2357 | 0.1944 | 0.225388 | 0.8705 | NaN | 0.1128 | 0.1223 | 0.356357 | 0.79 | -0.0204 | 0.1312 | 0.876238 | 0.9692 | 0.2075 | 0.1961 | 0.290054 | 0.9039 | NaN | 0.1287 | 0.1234 | 0.297179 | 0.7481 | -0.0432 | 0.1343 | 0.747968 | 0.9096 | 0.2473 | 0.1961 | 0.207225 | 0.8424 |
| pterin | 163.067 | 1.601121 | Cofactors and Vitamins | Pterin Metabolism | -0.1584 | 0.1313 | 0.227546 | 0.6042 | -0.0291 | 0.136 | 0.830806 | 0.932 | -0.2566 | 0.2164 | 0.235827 | 0.735 | NaN | -0.0943 | 0.1222 | 0.440275 | 0.8498 | -0.0203 | 0.1193 | 0.864812 | 0.9729 | -0.1281 | 0.2069 | 0.535852 | 0.954 | NaN | -0.1291 | 0.1214 | 0.287449 | 0.7865 | -0.053 | 0.1171 | 0.65058 | 0.9053 | -0.1811 | 0.2061 | 0.379403 | 0.9786 | NaN | -0.1461 | 0.1242 | 0.239224 | 0.7062 | -0.0959 | 0.1249 | 0.442914 | 0.7319 | -0.1444 | 0.2095 | 0.490659 | 0.9375 | NaN | -0.102 | 0.1237 | 0.409891 | 0.8283 | -0.0163 | 0.1196 | 0.891306 | 0.9727 | -0.1586 | 0.2098 | 0.44969 | 0.9359 | NaN | -0.1479 | 0.1244 | 0.234583 | 0.7013 | -0.088 | 0.1228 | 0.473518 | 0.7643 | -0.1723 | 0.2104 | 0.412788 | 0.8887 |
| riboflavin | 376.1322 | 14.122794 | Cofactors and Vitamins | Riboflavin Metabolism | -0.06 | 0.12 | 0.617063 | 0.8645 | 0.0643 | 0.1242 | 0.604448 | 0.8198 | -0.2283 | 0.2039 | 0.262783 | 0.7397 | NaN | -0.0147 | 0.1113 | 0.894967 | 0.9705 | 0.033 | 0.1092 | 0.762567 | 0.9545 | -0.106 | 0.1949 | 0.586546 | 0.954 | NaN | -0.0123 | 0.1112 | 0.911844 | 0.9717 | 0.04 | 0.1071 | 0.708623 | 0.9195 | -0.0967 | 0.1971 | 0.623667 | 0.9894 | NaN | 0.0162 | 0.1146 | 0.887325 | 0.9771 | 0.06 | 0.1136 | 0.597373 | 0.8188 | -0.0803 | 0.2001 | 0.688121 | 0.9476 | NaN | 0.0083 | 0.1133 | 0.941617 | 0.9796 | 0.0439 | 0.1093 | 0.687748 | 0.8735 | -0.0812 | 0.2015 | 0.687068 | 0.9621 | NaN | -0.0056 | 0.1143 | 0.960725 | 0.9855 | 0.0165 | 0.1125 | 0.883252 | 0.9667 | -0.0896 | 0.2025 | 0.658034 | 0.9459 |
| thyroxine | 776.6865 | 16.140047 | Cofactors and Vitamins | Thyroxine Metabolism | 0.0068 | 0.1392 | 0.960976 | 0.9911 | -0.0514 | 0.1567 | 0.742688 | 0.9087 | 0.0567 | 0.2148 | 0.791914 | 0.9647 | NaN | -0.016 | 0.1288 | 0.901024 | 0.972 | -0.1149 | 0.1376 | 0.403602 | 0.847 | 0.0714 | 0.2014 | 0.723078 | 0.954 | NaN | 0.008 | 0.1286 | 0.95017 | 0.9728 | -0.0877 | 0.1349 | 0.515482 | 0.9053 | 0.085 | 0.2028 | 0.675217 | 0.9894 | NaN | -0.0207 | 0.1317 | 0.875406 | 0.9749 | -0.1423 | 0.1441 | 0.323687 | 0.6497 | 0.09 | 0.2043 | 0.659418 | 0.9381 | NaN | -0.0211 | 0.1306 | 0.871855 | 0.9672 | -0.1066 | 0.1378 | 0.439351 | 0.8205 | 0.0504 | 0.2051 | 0.805749 | 0.9621 | NaN | -0.0427 | 0.1323 | 0.746998 | 0.9266 | -0.1524 | 0.1419 | 0.28279 | 0.652 | 0.0482 | 0.2061 | 0.814993 | 0.9641 |
| alpha-tocopherol | 430.3784 | 24.493536 | Cofactors and Vitamins | Tocopherol Metabolism | 0.0191 | 0.1363 | 0.888256 | 0.9809 | 0.0617 | 0.1493 | 0.679194 | 0.8622 | -0.0223 | 0.2134 | 0.916849 | 0.9838 | NaN | 0.0042 | 0.1261 | 0.973679 | 0.9952 | -0.0626 | 0.133 | 0.63804 | 0.9073 | 0.0579 | 0.2012 | 0.773637 | 0.954 | NaN | -0.0165 | 0.126 | 0.895559 | 0.9714 | -0.0728 | 0.1306 | 0.577194 | 0.9053 | 0.0226 | 0.2019 | 0.910766 | 0.9935 | NaN | 0.0062 | 0.1289 | 0.961911 | 0.9828 | -0.0493 | 0.139 | 0.722719 | 0.876 | 0.0505 | 0.2039 | 0.804423 | 0.9662 | NaN | 0.0368 | 0.1277 | 0.773379 | 0.938 | 0.0209 | 0.1316 | 0.873921 | 0.9687 | 0.0393 | 0.2046 | 0.847551 | 0.9621 | NaN | 0.0092 | 0.1291 | 0.943286 | 0.9794 | -0.0465 | 0.1365 | 0.733471 | 0.8984 | 0.0412 | 0.2058 | 0.841436 | 0.9641 |
| 4-pyridoxate | 183.0525 | 1.874988 | Cofactors and Vitamins | Vitamin B6 Metabolism | -0.0734 | 0.132 | 0.578547 | 0.8423 | -0.0344 | 0.1424 | 0.809307 | 0.932 | -0.1096 | 0.2097 | 0.601197 | 0.8909 | NaN | -0.0229 | 0.1225 | 0.851781 | 0.9705 | 0.0213 | 0.1254 | 0.865186 | 0.9729 | -0.0699 | 0.1971 | 0.722767 | 0.954 | NaN | -0.0464 | 0.1221 | 0.703675 | 0.9481 | -0.0192 | 0.1227 | 0.875594 | 0.9609 | -0.0767 | 0.1983 | 0.69909 | 0.9894 | NaN | -0.0079 | 0.1256 | 0.94976 | 0.9828 | 0.0567 | 0.1318 | 0.66694 | 0.8438 | -0.0747 | 0.1997 | 0.708501 | 0.9477 | NaN | 0.0264 | 0.1252 | 0.832805 | 0.9564 | 0.1044 | 0.1274 | 0.412736 | 0.8188 | -0.0422 | 0.2015 | 0.834178 | 0.9621 | NaN | -0.0108 | 0.1259 | 0.931854 | 0.9794 | 0.0405 | 0.1292 | 0.753705 | 0.9096 | -0.0621 | 0.202 | 0.758374 | 0.9525 |
| pyridoxamine | 168.091 | 2.715419 | Cofactors and Vitamins | Vitamin B6 Metabolism | 0.1028 | 0.1276 | 0.420483 | 0.7523 | 0.0277 | 0.1272 | 0.827625 | 0.932 | 0.1648 | 0.2178 | 0.449192 | 0.8098 | NaN | 0.0873 | 0.1181 | 0.459482 | 0.8498 | -0.012 | 0.1119 | 0.914947 | 0.9729 | 0.1733 | 0.2041 | 0.395792 | 0.9398 | NaN | 0.0845 | 0.1179 | 0.473641 | 0.8967 | -0.0126 | 0.1098 | 0.908596 | 0.973 | 0.1716 | 0.2055 | 0.403635 | 0.9816 | NaN | 0.0849 | 0.1207 | 0.481749 | 0.8009 | -0.0148 | 0.1168 | 0.8994 | 0.9695 | 0.1657 | 0.2069 | 0.423329 | 0.9375 | NaN | 0.0779 | 0.1197 | 0.515508 | 0.8625 | -0.0232 | 0.1123 | 0.836227 | 0.9459 | 0.162 | 0.2079 | 0.435829 | 0.9359 | NaN | 0.0835 | 0.121 | 0.490319 | 0.8278 | -0.0323 | 0.1153 | 0.779395 | 0.9173 | 0.1793 | 0.2089 | 0.390608 | 0.8887 |
| biotin | 244.0928 | 4.970581 | Cofactors and Vitamins | Vitamin B7 metabolism | 0.0149 | 0.1326 | 0.910257 | 0.9809 | -0.0057 | 0.1341 | 0.966207 | 0.987 | 0.0559 | 0.224 | 0.803021 | 0.9678 | NaN | -0.0443 | 0.123 | 0.718881 | 0.9325 | -0.1133 | 0.1188 | 0.340111 | 0.8095 | 0.061 | 0.2101 | 0.771419 | 0.954 | NaN | -0.0238 | 0.1226 | 0.846163 | 0.9714 | -0.0473 | 0.1156 | 0.682165 | 0.9195 | 0.0195 | 0.2118 | 0.926747 | 0.9935 | NaN | 0.0063 | 0.1253 | 0.960151 | 0.9828 | -0.0753 | 0.1234 | 0.541642 | 0.7845 | 0.1422 | 0.214 | 0.506471 | 0.9375 | NaN | 0.0074 | 0.1242 | 0.95234 | 0.9796 | -0.0532 | 0.1181 | 0.652684 | 0.8623 | 0.0939 | 0.2141 | 0.660975 | 0.9621 | NaN | 0.0118 | 0.1256 | 0.924862 | 0.9775 | -0.0711 | 0.1213 | 0.557892 | 0.8092 | 0.1331 | 0.2161 | 0.537934 | 0.8971 |
| 5-methyltetrahydrofolate | 459.1865 | 3.632105 | Cofactors and Vitamins | Vitamin B9 Metabolism | -0.0618 | 0.1294 | 0.63299 | 0.8678 | -0.096 | 0.1426 | 0.500889 | 0.7575 | -0.0521 | 0.2022 | 0.796733 | 0.9647 | NaN | 0.0286 | 0.1207 | 0.812591 | 0.9614 | -0.0803 | 0.1252 | 0.52127 | 0.8967 | 0.1035 | 0.1936 | 0.592861 | 0.954 | NaN | -0.0181 | 0.1197 | 0.880121 | 0.9714 | -0.0363 | 0.1235 | 0.768762 | 0.9284 | -0.0165 | 0.1912 | 0.931402 | 0.9935 | NaN | 0.0219 | 0.1235 | 0.858976 | 0.9696 | -0.1035 | 0.1303 | 0.426971 | 0.7208 | 0.1155 | 0.198 | 0.559747 | 0.9375 | NaN | -0.0004 | 0.1218 | 0.997488 | 0.9991 | -0.0815 | 0.1254 | 0.516006 | 0.8496 | 0.0417 | 0.1952 | 0.830991 | 0.9621 | NaN | -0.0014 | 0.1233 | 0.991213 | 0.9956 | -0.1351 | 0.1282 | 0.292265 | 0.6559 | 0.0832 | 0.1989 | 0.675534 | 0.9459 |
| cis-aconitate | 174.0164 | 1.361663 | Energy | TCA Cycle | 0.1869 | 0.1366 | 0.171241 | 0.531 | 0.1194 | 0.1433 | 0.404923 | 0.6737 | 0.2535 | 0.2212 | 0.251726 | 0.7397 | NaN | 0.1751 | 0.1264 | 0.165681 | 0.7251 | 0.0406 | 0.127 | 0.749076 | 0.949 | 0.3069 | 0.207 | 0.138323 | 0.8611 | NaN | 0.1278 | 0.1268 | 0.313598 | 0.7952 | 0.034 | 0.1247 | 0.785398 | 0.935 | 0.2069 | 0.2096 | 0.323648 | 0.9479 | NaN | 0.1877 | 0.1291 | 0.145982 | 0.6151 | 0.114 | 0.131 | 0.384273 | 0.6816 | 0.2587 | 0.2101 | 0.218116 | 0.8705 | NaN | 0.1933 | 0.1279 | 0.130792 | 0.6708 | 0.0698 | 0.1266 | 0.581676 | 0.8623 | 0.3044 | 0.211 | 0.149067 | 0.8056 | NaN | 0.2218 | 0.1293 | 0.086263 | 0.5441 | 0.1298 | 0.1289 | 0.313845 | 0.6715 | 0.3097 | 0.2122 | 0.144469 | 0.7588 |
| citramalate | 148.0374 | 1.446943 | Energy | TCA Cycle | 0.1985 | 0.1389 | 0.1531 | 0.5192 | 0.1815 | 0.1404 | 0.196149 | 0.4993 | 0.2203 | 0.2326 | 0.34369 | 0.7534 | NaN | 0.1845 | 0.1285 | 0.151089 | 0.6956 | 0.1498 | 0.1235 | 0.225177 | 0.7475 | 0.2367 | 0.218 | 0.277502 | 0.9223 | NaN | 0.1816 | 0.1283 | 0.157111 | 0.6683 | 0.1914 | 0.1204 | 0.112009 | 0.6578 | 0.1843 | 0.2201 | 0.402511 | 0.9816 | NaN | 0.1932 | 0.1313 | 0.141297 | 0.6148 | 0.1622 | 0.1286 | 0.207225 | 0.5478 | 0.2446 | 0.2209 | 0.268214 | 0.8705 | NaN | 0.1868 | 0.1302 | 0.151317 | 0.6753 | 0.1622 | 0.1235 | 0.188956 | 0.6684 | 0.2229 | 0.222 | 0.315394 | 0.9106 | NaN | 0.1915 | 0.1316 | 0.145762 | 0.6152 | 0.136 | 0.1272 | 0.28513 | 0.6531 | 0.2644 | 0.2232 | 0.236068 | 0.8424 |
| trans-aconitate | 174.0161 | 1.145015 | Energy | TCA Cycle | 0.0794 | 0.1291 | 0.538806 | 0.825 | -0.0379 | 0.1263 | 0.764055 | 0.9167 | 0.2032 | 0.2229 | 0.361917 | 0.7534 | NaN | 0.1229 | 0.1194 | 0.303434 | 0.7864 | -0.0439 | 0.1108 | 0.691676 | 0.9312 | 0.312 | 0.2095 | 0.136298 | 0.8611 | NaN | 0.068 | 0.1193 | 0.568285 | 0.9125 | -0.0329 | 0.1088 | 0.762018 | 0.9284 | 0.1718 | 0.2108 | 0.41497 | 0.9816 | NaN | 0.1019 | 0.1221 | 0.403794 | 0.7795 | -0.0427 | 0.1155 | 0.711523 | 0.8729 | 0.26 | 0.2118 | 0.219751 | 0.8705 | NaN | 0.1535 | 0.1214 | 0.206114 | 0.6855 | 0.0077 | 0.1114 | 0.945231 | 0.9923 | 0.3087 | 0.2138 | 0.148846 | 0.8056 | NaN | 0.1324 | 0.1226 | 0.28014 | 0.7337 | -0.0359 | 0.1138 | 0.752618 | 0.9096 | 0.32 | 0.2155 | 0.137534 | 0.7588 |
| citrate | 192.0271 | 0.984674 | Energy | TCA Cycle | 0.1572 | 0.1371 | 0.251803 | 0.6204 | -0.1261 | 0.1429 | 0.37785 | 0.6477 | 0.3891 | 0.2206 | 0.077768 | 0.4717 | NaN | 0.1675 | 0.1267 | 0.186245 | 0.7251 | -0.1378 | 0.1252 | 0.271084 | 0.7967 | 0.423 | 0.2061 | 0.040101 | 0.5676 | NaN | 0.1165 | 0.127 | 0.358737 | 0.8251 | -0.1057 | 0.1232 | 0.390873 | 0.8818 | 0.3009 | 0.2109 | 0.153583 | 0.7677 | NaN | 0.1806 | 0.1295 | 0.163331 | 0.6495 | -0.117 | 0.1307 | 0.371007 | 0.6762 | 0.4267 | 0.209 | 0.041167 | 0.5138 | NaN | 0.2014 | 0.1284 | 0.116764 | 0.6708 | -0.0752 | 0.1263 | 0.551776 | 0.8618 | 0.4276 | 0.21 | 0.041703 | 0.4772 | NaN | 0.2082 | 0.1299 | 0.109084 | 0.554 | -0.1062 | 0.1289 | 0.409759 | 0.725 | 0.4727 | 0.2114 | 0.025323 | 0.4368 |
| isocitrate | 192.0271 | 0.942504 | Energy | TCA Cycle | -0.1248 | 0.1325 | 0.34633 | 0.7081 | -0.064 | 0.149 | 0.667405 | 0.8568 | -0.1447 | 0.2053 | 0.480732 | 0.8319 | NaN | -0.0871 | 0.1229 | 0.478212 | 0.8571 | -0.1038 | 0.1307 | 0.427123 | 0.847 | -0.0533 | 0.1944 | 0.784011 | 0.9554 | NaN | -0.0662 | 0.123 | 0.590156 | 0.9125 | -0.0131 | 0.1287 | 0.919258 | 0.973 | -0.1004 | 0.1944 | 0.605629 | 0.9894 | NaN | -0.1028 | 0.1255 | 0.412513 | 0.7798 | -0.1161 | 0.1364 | 0.394658 | 0.689 | -0.0623 | 0.197 | 0.751947 | 0.9586 | NaN | -0.0767 | 0.1247 | 0.538264 | 0.8632 | -0.0958 | 0.1309 | 0.464408 | 0.8272 | -0.0517 | 0.1986 | 0.794706 | 0.9621 | NaN | -0.0898 | 0.1259 | 0.475792 | 0.8278 | -0.1048 | 0.1342 | 0.434969 | 0.7458 | -0.0591 | 0.1994 | 0.76687 | 0.9525 |
| malate | 134.0217 | 0.867725 | Energy | TCA Cycle | 0.0512 | 0.1336 | 0.701772 | 0.9136 | 0.0706 | 0.1274 | 0.579603 | 0.8019 | 0.039 | 0.2379 | 0.869863 | 0.974 | NaN | 0.0544 | 0.1235 | 0.659556 | 0.9185 | 0.0271 | 0.1122 | 0.808967 | 0.965 | 0.1118 | 0.2236 | 0.617153 | 0.954 | NaN | 0.0399 | 0.1234 | 0.746172 | 0.96 | 0.0772 | 0.1096 | 0.481086 | 0.9053 | -0.0015 | 0.2249 | 0.994662 | 0.9976 | NaN | 0.0191 | 0.1265 | 0.879967 | 0.9749 | 0.0023 | 0.1178 | 0.984335 | 0.9926 | 0.0679 | 0.2262 | 0.763981 | 0.9594 | NaN | 0.0637 | 0.1252 | 0.610937 | 0.8964 | 0.0588 | 0.112 | 0.599696 | 0.8623 | 0.0805 | 0.2274 | 0.723352 | 0.9621 | NaN | 0.0372 | 0.1266 | 0.7692 | 0.9344 | -0.008 | 0.1161 | 0.944959 | 0.9823 | 0.1122 | 0.2292 | 0.62439 | 0.9459 |
| succinate | 118.027 | 1.295398 | Energy | TCA Cycle | -0.0024 | 0.1311 | 0.985263 | 0.9936 | 0.2989 | 0.2168 | 0.168109 | 0.4833 | -0.0581 | 0.1737 | 0.737933 | 0.9647 | NaN | -0.0158 | 0.1213 | 0.896148 | 0.9705 | 0.25 | 0.1907 | 0.189858 | 0.7154 | -0.059 | 0.1629 | 0.717189 | 0.954 | NaN | -0.0076 | 0.1211 | 0.950074 | 0.9728 | 0.3164 | 0.1859 | 0.088701 | 0.6214 | -0.0699 | 0.164 | 0.669932 | 0.9894 | NaN | -0.0293 | 0.1241 | 0.813362 | 0.9445 | 0.2298 | 0.1996 | 0.249528 | 0.5831 | -0.0677 | 0.1651 | 0.681797 | 0.9476 | NaN | -0.0292 | 0.123 | 0.812025 | 0.952 | 0.2775 | 0.1905 | 0.14529 | 0.631 | -0.0841 | 0.166 | 0.612501 | 0.9621 | NaN | -0.0298 | 0.1243 | 0.810732 | 0.9477 | 0.1922 | 0.1977 | 0.330868 | 0.6739 | -0.0614 | 0.1667 | 0.712818 | 0.9459 |
| hippurate | 179.0586 | 4.79845 | Exogenous | Benzoate Metabolism | -0.0651 | 0.1322 | 0.62256 | 0.8678 | -0.0761 | 0.1326 | 0.56615 | 0.7994 | -0.0296 | 0.2242 | 0.895097 | 0.9826 | NaN | -0.0196 | 0.1226 | 0.873073 | 0.9705 | 0.0315 | 0.1182 | 0.789952 | 0.9616 | -0.0688 | 0.2105 | 0.743869 | 0.954 | NaN | -0.0086 | 0.1225 | 0.943791 | 0.9728 | 0.0097 | 0.1153 | 0.933149 | 0.9756 | -0.0271 | 0.2117 | 0.898157 | 0.9935 | NaN | -0.0276 | 0.1253 | 0.825907 | 0.9538 | 0.0136 | 0.1232 | 0.912383 | 0.9712 | -0.0596 | 0.2133 | 0.77992 | 0.961 | NaN | -0.0351 | 0.1241 | 0.776982 | 0.938 | 0.033 | 0.1185 | 0.780602 | 0.9247 | -0.0872 | 0.2147 | 0.684608 | 0.9621 | NaN | -0.0197 | 0.1257 | 0.875741 | 0.9588 | 0.0101 | 0.121 | 0.933732 | 0.9823 | -0.0297 | 0.2152 | 0.890164 | 0.9702 |
| benzoin | 212.1031 | 6.033384 | Exogenous | Drug | 0.1709 | 0.1308 | 0.191411 | 0.5541 | 0.1703 | 0.1387 | 0.219768 | 0.5107 | 0.1706 | 0.211 | 0.418609 | 0.7762 | NaN | 0.1617 | 0.1209 | 0.181098 | 0.7251 | 0.0927 | 0.1233 | 0.451788 | 0.8559 | 0.2177 | 0.1977 | 0.270907 | 0.9223 | NaN | 0.0819 | 0.1221 | 0.502159 | 0.9053 | 0.0469 | 0.1223 | 0.701171 | 0.9195 | 0.0974 | 0.2007 | 0.62749 | 0.9894 | NaN | 0.172 | 0.1236 | 0.163969 | 0.6495 | 0.0665 | 0.1301 | 0.609189 | 0.8188 | 0.2721 | 0.2015 | 0.176831 | 0.8705 | NaN | 0.1808 | 0.1224 | 0.139656 | 0.6708 | 0.1144 | 0.1229 | 0.351952 | 0.7839 | 0.2265 | 0.2016 | 0.26111 | 0.9039 | NaN | 0.1832 | 0.1238 | 0.138953 | 0.605 | 0.0678 | 0.1278 | 0.595667 | 0.82 | 0.2785 | 0.204 | 0.172316 | 0.8194 |
| guaifenesin | 198.0869 | 3.703858 | Exogenous | Drug | 0.1183 | 0.1221 | 0.332683 | 0.6942 | 0.1862 | 0.1395 | 0.182078 | 0.4964 | 0.0852 | 0.1863 | 0.647366 | 0.911 | NaN | 0.0835 | 0.1132 | 0.460701 | 0.8498 | 0.0734 | 0.1253 | 0.557926 | 0.9009 | 0.0986 | 0.1747 | 0.572273 | 0.954 | NaN | 0.0601 | 0.1134 | 0.595931 | 0.9125 | 0.0793 | 0.1225 | 0.517706 | 0.9053 | 0.0435 | 0.1764 | 0.805077 | 0.9935 | NaN | 0.1145 | 0.1155 | 0.321261 | 0.741 | 0.0789 | 0.1312 | 0.547438 | 0.7845 | 0.158 | 0.1778 | 0.374197 | 0.926 | NaN | 0.0863 | 0.1147 | 0.451642 | 0.8543 | 0.1053 | 0.1244 | 0.396993 | 0.8162 | 0.0754 | 0.1779 | 0.671547 | 0.9621 | NaN | 0.1083 | 0.1158 | 0.34927 | 0.7531 | 0.0671 | 0.1294 | 0.604082 | 0.8254 | 0.1414 | 0.1793 | 0.430259 | 0.8887 |
| chlorpheniramine | 274.1192 | 13.793018 | Exogenous | Drug | 0.2231 | 0.1307 | 0.087896 | 0.4294 | 0.2956 | 0.1498 | 0.048388 | 0.2996 | 0.1726 | 0.1983 | 0.384082 | 0.7534 | NaN | 0.1439 | 0.1221 | 0.238567 | 0.7495 | 0.1437 | 0.1367 | 0.293164 | 0.8051 | 0.1427 | 0.1863 | 0.443637 | 0.9478 | NaN | 0.1067 | 0.123 | 0.386018 | 0.8422 | 0.1982 | 0.1312 | 0.13093 | 0.6741 | 0.0418 | 0.1915 | 0.827121 | 0.9935 | NaN | 0.182 | 0.1241 | 0.142557 | 0.6148 | 0.163 | 0.1427 | 0.253465 | 0.5879 | 0.1971 | 0.1883 | 0.295301 | 0.8823 | NaN | 0.1534 | 0.1237 | 0.21468 | 0.689 | 0.1521 | 0.1365 | 0.265468 | 0.7359 | 0.1461 | 0.1896 | 0.44112 | 0.9359 | NaN | 0.1809 | 0.1244 | 0.145995 | 0.6152 | 0.1356 | 0.1418 | 0.339121 | 0.6758 | 0.2036 | 0.1902 | 0.284498 | 0.8424 |
| ibuprofen carboxylic acid | 236.1035 | 9.971766 | Exogenous | Drug | 0.182 | 0.1325 | 0.16963 | 0.531 | 0.2832 | 0.1494 | 0.058085 | 0.3054 | 0.1161 | 0.2031 | 0.567503 | 0.8726 | NaN | 0.0997 | 0.1237 | 0.420338 | 0.8498 | 0.139 | 0.1359 | 0.306463 | 0.8095 | 0.0723 | 0.191 | 0.705258 | 0.954 | NaN | 0.0761 | 0.1241 | 0.539862 | 0.9125 | 0.152 | 0.1324 | 0.250969 | 0.8037 | 0.0183 | 0.194 | 0.9248 | 0.9935 | NaN | 0.1328 | 0.1259 | 0.291536 | 0.7388 | 0.1581 | 0.1418 | 0.2648 | 0.5966 | 0.1172 | 0.1931 | 0.543968 | 0.9375 | NaN | 0.0949 | 0.1257 | 0.450207 | 0.8543 | 0.1312 | 0.1367 | 0.337109 | 0.7819 | 0.0642 | 0.1948 | 0.741617 | 0.9621 | NaN | 0.1305 | 0.1262 | 0.301169 | 0.7481 | 0.129 | 0.141 | 0.360459 | 0.6888 | 0.1254 | 0.1949 | 0.51995 | 0.8946 |
| salicyluric acid | 195.054 | 2.946303 | Exogenous | Drug | 0.0753 | 0.1369 | 0.582088 | 0.8423 | -0.1482 | 0.1479 | 0.316313 | 0.6107 | 0.2451 | 0.2149 | 0.254071 | 0.7397 | NaN | 0.0609 | 0.1266 | 0.630473 | 0.9079 | -0.1519 | 0.1296 | 0.241058 | 0.7677 | 0.214 | 0.2019 | 0.289044 | 0.9223 | NaN | 0.0821 | 0.1263 | 0.515829 | 0.9068 | -0.1321 | 0.1274 | 0.299845 | 0.8336 | 0.2342 | 0.2029 | 0.248439 | 0.9 | NaN | 0.0965 | 0.1294 | 0.455736 | 0.7844 | -0.107 | 0.1359 | 0.430915 | 0.723 | 0.241 | 0.2042 | 0.237898 | 0.8705 | NaN | 0.0558 | 0.1283 | 0.663977 | 0.9055 | -0.1685 | 0.1297 | 0.193748 | 0.6684 | 0.2203 | 0.2055 | 0.283602 | 0.9039 | NaN | 0.0999 | 0.1297 | 0.441098 | 0.801 | -0.1232 | 0.1334 | 0.355787 | 0.6867 | 0.264 | 0.206 | 0.20001 | 0.8424 |
| tricarballylic acid | 176.0311 | 1.087867 | Exogenous | Food Component/Plant | -0.1164 | 0.1328 | 0.38072 | 0.7222 | -0.0911 | 0.1546 | 0.55575 | 0.7957 | -0.1149 | 0.2008 | 0.567232 | 0.8726 | NaN | -0.1871 | 0.1229 | 0.127889 | 0.6772 | -0.173 | 0.1356 | 0.201946 | 0.7286 | -0.1787 | 0.1886 | 0.343323 | 0.9223 | NaN | -0.1195 | 0.1226 | 0.329699 | 0.8017 | -0.1575 | 0.1329 | 0.235914 | 0.8003 | -0.0868 | 0.1899 | 0.647487 | 0.9894 | NaN | -0.1441 | 0.1255 | 0.250931 | 0.714 | -0.1496 | 0.1415 | 0.290375 | 0.6165 | -0.1144 | 0.1909 | 0.54881 | 0.9375 | NaN | -0.1458 | 0.1244 | 0.241129 | 0.7156 | -0.0701 | 0.1361 | 0.606343 | 0.8623 | -0.1758 | 0.1922 | 0.360261 | 0.9106 | NaN | -0.1439 | 0.1258 | 0.252597 | 0.7187 | -0.1281 | 0.1391 | 0.357258 | 0.6871 | -0.1328 | 0.1927 | 0.490576 | 0.8887 |
| 2-acetyl-pyrrolidine | 113.0845 | 4.492652 | Exogenous | Food Component/Plant | -0.0134 | 0.1275 | 0.916399 | 0.9809 | 0.0593 | 0.1772 | 0.737843 | 0.9065 | -0.0347 | 0.1787 | 0.845961 | 0.9732 | NaN | -0.0157 | 0.1179 | 0.893969 | 0.9705 | 0.174 | 0.156 | 0.264609 | 0.7853 | -0.0758 | 0.1678 | 0.651382 | 0.954 | NaN | -0.007 | 0.1178 | 0.95228 | 0.9728 | 0.0937 | 0.1525 | 0.538755 | 0.9053 | -0.0292 | 0.1688 | 0.86287 | 0.9935 | NaN | 0.001 | 0.1206 | 0.993611 | 0.9985 | 0.1479 | 0.1627 | 0.363302 | 0.6762 | -0.0374 | 0.1699 | 0.825946 | 0.9721 | NaN | -0.0037 | 0.1195 | 0.974987 | 0.9861 | 0.1953 | 0.1566 | 0.212486 | 0.6963 | -0.0602 | 0.1708 | 0.724457 | 0.9621 | NaN | -0.0185 | 0.1208 | 0.878617 | 0.9588 | 0.1328 | 0.1598 | 0.406247 | 0.7211 | -0.0579 | 0.1716 | 0.735764 | 0.9467 |
| 2-piperidinone | 99.0691 | 2.676115 | Exogenous | Food Component/Plant | 0.1299 | 0.1335 | 0.330548 | 0.6942 | 0.1251 | 0.1278 | 0.327602 | 0.6183 | 0.1508 | 0.2364 | 0.523489 | 0.8655 | NaN | 0.1585 | 0.1233 | 0.198799 | 0.7316 | 0.0709 | 0.1129 | 0.530077 | 0.8967 | 0.3034 | 0.2235 | 0.174562 | 0.879 | NaN | 0.1778 | 0.1232 | 0.14898 | 0.6683 | 0.1231 | 0.1099 | 0.262735 | 0.8057 | 0.2528 | 0.224 | 0.259122 | 0.9 | NaN | 0.1641 | 0.1262 | 0.193319 | 0.6616 | 0.0979 | 0.1172 | 0.403392 | 0.6937 | 0.2867 | 0.2267 | 0.205893 | 0.8705 | NaN | 0.1216 | 0.1251 | 0.330904 | 0.7669 | 0.0536 | 0.1136 | 0.636992 | 0.8623 | 0.2175 | 0.2261 | 0.336082 | 0.9106 | NaN | 0.1434 | 0.1264 | 0.256721 | 0.7205 | 0.0813 | 0.1158 | 0.482545 | 0.7743 | 0.2423 | 0.2279 | 0.287721 | 0.8424 |
| 5-aminolevulinate | 131.0586 | 0.616781 | Exogenous | Food Component/Plant | 0.1037 | 0.1321 | 0.432432 | 0.7622 | 0.0657 | 0.1297 | 0.612811 | 0.8251 | 0.1487 | 0.2281 | 0.514635 | 0.8635 | NaN | 0.1498 | 0.1221 | 0.220056 | 0.7495 | 0.108 | 0.1138 | 0.34252 | 0.8095 | 0.2079 | 0.214 | 0.331201 | 0.9223 | NaN | 0.0855 | 0.122 | 0.483506 | 0.8967 | 0.0684 | 0.1117 | 0.540147 | 0.9053 | 0.1149 | 0.2158 | 0.594307 | 0.9894 | NaN | 0.1377 | 0.1249 | 0.270251 | 0.7313 | 0.1008 | 0.1187 | 0.395683 | 0.689 | 0.1932 | 0.2169 | 0.373022 | 0.926 | NaN | 0.1656 | 0.1239 | 0.181583 | 0.6753 | 0.1347 | 0.1141 | 0.237868 | 0.7254 | 0.2104 | 0.2181 | 0.334698 | 0.9106 | NaN | 0.15 | 0.1252 | 0.231084 | 0.697 | 0.1112 | 0.1169 | 0.341503 | 0.6781 | 0.2078 | 0.2192 | 0.343184 | 0.8785 |
| 5-hydroxy-1,4-naphthoquinone | 174.0272 | 4.803483 | Exogenous | Food Component/Plant | -0.1778 | 0.1299 | 0.171042 | 0.531 | 0.211 | 0.1594 | 0.185621 | 0.4974 | -0.3742 | 0.1885 | 0.047084 | 0.3661 | NaN | -0.2334 | 0.1199 | 0.051587 | 0.4443 | 0.0735 | 0.1435 | 0.608473 | 0.9043 | -0.3671 | 0.1765 | 0.037505 | 0.5448 | NaN | -0.2341 | 0.1197 | 0.050485 | 0.3667 | 0.1962 | 0.1371 | 0.152455 | 0.7183 | -0.4428 | 0.177 | 0.01236 | 0.234 | NaN | -0.2197 | 0.1227 | 0.073258 | 0.4957 | 0.0051 | 0.1555 | 0.97394 | 0.9926 | -0.304 | 0.1814 | 0.0937 | 0.7393 | NaN | -0.2385 | 0.1216 | 0.049897 | 0.4313 | 0.0696 | 0.1439 | 0.628963 | 0.8623 | -0.3817 | 0.1795 | 0.033461 | 0.4772 | NaN | -0.2356 | 0.123 | 0.055572 | 0.4446 | -0.0259 | 0.1541 | 0.866602 | 0.9586 | -0.3282 | 0.1821 | 0.071461 | 0.6024 |
| methyl-jasmonate | 224.141 | 16.080898 | Exogenous | Food Component/Plants | -0.0714 | 0.1299 | 0.582762 | 0.8423 | -0.0301 | 0.1346 | 0.82296 | 0.932 | -0.0673 | 0.2171 | 0.756401 | 0.9647 | NaN | -0.1009 | 0.1201 | 0.40099 | 0.8498 | -0.0613 | 0.1181 | 0.603877 | 0.9043 | -0.1121 | 0.2038 | 0.582116 | 0.954 | NaN | -0.0865 | 0.1199 | 0.470566 | 0.8967 | 0.0024 | 0.1161 | 0.983558 | 0.9907 | -0.173 | 0.2064 | 0.401844 | 0.9816 | NaN | -0.1499 | 0.1235 | 0.224631 | 0.7062 | -0.1549 | 0.1252 | 0.216052 | 0.5546 | -0.1031 | 0.2065 | 0.617678 | 0.9375 | NaN | -0.0814 | 0.1217 | 0.50345 | 0.8625 | -0.0671 | 0.1184 | 0.570683 | 0.8623 | -0.0682 | 0.2073 | 0.742044 | 0.9621 | NaN | -0.1246 | 0.1234 | 0.312346 | 0.7485 | -0.1495 | 0.1228 | 0.223433 | 0.5901 | -0.0697 | 0.2083 | 0.737955 | 0.9473 |
| 1,3,7-trimethyluric acid | 210.0867 | 5.631745 | Exogenous | Xanthine Metabolism | 0.1626 | 0.1261 | 0.197296 | 0.5585 | 0.1685 | 0.1459 | 0.248061 | 0.5391 | 0.1401 | 0.1917 | 0.4647 | 0.8207 | NaN | 0.1231 | 0.117 | 0.29256 | 0.7802 | 0.1219 | 0.1286 | 0.343168 | 0.8095 | 0.1048 | 0.1802 | 0.560668 | 0.954 | NaN | 0.1096 | 0.117 | 0.349108 | 0.8224 | 0.1393 | 0.1258 | 0.268365 | 0.806 | 0.0814 | 0.182 | 0.654903 | 0.9894 | NaN | 0.1089 | 0.12 | 0.364138 | 0.7543 | 0.135 | 0.1338 | 0.313071 | 0.6401 | 0.0595 | 0.1842 | 0.746467 | 0.9572 | NaN | 0.116 | 0.1187 | 0.328509 | 0.7669 | 0.1323 | 0.1286 | 0.303762 | 0.7544 | 0.0881 | 0.184 | 0.632194 | 0.9621 | NaN | 0.1127 | 0.1202 | 0.348102 | 0.7531 | 0.1156 | 0.1323 | 0.382269 | 0.6983 | 0.0855 | 0.1851 | 0.64406 | 0.9459 |
| 7-methylxanthine | 166.0541 | 2.619145 | Exogenous | Xanthine Metabolism | 0.0456 | 0.1322 | 0.730044 | 0.9287 | -0.0168 | 0.1446 | 0.907518 | 0.9578 | 0.0857 | 0.2075 | 0.679522 | 0.9354 | NaN | 0.0444 | 0.1223 | 0.716335 | 0.9325 | -0.0203 | 0.1269 | 0.873017 | 0.9729 | 0.0933 | 0.1946 | 0.631391 | 0.954 | NaN | 0.0461 | 0.1221 | 0.705841 | 0.9481 | -0.0414 | 0.1245 | 0.739714 | 0.9241 | 0.1156 | 0.1959 | 0.555267 | 0.9894 | NaN | 0.0592 | 0.125 | 0.635812 | 0.8611 | -0.0575 | 0.1324 | 0.66388 | 0.8438 | 0.1577 | 0.1979 | 0.42563 | 0.9375 | NaN | 0.0444 | 0.1239 | 0.720031 | 0.9229 | -0.0254 | 0.1271 | 0.841443 | 0.946 | 0.0955 | 0.1981 | 0.629873 | 0.9621 | NaN | 0.0414 | 0.1253 | 0.741325 | 0.9216 | -0.0443 | 0.1303 | 0.734 | 0.8984 | 0.105 | 0.1991 | 0.59783 | 0.9357 |
| caffeine | 194.081 | 5.866517 | Exogenous | Xanthine Metabolism | 0.1409 | 0.1382 | 0.307804 | 0.6742 | 0.2156 | 0.1437 | 0.133427 | 0.4282 | 0.0937 | 0.2246 | 0.676628 | 0.935 | NaN | 0.0708 | 0.1286 | 0.582047 | 0.9079 | 0.1455 | 0.1274 | 0.253448 | 0.7821 | 0.0149 | 0.2118 | 0.943852 | 0.9911 | NaN | 0.0937 | 0.128 | 0.463966 | 0.8953 | 0.1552 | 0.1246 | 0.213086 | 0.7942 | 0.041 | 0.2127 | 0.846984 | 0.9935 | NaN | 0.1246 | 0.1307 | 0.340437 | 0.741 | 0.1937 | 0.1315 | 0.140823 | 0.4798 | 0.0774 | 0.2136 | 0.717174 | 0.9477 | NaN | 0.0767 | 0.1303 | 0.555961 | 0.872 | 0.1203 | 0.1286 | 0.349339 | 0.7839 | 0.0485 | 0.215 | 0.821494 | 0.9621 | NaN | 0.1196 | 0.131 | 0.361476 | 0.7576 | 0.171 | 0.1301 | 0.18877 | 0.5692 | 0.087 | 0.2156 | 0.686485 | 0.9459 |
| paraxanthine | 180.0652 | 4.203445 | Exogenous | Xanthine Metabolism | 0.112 | 0.1254 | 0.372171 | 0.7183 | 0.2392 | 0.1221 | 0.050045 | 0.2996 | -0.0157 | 0.2171 | 0.942485 | 0.9887 | NaN | 0.0465 | 0.1167 | 0.690323 | 0.9297 | 0.176 | 0.1085 | 0.104699 | 0.6118 | -0.1004 | 0.2046 | 0.623426 | 0.954 | NaN | 0.0675 | 0.1162 | 0.561604 | 0.9125 | 0.1772 | 0.1063 | 0.095451 | 0.6274 | -0.0616 | 0.2053 | 0.76403 | 0.9935 | NaN | 0.1146 | 0.1186 | 0.333847 | 0.741 | 0.2369 | 0.1113 | 0.033247 | 0.2362 | -0.0252 | 0.2064 | 0.902852 | 0.99 | NaN | 0.0722 | 0.1179 | 0.540112 | 0.8632 | 0.203 | 0.1077 | 0.059455 | 0.4149 | -0.0744 | 0.208 | 0.720582 | 0.9621 | NaN | 0.1032 | 0.1189 | 0.385244 | 0.7698 | 0.2299 | 0.1097 | 0.036091 | 0.2621 | -0.041 | 0.2085 | 0.844272 | 0.9641 |
| theobromine | 180.065 | 3.297352 | Exogenous | Xanthine Metabolism | -0.2368 | 0.1351 | 0.079733 | 0.4001 | -0.1435 | 0.1517 | 0.344037 | 0.6309 | -0.2832 | 0.2101 | 0.177826 | 0.6772 | NaN | -0.118 | 0.1274 | 0.354482 | 0.8434 | -0.0172 | 0.1359 | 0.899286 | 0.9729 | -0.1796 | 0.2 | 0.369234 | 0.9312 | NaN | -0.1141 | 0.1273 | 0.369927 | 0.8283 | 0.0128 | 0.1341 | 0.924117 | 0.973 | -0.2044 | 0.2004 | 0.307753 | 0.9479 | NaN | -0.1487 | 0.1296 | 0.251302 | 0.714 | -0.0703 | 0.1402 | 0.61633 | 0.8228 | -0.1847 | 0.203 | 0.362815 | 0.9223 | NaN | -0.1354 | 0.1288 | 0.29294 | 0.7524 | -0.0084 | 0.1365 | 0.950803 | 0.9923 | -0.213 | 0.2026 | 0.292947 | 0.9039 | NaN | -0.1466 | 0.1301 | 0.259817 | 0.7205 | -0.0513 | 0.1386 | 0.711182 | 0.8887 | -0.1985 | 0.2046 | 0.331884 | 0.8727 |
| theophylline | 180.0652 | 4.276442 | Exogenous | Xanthine Metabolism | 0.0519 | 0.1269 | 0.682395 | 0.9021 | 0.1736 | 0.12 | 0.147956 | 0.4588 | -0.0818 | 0.227 | 0.718761 | 0.9594 | NaN | 0.0583 | 0.1174 | 0.619056 | 0.9079 | 0.1616 | 0.1052 | 0.124364 | 0.6118 | -0.0628 | 0.213 | 0.768228 | 0.954 | NaN | 0.0606 | 0.1172 | 0.605155 | 0.9125 | 0.1814 | 0.1028 | 0.077701 | 0.5751 | -0.0952 | 0.2143 | 0.657021 | 0.9894 | NaN | 0.0889 | 0.1201 | 0.45899 | 0.7844 | 0.1666 | 0.1096 | 0.128549 | 0.4699 | 0.0116 | 0.2177 | 0.957559 | 0.99 | NaN | 0.0581 | 0.1189 | 0.625336 | 0.8971 | 0.1829 | 0.105 | 0.08167 | 0.4705 | -0.0915 | 0.2167 | 0.672757 | 0.9621 | NaN | 0.0849 | 0.1204 | 0.480368 | 0.8278 | 0.1691 | 0.1079 | 0.116947 | 0.4747 | -0.0103 | 0.2192 | 0.962364 | 0.9892 |
| quinolin-2-ol | 145.053 | 7.731086 | Exogenous | Bacteria Metabolism | 0.1709 | 0.1159 | 0.140246 | 0.5159 | 0.1688 | 0.1314 | 0.199001 | 0.4993 | 0.1646 | 0.1772 | 0.353092 | 0.7534 | NaN | 0.129 | 0.1076 | 0.230438 | 0.7495 | 0.0917 | 0.1169 | 0.43257 | 0.8528 | 0.1511 | 0.1663 | 0.363513 | 0.9312 | NaN | 0.0829 | 0.1085 | 0.444835 | 0.8801 | 0.1089 | 0.1141 | 0.3398 | 0.8587 | 0.0624 | 0.1704 | 0.71435 | 0.99 | NaN | 0.1393 | 0.1099 | 0.205029 | 0.6859 | 0.0718 | 0.1233 | 0.560157 | 0.789 | 0.1849 | 0.1683 | 0.271909 | 0.8705 | NaN | 0.1426 | 0.1089 | 0.190196 | 0.6753 | 0.0798 | 0.1176 | 0.497189 | 0.8419 | 0.1773 | 0.1691 | 0.29428 | 0.9039 | NaN | 0.1447 | 0.1101 | 0.188452 | 0.6463 | 0.0562 | 0.1218 | 0.644399 | 0.8613 | 0.1981 | 0.17 | 0.244048 | 0.8424 |
| honaucin A | 188.0495 | 0.965569 | Exogenous | Bacteria Metabolite | 0.1501 | 0.1334 | 0.260304 | 0.6341 | 0.0271 | 0.1187 | 0.819187 | 0.932 | 0.3746 | 0.2636 | 0.155315 | 0.6351 | NaN | 0.1638 | 0.1232 | 0.183796 | 0.7251 | 0.0555 | 0.1042 | 0.594133 | 0.904 | 0.3688 | 0.247 | 0.135427 | 0.8611 | NaN | 0.1988 | 0.123 | 0.106158 | 0.5635 | 0.0908 | 0.1024 | 0.375504 | 0.8818 | 0.4051 | 0.2483 | 0.102869 | 0.6251 | NaN | 0.1422 | 0.1261 | 0.259558 | 0.7164 | 0.0269 | 0.1085 | 0.804251 | 0.9172 | 0.3679 | 0.2504 | 0.141854 | 0.8157 | NaN | 0.1882 | 0.1249 | 0.131865 | 0.6708 | 0.0651 | 0.1044 | 0.533059 | 0.8528 | 0.4232 | 0.2512 | 0.09206 | 0.6515 | NaN | 0.1475 | 0.1263 | 0.243075 | 0.7034 | 0.0258 | 0.1069 | 0.808973 | 0.9294 | 0.3843 | 0.2527 | 0.128255 | 0.7588 |
| trimethylamine | 59.074 | 0.696045 | Exogenous | Bacteria Metabolite | -0.0047 | 0.1367 | 0.972752 | 0.9936 | -0.2139 | 0.1801 | 0.23505 | 0.5274 | 0.108 | 0.1952 | 0.58029 | 0.8849 | NaN | 0.0359 | 0.1266 | 0.77679 | 0.955 | -0.1683 | 0.1585 | 0.288259 | 0.7996 | 0.1357 | 0.183 | 0.458622 | 0.9478 | NaN | -0.0188 | 0.1262 | 0.881376 | 0.9714 | -0.2237 | 0.1546 | 0.147981 | 0.7153 | 0.0629 | 0.1849 | 0.733653 | 0.9927 | NaN | 0.0186 | 0.1293 | 0.885903 | 0.9771 | -0.1917 | 0.1648 | 0.245 | 0.5817 | 0.1294 | 0.1855 | 0.485404 | 0.9375 | NaN | 0.0257 | 0.1282 | 0.841398 | 0.9611 | -0.1536 | 0.1592 | 0.334578 | 0.7793 | 0.1147 | 0.1864 | 0.53821 | 0.9621 | NaN | 0.0379 | 0.1298 | 0.770195 | 0.9344 | -0.1533 | 0.1632 | 0.347405 | 0.6824 | 0.1384 | 0.1874 | 0.460064 | 0.8887 |
| N-cyclohexylformamide | 127.099 | 7.931769 | Exogenous | Bacteria Metabolism | 0.1206 | 0.1371 | 0.379284 | 0.7219 | 0.031 | 0.1503 | 0.836809 | 0.932 | 0.1941 | 0.215 | 0.366569 | 0.7534 | NaN | 0.1089 | 0.1268 | 0.390358 | 0.8498 | 0.0175 | 0.132 | 0.894748 | 0.9729 | 0.1894 | 0.2015 | 0.347278 | 0.9223 | NaN | 0.1251 | 0.1265 | 0.322886 | 0.8008 | 0.0422 | 0.1294 | 0.744175 | 0.9241 | 0.1951 | 0.2029 | 0.336223 | 0.957 | NaN | 0.0922 | 0.1298 | 0.477459 | 0.7987 | -0.0436 | 0.1385 | 0.75293 | 0.8953 | 0.2157 | 0.2041 | 0.290678 | 0.8768 | NaN | 0.1271 | 0.1284 | 0.322183 | 0.7669 | 0.0331 | 0.1322 | 0.801958 | 0.9326 | 0.2077 | 0.2051 | 0.311147 | 0.9106 | NaN | 0.0884 | 0.1302 | 0.496904 | 0.8285 | -0.0344 | 0.1361 | 0.800674 | 0.9273 | 0.1931 | 0.2062 | 0.349147 | 0.8785 |
| phenylephrine | 167.0945 | 0.944446 | Exogenous | Drug | 0.1268 | 0.1362 | 0.3521 | 0.7161 | -0.0071 | 0.1551 | 0.963643 | 0.987 | 0.214 | 0.2128 | 0.314708 | 0.7534 | NaN | 0.1393 | 0.1259 | 0.268359 | 0.7625 | 0.0523 | 0.1364 | 0.701257 | 0.9328 | 0.1679 | 0.2003 | 0.401749 | 0.94 | NaN | 0.1315 | 0.1257 | 0.295342 | 0.7865 | 0.0103 | 0.1336 | 0.938315 | 0.9765 | 0.19 | 0.2012 | 0.345005 | 0.957 | NaN | 0.1757 | 0.1288 | 0.172655 | 0.6514 | 0.0083 | 0.1419 | 0.953066 | 0.987 | 0.268 | 0.2022 | 0.185111 | 0.8705 | NaN | 0.1595 | 0.1276 | 0.211114 | 0.6855 | 0.0675 | 0.1369 | 0.621905 | 0.8623 | 0.2034 | 0.2033 | 0.31702 | 0.9106 | NaN | 0.1652 | 0.1291 | 0.200375 | 0.6623 | 0.0041 | 0.1397 | 0.976552 | 0.9946 | 0.2513 | 0.2041 | 0.218244 | 0.8424 |
| debrisoquin | 175.1106 | 3.15226 | Exogenous | Drug | 0.2135 | 0.1333 | 0.109172 | 0.4745 | 0.2627 | 0.1479 | 0.075785 | 0.357 | 0.1832 | 0.2068 | 0.375701 | 0.7534 | NaN | 0.1812 | 0.1235 | 0.142413 | 0.6828 | 0.1559 | 0.1326 | 0.239795 | 0.7677 | 0.2035 | 0.1937 | 0.293368 | 0.9223 | NaN | 0.1252 | 0.1245 | 0.314707 | 0.7952 | 0.1933 | 0.1286 | 0.132671 | 0.6741 | 0.0688 | 0.1985 | 0.728929 | 0.9927 | NaN | 0.2108 | 0.126 | 0.094158 | 0.5372 | 0.1688 | 0.1383 | 0.22241 | 0.5606 | 0.2541 | 0.1968 | 0.196608 | 0.8705 | NaN | 0.1855 | 0.1251 | 0.138146 | 0.6708 | 0.1502 | 0.1332 | 0.259405 | 0.7339 | 0.2067 | 0.1973 | 0.294747 | 0.9039 | NaN | 0.2171 | 0.1262 | 0.085268 | 0.5441 | 0.1587 | 0.1365 | 0.244935 | 0.6202 | 0.262 | 0.1991 | 0.188069 | 0.8372 |
| diethyl-2-methyl-3-oxosuccinate | 202.0845 | 3.062651 | Exogenous | Food Component/Plant | 0.1794 | 0.1331 | 0.177685 | 0.5449 | -0.0015 | 0.1594 | 0.992475 | 0.9963 | 0.2679 | 0.1994 | 0.178993 | 0.6772 | NaN | 0.1359 | 0.1235 | 0.270862 | 0.7625 | -0.1065 | 0.1408 | 0.449593 | 0.8558 | 0.2508 | 0.1871 | 0.179933 | 0.879 | NaN | 0.0969 | 0.124 | 0.434642 | 0.8788 | -0.0333 | 0.1374 | 0.808673 | 0.9363 | 0.151 | 0.1923 | 0.432395 | 0.9816 | NaN | 0.1501 | 0.1261 | 0.233741 | 0.7062 | -0.1242 | 0.1479 | 0.40101 | 0.6937 | 0.2807 | 0.1892 | 0.137941 | 0.8157 | NaN | 0.1512 | 0.1249 | 0.226113 | 0.7052 | -0.0735 | 0.1406 | 0.601439 | 0.8623 | 0.2553 | 0.1904 | 0.180029 | 0.8608 | NaN | 0.1532 | 0.1263 | 0.225178 | 0.6905 | -0.1532 | 0.1462 | 0.294504 | 0.6559 | 0.2969 | 0.191 | 0.120112 | 0.7513 |
| pinitol | 194.0788 | 0.882718 | Exogenous | Food Component/Plant | -0.1327 | 0.1326 | 0.316835 | 0.6805 | -0.1054 | 0.1391 | 0.448473 | 0.7196 | -0.1378 | 0.2161 | 0.523638 | 0.8655 | NaN | -0.0943 | 0.1229 | 0.442689 | 0.8498 | -0.0498 | 0.1228 | 0.68471 | 0.9267 | -0.1114 | 0.2029 | 0.582962 | 0.954 | NaN | -0.1717 | 0.1223 | 0.16031 | 0.6683 | -0.0663 | 0.1202 | 0.581294 | 0.9053 | -0.2575 | 0.2054 | 0.210024 | 0.8462 | NaN | -0.1314 | 0.1253 | 0.294452 | 0.7388 | -0.1149 | 0.1271 | 0.365693 | 0.6762 | -0.1116 | 0.2057 | 0.587348 | 0.9375 | NaN | -0.0924 | 0.1246 | 0.458292 | 0.8605 | -0.0511 | 0.123 | 0.677611 | 0.8638 | -0.1057 | 0.2067 | 0.609143 | 0.9621 | NaN | -0.112 | 0.1257 | 0.372841 | 0.7624 | -0.099 | 0.1253 | 0.42909 | 0.7448 | -0.0938 | 0.2081 | 0.65209 | 0.9459 |
| 4-nitrophenol | 139.027 | 7.010404 | Exogenous | Pesticide Metabolism | 0.0701 | 0.1298 | 0.589185 | 0.8448 | 0.0804 | 0.1249 | 0.519617 | 0.7731 | 0.0892 | 0.23 | 0.69812 | 0.9492 | NaN | 0.0844 | 0.12 | 0.481978 | 0.8576 | 0.0637 | 0.1097 | 0.561431 | 0.9009 | 0.1417 | 0.2159 | 0.51151 | 0.954 | NaN | 0.0594 | 0.1199 | 0.620352 | 0.9181 | 0.0796 | 0.1075 | 0.458934 | 0.8952 | 0.0436 | 0.2177 | 0.841172 | 0.9935 | NaN | 0.0804 | 0.1227 | 0.512413 | 0.8197 | 0.0531 | 0.1145 | 0.642955 | 0.8371 | 0.1616 | 0.2193 | 0.461156 | 0.9375 | NaN | 0.0869 | 0.1216 | 0.474781 | 0.8625 | 0.0507 | 0.1101 | 0.645408 | 0.8623 | 0.1564 | 0.2202 | 0.477676 | 0.9403 | NaN | 0.0845 | 0.123 | 0.491761 | 0.8278 | 0.039 | 0.113 | 0.730169 | 0.8984 | 0.1787 | 0.2221 | 0.420939 | 0.8887 |
| estradiol valerate | 356.2358 | 21.2267 | Exogenous | Synthetic estrodiol | 0.0134 | 0.131 | 0.918699 | 0.9809 | -0.3036 | 0.1369 | 0.026522 | 0.2481 | 0.2543 | 0.2077 | 0.220848 | 0.7251 | NaN | 0.0248 | 0.1211 | 0.837625 | 0.9673 | -0.224 | 0.122 | 0.066319 | 0.4801 | 0.1915 | 0.196 | 0.328553 | 0.9223 | NaN | 0.0147 | 0.1209 | 0.903292 | 0.9717 | -0.2029 | 0.1205 | 0.092135 | 0.6246 | 0.1656 | 0.1985 | 0.404018 | 0.9816 | NaN | -0.0382 | 0.1242 | 0.758747 | 0.9246 | -0.3042 | 0.1245 | 0.014567 | 0.1422 | 0.1439 | 0.2012 | 0.4745 | 0.9375 | NaN | 0.0276 | 0.1227 | 0.821882 | 0.9564 | -0.2386 | 0.1216 | 0.049796 | 0.3844 | 0.2216 | 0.1988 | 0.26491 | 0.9039 | NaN | -0.0182 | 0.1243 | 0.88344 | 0.9588 | -0.3073 | 0.1224 | 0.012077 | 0.1359 | 0.1916 | 0.201 | 0.3404 | 0.8785 |
| phytanate | 312.3016 | 23.236364 | Lipid | Branched Chain Fatty Acid | -0.1145 | 0.1349 | 0.396026 | 0.7287 | -0.2038 | 0.1351 | 0.131352 | 0.424 | -0.0029 | 0.2277 | 0.989851 | 0.9935 | NaN | -0.1052 | 0.1248 | 0.398984 | 0.8498 | -0.1348 | 0.1199 | 0.260946 | 0.7828 | -0.0794 | 0.2143 | 0.710978 | 0.954 | NaN | -0.0801 | 0.1248 | 0.521052 | 0.9101 | -0.071 | 0.1199 | 0.553769 | 0.9053 | -0.1017 | 0.2165 | 0.638494 | 0.9894 | NaN | -0.1441 | 0.1275 | 0.258395 | 0.7164 | -0.1993 | 0.1233 | 0.106149 | 0.4378 | -0.0806 | 0.2175 | 0.711098 | 0.9477 | NaN | -0.0882 | 0.1266 | 0.486138 | 0.8625 | -0.1262 | 0.1204 | 0.294623 | 0.7544 | -0.0392 | 0.2177 | 0.856954 | 0.9621 | NaN | -0.1252 | 0.1277 | 0.327156 | 0.7485 | -0.1929 | 0.1215 | 0.112466 | 0.4653 | -0.0432 | 0.2189 | 0.843479 | 0.9641 |
| Cer 35:0 | 569.5027 | 24.040377 | Lipid | Ceramide | -0.0104 | 0.1337 | 0.938016 | 0.9847 | -0.2951 | 0.1428 | 0.038819 | 0.2877 | 0.2009 | 0.209 | 0.336559 | 0.7534 | NaN | -0.0164 | 0.1237 | 0.894531 | 0.9705 | -0.2066 | 0.1276 | 0.105303 | 0.6118 | 0.1063 | 0.1982 | 0.591868 | 0.954 | NaN | 0.0367 | 0.1237 | 0.766947 | 0.96 | -0.1407 | 0.1282 | 0.272401 | 0.806 | 0.153 | 0.1981 | 0.439811 | 0.9816 | NaN | -0.0659 | 0.1268 | 0.603244 | 0.8573 | -0.273 | 0.1307 | 0.036676 | 0.2538 | 0.0722 | 0.2033 | 0.72247 | 0.9518 | NaN | -0.0352 | 0.1254 | 0.778775 | 0.938 | -0.2537 | 0.126 | 0.044044 | 0.357 | 0.1257 | 0.2015 | 0.532629 | 0.9608 | NaN | -0.0496 | 0.1269 | 0.695747 | 0.9035 | -0.2671 | 0.1288 | 0.038045 | 0.2692 | 0.1081 | 0.2036 | 0.595495 | 0.9357 |
| Cer 36:0 | 583.5183 | 24.290825 | Lipid | Ceramide | -0.1969 | 0.1317 | 0.134867 | 0.5064 | -0.2263 | 0.1337 | 0.090481 | 0.3727 | -0.1966 | 0.2204 | 0.372296 | 0.7534 | NaN | -0.1798 | 0.1218 | 0.139957 | 0.6828 | -0.1404 | 0.1194 | 0.23964 | 0.7677 | -0.2427 | 0.2065 | 0.239826 | 0.9223 | NaN | -0.1725 | 0.1217 | 0.156345 | 0.6683 | -0.1512 | 0.1166 | 0.194854 | 0.7683 | -0.1925 | 0.2081 | 0.354969 | 0.9578 | NaN | -0.2081 | 0.1243 | 0.09413 | 0.5372 | -0.1826 | 0.1231 | 0.138139 | 0.4784 | -0.2646 | 0.2096 | 0.206956 | 0.8705 | NaN | -0.1956 | 0.1233 | 0.112584 | 0.6708 | -0.1854 | 0.1181 | 0.116435 | 0.5766 | -0.2181 | 0.2103 | 0.299681 | 0.9106 | NaN | -0.2014 | 0.1246 | 0.106171 | 0.5529 | -0.1823 | 0.1212 | 0.13244 | 0.5077 | -0.2387 | 0.2115 | 0.258951 | 0.8424 |
| Cer 37:0 | 597.5333 | 24.592678 | Lipid | Ceramide | -0.2827 | 0.1365 | 0.038282 | 0.2818 | -0.3915 | 0.1495 | 0.008845 | 0.1684 | -0.2075 | 0.2128 | 0.329513 | 0.7534 | NaN | -0.2763 | 0.126 | 0.028355 | 0.3293 | -0.2457 | 0.1369 | 0.072655 | 0.4865 | -0.3185 | 0.2 | 0.111348 | 0.7818 | NaN | -0.2594 | 0.1261 | 0.039673 | 0.316 | -0.2252 | 0.1351 | 0.095478 | 0.6274 | -0.2886 | 0.2011 | 0.151163 | 0.7655 | NaN | -0.307 | 0.1287 | 0.017035 | 0.2098 | -0.3306 | 0.1383 | 0.016838 | 0.1575 | -0.2983 | 0.2028 | 0.141229 | 0.8157 | NaN | -0.2741 | 0.1278 | 0.031957 | 0.332 | -0.2767 | 0.1352 | 0.040691 | 0.3563 | -0.2694 | 0.2033 | 0.185018 | 0.8608 | NaN | -0.2991 | 0.129 | 0.020413 | 0.2397 | -0.3287 | 0.1361 | 0.015691 | 0.1579 | -0.2741 | 0.2045 | 0.180098 | 0.8194 |
| Cer 38:0 | 611.5497 | 24.956318 | Lipid | Ceramide | -0.0605 | 0.1304 | 0.642841 | 0.8731 | -0.2383 | 0.1385 | 0.08542 | 0.3625 | 0.063 | 0.2091 | 0.763262 | 0.9647 | NaN | -0.1408 | 0.121 | 0.244689 | 0.7495 | -0.2187 | 0.1215 | 0.071755 | 0.4865 | -0.0963 | 0.2003 | 0.630752 | 0.954 | NaN | -0.0876 | 0.1204 | 0.467206 | 0.8955 | -0.1737 | 0.1204 | 0.149022 | 0.7153 | -0.0162 | 0.1988 | 0.934935 | 0.9935 | NaN | -0.1631 | 0.1245 | 0.190138 | 0.6616 | -0.2623 | 0.1259 | 0.037235 | 0.2538 | -0.1055 | 0.2047 | 0.606236 | 0.9375 | NaN | -0.1339 | 0.1227 | 0.274917 | 0.7462 | -0.2475 | 0.1211 | 0.040932 | 0.3563 | -0.0458 | 0.2026 | 0.821102 | 0.9621 | NaN | -0.1494 | 0.1245 | 0.230105 | 0.697 | -0.2512 | 0.1241 | 0.042982 | 0.2805 | -0.0773 | 0.2058 | 0.707339 | 0.9459 |
| Cer 40:0 | 639.5812 | 25.886269 | Lipid | Ceramide | 0.0882 | 0.132 | 0.504186 | 0.8067 | -0.1823 | 0.1411 | 0.196375 | 0.4993 | 0.3084 | 0.2079 | 0.138016 | 0.6043 | NaN | 0.0761 | 0.1221 | 0.533274 | 0.8926 | -0.0777 | 0.1263 | 0.538345 | 0.8967 | 0.1836 | 0.1992 | 0.356708 | 0.9223 | NaN | 0.1081 | 0.1218 | 0.374777 | 0.8283 | -0.0494 | 0.1248 | 0.69214 | 0.9195 | 0.2223 | 0.1987 | 0.263259 | 0.9 | NaN | 0.0245 | 0.1256 | 0.845388 | 0.962 | -0.1515 | 0.1295 | 0.241872 | 0.5805 | 0.1536 | 0.2052 | 0.454034 | 0.9375 | NaN | 0.0614 | 0.1238 | 0.61982 | 0.8971 | -0.1182 | 0.1252 | 0.345134 | 0.7839 | 0.2093 | 0.2022 | 0.300536 | 0.9106 | NaN | 0.049 | 0.1254 | 0.695945 | 0.9035 | -0.1371 | 0.1278 | 0.283474 | 0.652 | 0.1998 | 0.2043 | 0.328023 | 0.8727 |
| Cer 41:0 | 653.5953 | 26.49853 | Lipid | Ceramide | 0.031 | 0.1315 | 0.813428 | 0.9656 | -0.2237 | 0.1412 | 0.113161 | 0.3941 | 0.2328 | 0.2063 | 0.259012 | 0.7397 | NaN | -0.0001 | 0.1218 | 0.999578 | 0.9999 | -0.1141 | 0.1268 | 0.368095 | 0.824 | 0.0731 | 0.1993 | 0.713858 | 0.954 | NaN | 0.0583 | 0.1215 | 0.631423 | 0.9254 | -0.0673 | 0.1263 | 0.5938 | 0.9053 | 0.1473 | 0.1969 | 0.454403 | 0.9816 | NaN | -0.0639 | 0.1258 | 0.611553 | 0.8573 | -0.2127 | 0.1291 | 0.099323 | 0.4326 | 0.042 | 0.206 | 0.838627 | 0.9726 | NaN | -0.0245 | 0.1237 | 0.842723 | 0.9611 | -0.1735 | 0.1249 | 0.164807 | 0.631 | 0.0998 | 0.2026 | 0.622276 | 0.9621 | NaN | -0.0389 | 0.1255 | 0.756527 | 0.9321 | -0.194 | 0.1275 | 0.128107 | 0.498 | 0.0876 | 0.2053 | 0.669772 | 0.9459 |
| Cer 42:0 | 667.6126 | 27.104397 | Lipid | Ceramide | 0.0041 | 0.1332 | 0.975494 | 0.9936 | -0.231 | 0.1407 | 0.100566 | 0.3816 | 0.2129 | 0.2125 | 0.316508 | 0.7534 | NaN | -0.0038 | 0.1232 | 0.975654 | 0.9952 | -0.0972 | 0.1275 | 0.446071 | 0.8547 | 0.0624 | 0.2042 | 0.759949 | 0.954 | NaN | 0.0361 | 0.1231 | 0.769351 | 0.9608 | -0.0836 | 0.1255 | 0.505285 | 0.9053 | 0.1279 | 0.2027 | 0.527856 | 0.9894 | NaN | -0.0837 | 0.1271 | 0.510234 | 0.8197 | -0.2028 | 0.129 | 0.115837 | 0.445 | 0.0103 | 0.2124 | 0.961473 | 0.99 | NaN | -0.0236 | 0.1249 | 0.850145 | 0.962 | -0.1461 | 0.1256 | 0.244972 | 0.7302 | 0.0915 | 0.2074 | 0.659201 | 0.9621 | NaN | -0.0488 | 0.1267 | 0.70013 | 0.9035 | -0.176 | 0.1278 | 0.168291 | 0.5465 | 0.0696 | 0.2107 | 0.741321 | 0.9477 |
| Cer 43:0 | 681.6278 | 27.911722 | Lipid | Ceramide | -0.0118 | 0.1347 | 0.930366 | 0.982 | -0.1808 | 0.1404 | 0.197811 | 0.4993 | 0.1571 | 0.2188 | 0.472849 | 0.8234 | NaN | -0.0144 | 0.1246 | 0.907768 | 0.9737 | -0.0469 | 0.1268 | 0.711736 | 0.934 | 0.0083 | 0.2094 | 0.968436 | 0.9911 | NaN | 0.0244 | 0.1246 | 0.844695 | 0.9714 | -0.0419 | 0.1244 | 0.736033 | 0.9241 | 0.0815 | 0.208 | 0.69513 | 0.9894 | NaN | -0.1007 | 0.1284 | 0.432901 | 0.7844 | -0.1585 | 0.1286 | 0.217766 | 0.5546 | -0.0515 | 0.2177 | 0.812851 | 0.9674 | NaN | -0.0359 | 0.1263 | 0.776531 | 0.938 | -0.0965 | 0.1252 | 0.440621 | 0.8205 | 0.0358 | 0.2129 | 0.866421 | 0.9621 | NaN | -0.0685 | 0.1281 | 0.592982 | 0.8765 | -0.1331 | 0.1272 | 0.295536 | 0.6559 | 0.0053 | 0.2166 | 0.980402 | 0.9967 |
| Cer 44:0 | 695.6444 | 28.868212 | Lipid | Ceramide | -0.0045 | 0.1355 | 0.973709 | 0.9936 | -0.1683 | 0.1426 | 0.238053 | 0.5299 | 0.1612 | 0.2189 | 0.461643 | 0.8194 | NaN | 0.0004 | 0.1253 | 0.997542 | 0.9999 | -0.0322 | 0.1287 | 0.802291 | 0.965 | 0.0266 | 0.2089 | 0.898796 | 0.977 | NaN | 0.0299 | 0.1252 | 0.811084 | 0.9676 | -0.0365 | 0.1259 | 0.771826 | 0.9284 | 0.0852 | 0.2082 | 0.682514 | 0.9894 | NaN | -0.0903 | 0.1291 | 0.484316 | 0.8009 | -0.1467 | 0.1306 | 0.26136 | 0.5913 | -0.0397 | 0.2172 | 0.85502 | 0.9772 | NaN | -0.0228 | 0.127 | 0.857346 | 0.962 | -0.0806 | 0.1272 | 0.526044 | 0.8496 | 0.0472 | 0.2126 | 0.824285 | 0.9621 | NaN | -0.0547 | 0.1287 | 0.670687 | 0.9035 | -0.1169 | 0.1293 | 0.365834 | 0.6901 | 0.0184 | 0.2161 | 0.93196 | 0.9869 |
| Cer d38:1 (2OH) | 609.5342 | 24.481514 | Lipid | Ceramide | -0.0267 | 0.1324 | 0.839945 | 0.9778 | -0.2122 | 0.1447 | 0.142445 | 0.4519 | 0.0961 | 0.2059 | 0.640806 | 0.9104 | NaN | -0.1274 | 0.1232 | 0.301349 | 0.7864 | -0.2304 | 0.1263 | 0.068035 | 0.4801 | -0.069 | 0.1979 | 0.727536 | 0.954 | NaN | -0.0376 | 0.1222 | 0.758553 | 0.96 | -0.131 | 0.1261 | 0.299106 | 0.8336 | 0.0243 | 0.1956 | 0.901073 | 0.9935 | NaN | -0.1785 | 0.128 | 0.163247 | 0.6495 | -0.3009 | 0.1316 | 0.022259 | 0.192 | -0.1117 | 0.2049 | 0.585635 | 0.9375 | NaN | -0.1225 | 0.125 | 0.326993 | 0.7669 | -0.247 | 0.1263 | 0.050555 | 0.3844 | -0.0357 | 0.201 | 0.859184 | 0.9621 | NaN | -0.1618 | 0.1278 | 0.20549 | 0.6633 | -0.2904 | 0.1294 | 0.024793 | 0.2033 | -0.0786 | 0.2058 | 0.702619 | 0.9459 |
| Cer d40:1 (2OH) | 637.5656 | 25.195412 | Lipid | Ceramide | 0.0104 | 0.1347 | 0.938355 | 0.9847 | -0.1919 | 0.1437 | 0.181749 | 0.4964 | 0.1747 | 0.2132 | 0.412485 | 0.7762 | NaN | -0.0107 | 0.1246 | 0.931596 | 0.9861 | -0.1042 | 0.128 | 0.415322 | 0.847 | 0.0481 | 0.2033 | 0.813152 | 0.9632 | NaN | 0.0318 | 0.1244 | 0.798138 | 0.9641 | -0.0684 | 0.1267 | 0.589291 | 0.9053 | 0.1021 | 0.2027 | 0.614583 | 0.9894 | NaN | -0.0612 | 0.1281 | 0.633005 | 0.8606 | -0.1758 | 0.1315 | 0.181221 | 0.5327 | 0.0159 | 0.2089 | 0.939386 | 0.99 | NaN | -0.0202 | 0.1264 | 0.873222 | 0.9672 | -0.1315 | 0.1274 | 0.30183 | 0.7544 | 0.0715 | 0.2067 | 0.729372 | 0.9621 | NaN | -0.0392 | 0.128 | 0.759525 | 0.9324 | -0.1591 | 0.1298 | 0.220333 | 0.5853 | 0.0561 | 0.209 | 0.788415 | 0.9525 |
| Cer d42:1 (2OH) | 665.5972 | 26.210842 | Lipid | Ceramide | 0.0447 | 0.135 | 0.740672 | 0.9321 | -0.2158 | 0.1441 | 0.134211 | 0.4282 | 0.263 | 0.2131 | 0.217147 | 0.7178 | NaN | 0.036 | 0.1248 | 0.773191 | 0.9527 | -0.0875 | 0.13 | 0.50085 | 0.8931 | 0.1231 | 0.2045 | 0.547006 | 0.954 | NaN | 0.075 | 0.1247 | 0.54765 | 0.9125 | -0.0633 | 0.1284 | 0.621824 | 0.9053 | 0.1773 | 0.2034 | 0.383205 | 0.9793 | NaN | -0.0252 | 0.1284 | 0.844361 | 0.962 | -0.1715 | 0.1326 | 0.195738 | 0.5441 | 0.0851 | 0.2114 | 0.687177 | 0.9476 | NaN | 0.0169 | 0.1266 | 0.893812 | 0.9674 | -0.1423 | 0.1281 | 0.266629 | 0.7359 | 0.1551 | 0.2073 | 0.454412 | 0.9359 | NaN | 0.0007 | 0.1283 | 0.99558 | 0.9956 | -0.1572 | 0.1309 | 0.229754 | 0.6011 | 0.1371 | 0.2102 | 0.514209 | 0.8946 |
| Cer d43:1 (2OH) | 679.6125 | 26.850416 | Lipid | Ceramide | 0.0263 | 0.1377 | 0.848439 | 0.9778 | -0.1663 | 0.1466 | 0.256661 | 0.5494 | 0.2048 | 0.2198 | 0.351623 | 0.7534 | NaN | 0.0217 | 0.1274 | 0.864965 | 0.9705 | -0.0354 | 0.1319 | 0.788618 | 0.9616 | 0.0671 | 0.2102 | 0.749558 | 0.954 | NaN | 0.073 | 0.1273 | 0.566568 | 0.9125 | -0.0142 | 0.13 | 0.912995 | 0.973 | 0.1447 | 0.2086 | 0.487972 | 0.9848 | NaN | -0.0436 | 0.1309 | 0.739405 | 0.9111 | -0.1207 | 0.1349 | 0.371025 | 0.6762 | 0.0218 | 0.2172 | 0.920073 | 0.99 | NaN | 0.0018 | 0.1291 | 0.988645 | 0.9959 | -0.0951 | 0.1302 | 0.464848 | 0.8272 | 0.1011 | 0.2131 | 0.635064 | 0.9621 | NaN | -0.0159 | 0.1308 | 0.903183 | 0.9693 | -0.1068 | 0.1331 | 0.422358 | 0.7401 | 0.0788 | 0.216 | 0.715258 | 0.9459 |
| Cer d44:1 (2OH) | 693.6285 | 27.404913 | Lipid | Ceramide | -0.0264 | 0.135 | 0.84516 | 0.9778 | -0.2584 | 0.14 | 0.064884 | 0.3256 | 0.1897 | 0.2181 | 0.384357 | 0.7534 | NaN | -0.0037 | 0.1249 | 0.976144 | 0.9952 | -0.1025 | 0.1284 | 0.424768 | 0.847 | 0.0725 | 0.2075 | 0.726973 | 0.954 | NaN | 0.0246 | 0.1249 | 0.844017 | 0.9714 | -0.1089 | 0.1253 | 0.384665 | 0.8818 | 0.1355 | 0.2068 | 0.512254 | 0.9894 | NaN | -0.0677 | 0.1278 | 0.596512 | 0.8553 | -0.1843 | 0.1302 | 0.156893 | 0.5021 | 0.03 | 0.2137 | 0.88826 | 0.99 | NaN | -0.0244 | 0.1265 | 0.847184 | 0.962 | -0.16 | 0.1257 | 0.203284 | 0.6801 | 0.1074 | 0.2104 | 0.609777 | 0.9621 | NaN | -0.0389 | 0.1279 | 0.760985 | 0.9324 | -0.165 | 0.1289 | 0.200539 | 0.5756 | 0.085 | 0.2129 | 0.689851 | 0.9459 |
| Cer t34:0(2OH) | 571.4738 | 23.930481 | Lipid | Ceramide | 0.0296 | 0.1315 | 0.822056 | 0.9696 | -0.2744 | 0.1403 | 0.050458 | 0.2996 | 0.261 | 0.2061 | 0.205476 | 0.7107 | NaN | 0.0044 | 0.1217 | 0.971446 | 0.9952 | -0.1956 | 0.1249 | 0.117413 | 0.6118 | 0.1329 | 0.1975 | 0.501046 | 0.954 | NaN | 0.0625 | 0.1214 | 0.606864 | 0.9125 | -0.1166 | 0.1261 | 0.355088 | 0.8722 | 0.1776 | 0.1968 | 0.366706 | 0.9578 | NaN | -0.0471 | 0.1252 | 0.706802 | 0.8887 | -0.2732 | 0.1278 | 0.032599 | 0.2362 | 0.105 | 0.2032 | 0.605296 | 0.9375 | NaN | -0.0124 | 0.1234 | 0.920155 | 0.9796 | -0.2269 | 0.124 | 0.067285 | 0.4198 | 0.1478 | 0.2012 | 0.462548 | 0.9359 | NaN | -0.0267 | 0.1251 | 0.830732 | 0.9491 | -0.2577 | 0.1262 | 0.041153 | 0.2765 | 0.1418 | 0.2032 | 0.485349 | 0.8887 |
| Cer t36:0(2OH) | 599.5055 | 24.486198 | Lipid | Ceramide | 0.0527 | 0.1366 | 0.699588 | 0.9136 | 0.0195 | 0.1448 | 0.893159 | 0.9519 | 0.0629 | 0.2258 | 0.780674 | 0.9647 | NaN | -0.1588 | 0.1307 | 0.224514 | 0.7495 | -0.1242 | 0.1292 | 0.336572 | 0.8095 | -0.1993 | 0.2213 | 0.367782 | 0.9312 | NaN | -0.0314 | 0.1269 | 0.804357 | 0.9673 | -0.0197 | 0.1249 | 0.874494 | 0.9609 | -0.0231 | 0.2146 | 0.91429 | 0.9935 | NaN | -0.1652 | 0.1357 | 0.223512 | 0.7062 | -0.1389 | 0.1365 | 0.308617 | 0.6362 | -0.2117 | 0.2276 | 0.352408 | 0.9133 | NaN | -0.1393 | 0.1325 | 0.29305 | 0.7524 | -0.1293 | 0.1297 | 0.318519 | 0.7579 | -0.1509 | 0.2248 | 0.501921 | 0.9436 | NaN | -0.1725 | 0.1366 | 0.206873 | 0.6639 | -0.149 | 0.1342 | 0.266655 | 0.6386 | -0.2094 | 0.2324 | 0.367483 | 0.8858 |
| Cer t38:0(2OH) | 627.5368 | 25.20021 | Lipid | Ceramide | -0.0186 | 0.1317 | 0.888014 | 0.9809 | -0.1905 | 0.1371 | 0.164619 | 0.479 | 0.1293 | 0.2126 | 0.54301 | 0.8663 | NaN | -0.0667 | 0.122 | 0.584705 | 0.9079 | -0.1207 | 0.1216 | 0.321101 | 0.8095 | -0.0379 | 0.2045 | 0.853075 | 0.9765 | NaN | -0.0042 | 0.1217 | 0.972332 | 0.9794 | -0.0525 | 0.1217 | 0.666325 | 0.9112 | 0.032 | 0.2029 | 0.874713 | 0.9935 | NaN | -0.1208 | 0.1259 | 0.337388 | 0.741 | -0.2139 | 0.1249 | 0.086722 | 0.4127 | -0.0523 | 0.2095 | 0.802821 | 0.9662 | NaN | -0.0655 | 0.1237 | 0.596535 | 0.8924 | -0.1366 | 0.1214 | 0.260601 | 0.7339 | -0.0005 | 0.2074 | 0.998146 | 0.9999 | NaN | -0.0959 | 0.1256 | 0.445134 | 0.801 | -0.1908 | 0.1232 | 0.121428 | 0.4822 | -0.0136 | 0.2099 | 0.948384 | 0.9869 |
| Cer t40:0(2OH) | 655.5675 | 26.20871 | Lipid | Ceramide | 0.0496 | 0.136 | 0.71521 | 0.9246 | -0.2124 | 0.1461 | 0.145887 | 0.455 | 0.2639 | 0.2137 | 0.216722 | 0.7178 | NaN | 0.0419 | 0.1258 | 0.739129 | 0.9401 | -0.0737 | 0.1322 | 0.576879 | 0.904 | 0.1207 | 0.2052 | 0.556276 | 0.954 | NaN | 0.0863 | 0.1256 | 0.492087 | 0.9053 | -0.0467 | 0.1306 | 0.720583 | 0.9241 | 0.1834 | 0.2037 | 0.367838 | 0.9578 | NaN | -0.0113 | 0.1292 | 0.930472 | 0.9828 | -0.1608 | 0.1346 | 0.232125 | 0.572 | 0.0998 | 0.2107 | 0.635693 | 0.9375 | NaN | 0.0291 | 0.1275 | 0.81971 | 0.9564 | -0.1181 | 0.1306 | 0.365669 | 0.7947 | 0.1555 | 0.2079 | 0.454557 | 0.9359 | NaN | 0.0097 | 0.1291 | 0.940062 | 0.9794 | -0.1448 | 0.133 | 0.27632 | 0.649 | 0.1407 | 0.2105 | 0.503893 | 0.8946 |
| Cer t41:0(2OH) | 669.5838 | 26.84795 | Lipid | Ceramide | -0.0024 | 0.1353 | 0.985954 | 0.9936 | -0.2123 | 0.1387 | 0.126022 | 0.4166 | 0.2022 | 0.2211 | 0.360398 | 0.7534 | NaN | 0.0075 | 0.1251 | 0.952204 | 0.9952 | -0.0577 | 0.1268 | 0.6493 | 0.9079 | 0.0555 | 0.2118 | 0.793449 | 0.9605 | NaN | 0.043 | 0.1251 | 0.730826 | 0.9567 | -0.0502 | 0.1244 | 0.686536 | 0.9195 | 0.1252 | 0.2103 | 0.551589 | 0.9894 | NaN | -0.0521 | 0.1282 | 0.684498 | 0.877 | -0.1452 | 0.1286 | 0.258874 | 0.5881 | 0.0263 | 0.2177 | 0.903709 | 0.99 | NaN | -0.0096 | 0.1268 | 0.939577 | 0.9796 | -0.1042 | 0.1248 | 0.403679 | 0.8162 | 0.0915 | 0.2147 | 0.670111 | 0.9621 | NaN | -0.0282 | 0.1283 | 0.826003 | 0.9491 | -0.1305 | 0.1271 | 0.304576 | 0.6619 | 0.0785 | 0.217 | 0.717529 | 0.9459 |
| Cer t42:0(2OH) | 683.5993 | 27.302876 | Lipid | Ceramide | -0.0461 | 0.1335 | 0.729524 | 0.9287 | -0.3189 | 0.1367 | 0.01965 | 0.208 | 0.1946 | 0.2152 | 0.365728 | 0.7534 | NaN | -0.0326 | 0.1234 | 0.79197 | 0.9571 | -0.1623 | 0.1264 | 0.198961 | 0.7225 | 0.0531 | 0.206 | 0.796638 | 0.9617 | NaN | 0.0072 | 0.1236 | 0.953393 | 0.9728 | -0.1489 | 0.1243 | 0.230894 | 0.8003 | 0.1265 | 0.2045 | 0.536159 | 0.9894 | NaN | -0.0925 | 0.1264 | 0.464449 | 0.7864 | -0.2491 | 0.1271 | 0.050133 | 0.2976 | 0.0244 | 0.2118 | 0.90844 | 0.99 | NaN | -0.0474 | 0.125 | 0.70445 | 0.9116 | -0.2056 | 0.1239 | 0.097082 | 0.5203 | 0.0917 | 0.2086 | 0.660448 | 0.9621 | NaN | -0.0679 | 0.1265 | 0.591578 | 0.8765 | -0.2296 | 0.126 | 0.06856 | 0.357 | 0.0722 | 0.2113 | 0.732739 | 0.9459 |
| PE-Cer d34:1 | 660.5193 | 23.983944 | Lipid | Ceramide phosphoethanolamines | 0.0452 | 0.1344 | 0.736693 | 0.9321 | -0.1733 | 0.142 | 0.222402 | 0.5117 | 0.237 | 0.2146 | 0.26936 | 0.7397 | NaN | 0.0428 | 0.1243 | 0.730571 | 0.9367 | -0.0644 | 0.1272 | 0.612676 | 0.9043 | 0.1216 | 0.2044 | 0.552092 | 0.954 | NaN | 0.0642 | 0.1241 | 0.605024 | 0.9125 | -0.0486 | 0.1251 | 0.697762 | 0.9195 | 0.1507 | 0.2047 | 0.461595 | 0.9816 | NaN | -0.0072 | 0.1276 | 0.954752 | 0.9828 | -0.1212 | 0.1309 | 0.354449 | 0.6762 | 0.0784 | 0.2108 | 0.710076 | 0.9477 | NaN | 0.0234 | 0.126 | 0.852974 | 0.962 | -0.1092 | 0.126 | 0.386051 | 0.8103 | 0.1425 | 0.2078 | 0.492954 | 0.9434 | NaN | 0.0216 | 0.1275 | 0.865461 | 0.9576 | -0.0999 | 0.1295 | 0.440266 | 0.7458 | 0.1298 | 0.21 | 0.5364 | 0.8971 |
| PE-Cer d36:1 | 688.5503 | 23.996895 | Lipid | Ceramide phosphoethanolamines | 0.3236 | 0.1295 | 0.012445 | 0.1478 | -0.1559 | 0.1715 | 0.363049 | 0.6403 | 0.5406 | 0.1801 | 0.002685 | 0.1058 | NaN | 0.2251 | 0.1218 | 0.064664 | 0.5099 | -0.1266 | 0.1507 | 0.400778 | 0.847 | 0.3907 | 0.1782 | 0.028347 | 0.5113 | NaN | 0.2871 | 0.1199 | 0.016621 | 0.2039 | -0.0372 | 0.1497 | 0.804052 | 0.9363 | 0.4379 | 0.175 | 0.012362 | 0.234 | NaN | 0.1921 | 0.127 | 0.130415 | 0.5901 | -0.2137 | 0.1565 | 0.172078 | 0.5146 | 0.3851 | 0.1846 | 0.037008 | 0.5138 | NaN | 0.2137 | 0.1243 | 0.085413 | 0.5831 | -0.1735 | 0.1504 | 0.248637 | 0.7302 | 0.4117 | 0.182 | 0.023698 | 0.4673 | NaN | 0.2077 | 0.1265 | 0.10058 | 0.5529 | -0.2357 | 0.1541 | 0.126179 | 0.494 | 0.4223 | 0.1825 | 0.020672 | 0.4132 |
| PE-Cer d32:3 | 628.4845 | 25.65966 | Lipid | Ceramide phosphoethanolamines | 0.2532 | 0.1272 | 0.046457 | 0.3127 | 0.0238 | 0.1316 | 0.856651 | 0.932 | 0.4856 | 0.2078 | 0.019424 | 0.2331 | NaN | 0.1176 | 0.1209 | 0.330718 | 0.8078 | 0.0046 | 0.1156 | 0.968507 | 0.9891 | 0.2413 | 0.2127 | 0.25661 | 0.9223 | NaN | 0.208 | 0.1179 | 0.077768 | 0.5097 | 0.1173 | 0.1139 | 0.302859 | 0.8336 | 0.3146 | 0.2063 | 0.127339 | 0.7073 | NaN | 0.1047 | 0.1255 | 0.404066 | 0.7795 | -0.0624 | 0.1218 | 0.608647 | 0.8188 | 0.2822 | 0.214 | 0.187201 | 0.8705 | NaN | 0.1362 | 0.1222 | 0.264963 | 0.7442 | -0.0023 | 0.1158 | 0.984337 | 0.9923 | 0.3045 | 0.2129 | 0.15278 | 0.8056 | NaN | 0.1172 | 0.1252 | 0.349094 | 0.7531 | -0.0593 | 0.1197 | 0.620339 | 0.8372 | 0.3144 | 0.2144 | 0.142428 | 0.7588 |
| PE-Cer d34:2 | 658.5018 | 23.675238 | Lipid | Ceramide phosphoethanolamines | 0.0524 | 0.1259 | 0.677199 | 0.8986 | -0.1761 | 0.1338 | 0.187877 | 0.4993 | 0.2315 | 0.1997 | 0.246359 | 0.7391 | NaN | 0.0727 | 0.1164 | 0.532329 | 0.8926 | -0.0706 | 0.12 | 0.556099 | 0.9009 | 0.1634 | 0.1887 | 0.3865 | 0.9389 | NaN | 0.1234 | 0.1166 | 0.289737 | 0.7865 | -0.006 | 0.1202 | 0.960059 | 0.9785 | 0.2094 | 0.1887 | 0.267346 | 0.9 | NaN | 0.023 | 0.1192 | 0.847369 | 0.962 | -0.1108 | 0.1239 | 0.371182 | 0.6762 | 0.1013 | 0.195 | 0.603411 | 0.9375 | NaN | 0.0555 | 0.118 | 0.637949 | 0.8992 | -0.0939 | 0.1194 | 0.431382 | 0.8205 | 0.1675 | 0.1923 | 0.383599 | 0.9106 | NaN | 0.0437 | 0.1193 | 0.714488 | 0.9116 | -0.0977 | 0.1224 | 0.424522 | 0.7416 | 0.1445 | 0.1946 | 0.457737 | 0.8887 |
| PE-Cer d36:2 | 686.5345 | 23.691633 | Lipid | Ceramide phosphoethanolamines | 0.0483 | 0.1339 | 0.718152 | 0.9262 | -0.078 | 0.1485 | 0.599653 | 0.8193 | 0.1551 | 0.2135 | 0.467549 | 0.8207 | NaN | 0.0386 | 0.1239 | 0.755102 | 0.9509 | -0.0532 | 0.1305 | 0.683634 | 0.9267 | 0.0863 | 0.2014 | 0.668045 | 0.954 | NaN | 0.0806 | 0.1237 | 0.514591 | 0.9068 | 0.0526 | 0.13 | 0.685986 | 0.9195 | 0.0779 | 0.2031 | 0.701442 | 0.9894 | NaN | 0.0124 | 0.1268 | 0.921927 | 0.9828 | -0.0941 | 0.1358 | 0.48838 | 0.7494 | 0.0696 | 0.2049 | 0.734271 | 0.9559 | NaN | 0.0354 | 0.1255 | 0.777995 | 0.938 | -0.051 | 0.1308 | 0.696415 | 0.8748 | 0.0903 | 0.2052 | 0.659934 | 0.9621 | NaN | 0.0255 | 0.127 | 0.841022 | 0.9513 | -0.0831 | 0.1337 | 0.534271 | 0.8003 | 0.0916 | 0.2063 | 0.657132 | 0.9459 |
| PE-Cer d34:3 | 656.5162 | 26.70364 | Lipid | Ceramide phosphoethanolamines | 0.1712 | 0.1317 | 0.193839 | 0.5541 | -0.0972 | 0.1442 | 0.50027 | 0.7575 | 0.3801 | 0.2048 | 0.063458 | 0.4426 | NaN | 0.0951 | 0.1229 | 0.439016 | 0.8498 | -0.0426 | 0.1272 | 0.737878 | 0.9428 | 0.1919 | 0.2017 | 0.341417 | 0.9223 | NaN | 0.1679 | 0.1216 | 0.167186 | 0.6736 | 0.0358 | 0.1266 | 0.77715 | 0.9309 | 0.2646 | 0.1978 | 0.181013 | 0.8127 | NaN | 0.0612 | 0.1271 | 0.630275 | 0.8606 | -0.1197 | 0.1318 | 0.36371 | 0.6762 | 0.1937 | 0.2067 | 0.348877 | 0.9127 | NaN | 0.1023 | 0.1245 | 0.411135 | 0.8283 | -0.0463 | 0.1274 | 0.716323 | 0.8866 | 0.23 | 0.2043 | 0.260299 | 0.9039 | NaN | 0.079 | 0.1268 | 0.533259 | 0.8482 | -0.102 | 0.1298 | 0.432066 | 0.7453 | 0.2263 | 0.2069 | 0.274205 | 0.8424 |
| DG 36:0 | 646.5518 | 29.627296 | Lipid | Diacylglycerol | 0.0267 | 0.1426 | 0.851628 | 0.9778 | 0.0526 | 0.1875 | 0.778904 | 0.9266 | 0.0375 | 0.2036 | 0.853751 | 0.9732 | NaN | -0.0163 | 0.132 | 0.901545 | 0.972 | -0.0156 | 0.1651 | 0.924795 | 0.9729 | -0.007 | 0.1914 | 0.97071 | 0.9911 | NaN | -0.0048 | 0.1318 | 0.970931 | 0.9794 | 0.0001 | 0.1619 | 0.999395 | 0.9994 | -0.0093 | 0.1928 | 0.961692 | 0.9976 | NaN | -0.0142 | 0.135 | 0.916337 | 0.9828 | 0.0042 | 0.172 | 0.980529 | 0.9926 | -0.0092 | 0.1941 | 0.962098 | 0.99 | NaN | -0.0075 | 0.1338 | 0.955498 | 0.9796 | -0.0464 | 0.166 | 0.779593 | 0.9247 | 0.0194 | 0.1945 | 0.920367 | 0.977 | NaN | -0.015 | 0.1354 | 0.911555 | 0.9714 | -0.0204 | 0.1697 | 0.904484 | 0.9732 | 0.0004 | 0.1958 | 0.998184 | 0.9991 |
| DG 33:1 | 602.4901 | 25.90679 | Lipid | Diacylglycerol | 0.336 | 0.1306 | 0.010118 | 0.1269 | 0.0858 | 0.1375 | 0.532682 | 0.7813 | 0.5563 | 0.21 | 0.008081 | 0.1612 | NaN | 0.1489 | 0.1272 | 0.242057 | 0.7495 | -0.0343 | 0.123 | 0.780376 | 0.9615 | 0.3179 | 0.2154 | 0.14002 | 0.8611 | NaN | 0.2555 | 0.1221 | 0.03635 | 0.2995 | 0.0626 | 0.1186 | 0.597734 | 0.9053 | 0.4303 | 0.2043 | 0.035248 | 0.3815 | NaN | 0.1556 | 0.1319 | 0.238189 | 0.7062 | -0.0786 | 0.1314 | 0.54981 | 0.7845 | 0.3582 | 0.2167 | 0.098232 | 0.7531 | NaN | 0.189 | 0.1274 | 0.13793 | 0.6708 | -0.0123 | 0.1226 | 0.920383 | 0.9808 | 0.3847 | 0.2147 | 0.073173 | 0.6055 | NaN | 0.1589 | 0.1322 | 0.229444 | 0.697 | -0.0835 | 0.1289 | 0.517383 | 0.7933 | 0.3787 | 0.2195 | 0.084551 | 0.6395 |
| DG 35:1 | 630.5215 | 27.154875 | Lipid | Diacylglycerol | 0.3168 | 0.1301 | 0.014866 | 0.1566 | 0.1387 | 0.1594 | 0.384324 | 0.6568 | 0.4198 | 0.1902 | 0.027322 | 0.3016 | NaN | 0.1432 | 0.1258 | 0.255006 | 0.7495 | -0.002 | 0.143 | 0.988952 | 0.9953 | 0.2203 | 0.1911 | 0.248845 | 0.9223 | NaN | 0.2065 | 0.1225 | 0.091943 | 0.5342 | 0.1045 | 0.1376 | 0.447707 | 0.8947 | 0.2639 | 0.1886 | 0.161596 | 0.7677 | NaN | 0.1717 | 0.1284 | 0.18103 | 0.6574 | -0.0194 | 0.1511 | 0.89766 | 0.9695 | 0.2696 | 0.1903 | 0.156572 | 0.8679 | NaN | 0.1729 | 0.1265 | 0.171759 | 0.6753 | 0.0194 | 0.1426 | 0.891929 | 0.9727 | 0.2668 | 0.1925 | 0.165777 | 0.8292 | NaN | 0.1773 | 0.1285 | 0.167732 | 0.6299 | -0.0213 | 0.1483 | 0.88555 | 0.9667 | 0.2855 | 0.1921 | 0.13712 | 0.7588 |
| DG 34:2 | 614.4888 | 25.732864 | Lipid | Diacylglycerol | 0.3173 | 0.1292 | 0.014009 | 0.1558 | 0.0827 | 0.1411 | 0.557877 | 0.7957 | 0.5527 | 0.206 | 0.007298 | 0.1612 | NaN | 0.1262 | 0.126 | 0.316655 | 0.7898 | -0.0217 | 0.1256 | 0.862597 | 0.9729 | 0.3029 | 0.2141 | 0.157267 | 0.879 | NaN | 0.2069 | 0.1217 | 0.089179 | 0.5342 | 0.0554 | 0.1218 | 0.649337 | 0.9053 | 0.3796 | 0.2059 | 0.065259 | 0.5146 | NaN | 0.1335 | 0.1306 | 0.306956 | 0.741 | -0.0819 | 0.1345 | 0.54293 | 0.7845 | 0.3623 | 0.212 | 0.08742 | 0.7393 | NaN | 0.17 | 0.126 | 0.177233 | 0.6753 | -0.0026 | 0.1254 | 0.983401 | 0.9923 | 0.3779 | 0.2119 | 0.074606 | 0.6055 | NaN | 0.144 | 0.1304 | 0.269307 | 0.7315 | -0.081 | 0.1317 | 0.538679 | 0.8003 | 0.3867 | 0.2137 | 0.070391 | 0.6024 |
| DG 35:2 | 628.5046 | 26.1662 | Lipid | Diacylglycerol | 0.3235 | 0.1362 | 0.017556 | 0.1685 | 0.1001 | 0.1477 | 0.498047 | 0.7574 | 0.5025 | 0.2148 | 0.019334 | 0.2331 | NaN | 0.1004 | 0.1342 | 0.454105 | 0.8498 | -0.0602 | 0.1332 | 0.651431 | 0.9079 | 0.2379 | 0.2217 | 0.28322 | 0.9223 | NaN | 0.1966 | 0.1288 | 0.126988 | 0.6315 | 0.0749 | 0.1274 | 0.556638 | 0.9053 | 0.3097 | 0.2153 | 0.150303 | 0.7655 | NaN | 0.128 | 0.1378 | 0.35304 | 0.7467 | -0.0856 | 0.1418 | 0.546291 | 0.7845 | 0.297 | 0.2204 | 0.177832 | 0.8705 | NaN | 0.1509 | 0.1338 | 0.259499 | 0.7422 | -0.031 | 0.1325 | 0.814981 | 0.9396 | 0.3152 | 0.2202 | 0.152219 | 0.8056 | NaN | 0.137 | 0.1377 | 0.319724 | 0.7485 | -0.0946 | 0.1393 | 0.496857 | 0.7792 | 0.326 | 0.2215 | 0.141086 | 0.7588 |
| DG 35:3 | 626.49 | 25.472881 | Lipid | Diacylglycerol | 0.2072 | 0.1329 | 0.118944 | 0.4809 | 0.0382 | 0.1378 | 0.781792 | 0.9281 | 0.3546 | 0.2183 | 0.104376 | 0.5335 | NaN | -0.0181 | 0.1299 | 0.889226 | 0.9705 | -0.0679 | 0.1224 | 0.579166 | 0.904 | 0.0186 | 0.2291 | 0.935272 | 0.9911 | NaN | 0.1033 | 0.1245 | 0.406598 | 0.8502 | 0.0745 | 0.1186 | 0.53025 | 0.9053 | 0.1419 | 0.2182 | 0.515378 | 0.9894 | NaN | -0.0005 | 0.134 | 0.997127 | 0.9989 | -0.1287 | 0.1309 | 0.325573 | 0.6511 | 0.1096 | 0.2253 | 0.626736 | 0.9375 | NaN | 0.0229 | 0.1304 | 0.860554 | 0.962 | -0.0741 | 0.1228 | 0.546259 | 0.8618 | 0.1255 | 0.2258 | 0.578241 | 0.9621 | NaN | 0.0063 | 0.1341 | 0.962243 | 0.9855 | -0.1398 | 0.1287 | 0.277457 | 0.649 | 0.1414 | 0.2267 | 0.532652 | 0.8971 |
| DG 36:3 | 640.5052 | 25.970724 | Lipid | Diacylglycerol | 0.1786 | 0.1375 | 0.193709 | 0.5541 | -0.0927 | 0.1363 | 0.496519 | 0.7571 | 0.4995 | 0.2345 | 0.033202 | 0.3293 | NaN | 0.0227 | 0.1305 | 0.862023 | 0.9705 | -0.135 | 0.1194 | 0.25811 | 0.7828 | 0.2323 | 0.2378 | 0.328663 | 0.9223 | NaN | 0.0909 | 0.1282 | 0.478239 | 0.8967 | -0.0655 | 0.1176 | 0.577579 | 0.9053 | 0.2978 | 0.2333 | 0.201727 | 0.8462 | NaN | 0.0222 | 0.1346 | 0.868726 | 0.9747 | -0.1868 | 0.1252 | 0.135869 | 0.4784 | 0.2928 | 0.2371 | 0.216722 | 0.8705 | NaN | 0.0681 | 0.131 | 0.602967 | 0.8964 | -0.1213 | 0.1196 | 0.310379 | 0.7544 | 0.3251 | 0.2351 | 0.166744 | 0.8292 | NaN | 0.0471 | 0.1338 | 0.724573 | 0.9153 | -0.181 | 0.123 | 0.141085 | 0.5193 | 0.3421 | 0.2354 | 0.146219 | 0.7588 |
| DG 38:3 | 668.5383 | 27.205564 | Lipid | Diacylglycerol | 0.1271 | 0.1398 | 0.363173 | 0.7161 | -0.1339 | 0.1453 | 0.356846 | 0.6361 | 0.378 | 0.2263 | 0.0948 | 0.5081 | NaN | 0.0179 | 0.1309 | 0.891064 | 0.9705 | -0.1693 | 0.1271 | 0.182881 | 0.701 | 0.1956 | 0.2202 | 0.374517 | 0.9312 | NaN | 0.0608 | 0.1297 | 0.639553 | 0.929 | -0.1093 | 0.1253 | 0.383053 | 0.8818 | 0.2175 | 0.2207 | 0.324523 | 0.9479 | NaN | 0.002 | 0.1349 | 0.98814 | 0.9985 | -0.2194 | 0.1329 | 0.098915 | 0.4326 | 0.2149 | 0.2233 | 0.335722 | 0.9044 | NaN | 0.0492 | 0.132 | 0.709645 | 0.9131 | -0.1508 | 0.1275 | 0.236741 | 0.7254 | 0.2493 | 0.2218 | 0.261127 | 0.9039 | NaN | 0.0228 | 0.1345 | 0.865662 | 0.9576 | -0.2264 | 0.1308 | 0.083366 | 0.3967 | 0.2624 | 0.2224 | 0.23805 | 0.8424 |
| DG 36:4 | 638.4888 | 25.322704 | Lipid | Diacylglycerol | 0.1758 | 0.1353 | 0.193915 | 0.5541 | -0.0645 | 0.1707 | 0.705583 | 0.8832 | 0.3042 | 0.1957 | 0.119955 | 0.5912 | NaN | 0.0002 | 0.1294 | 0.999045 | 0.9999 | -0.0881 | 0.1497 | 0.556099 | 0.9009 | 0.0458 | 0.1998 | 0.818476 | 0.9653 | NaN | 0.0844 | 0.1263 | 0.504123 | 0.9053 | 0.0145 | 0.1478 | 0.921784 | 0.973 | 0.1324 | 0.1935 | 0.49372 | 0.9848 | NaN | 0.0319 | 0.132 | 0.808862 | 0.9433 | -0.1552 | 0.1568 | 0.322217 | 0.6497 | 0.134 | 0.1957 | 0.493409 | 0.9375 | NaN | 0.0551 | 0.1294 | 0.67011 | 0.9077 | -0.0947 | 0.15 | 0.528115 | 0.8496 | 0.1519 | 0.1955 | 0.437086 | 0.9359 | NaN | 0.05 | 0.1315 | 0.703661 | 0.9035 | -0.1519 | 0.1542 | 0.32442 | 0.6724 | 0.1685 | 0.1956 | 0.388963 | 0.8887 |
| DG 38:4 | 666.5223 | 26.351738 | Lipid | Diacylglycerol | 0.083 | 0.1355 | 0.540227 | 0.825 | -0.0766 | 0.1326 | 0.563384 | 0.7994 | 0.2775 | 0.2351 | 0.237936 | 0.735 | NaN | -0.0397 | 0.1271 | 0.754729 | 0.9509 | -0.1119 | 0.1162 | 0.335737 | 0.8095 | 0.0576 | 0.2299 | 0.802012 | 0.9617 | NaN | 0.0099 | 0.1258 | 0.93754 | 0.9728 | -0.0493 | 0.1144 | 0.666895 | 0.9112 | 0.094 | 0.2296 | 0.682158 | 0.9894 | NaN | -0.0368 | 0.1305 | 0.778053 | 0.936 | -0.1513 | 0.1217 | 0.213804 | 0.5546 | 0.117 | 0.2302 | 0.611347 | 0.9375 | NaN | -0.0174 | 0.1285 | 0.892532 | 0.9674 | -0.1253 | 0.1165 | 0.282015 | 0.7544 | 0.1322 | 0.2305 | 0.566407 | 0.9621 | NaN | -0.019 | 0.1302 | 0.884146 | 0.9588 | -0.1589 | 0.1198 | 0.184637 | 0.5692 | 0.1654 | 0.2298 | 0.471616 | 0.8887 |
| DG 36:5 | 636.472 | 24.87105 | Lipid | Diacylglycerol | 0.142 | 0.132 | 0.282334 | 0.6604 | 0.023 | 0.1316 | 0.861089 | 0.932 | 0.2598 | 0.2239 | 0.245845 | 0.7391 | NaN | 0.0381 | 0.1237 | 0.757975 | 0.9509 | 0.0281 | 0.1155 | 0.80798 | 0.965 | 0.0296 | 0.2205 | 0.89324 | 0.977 | NaN | 0.0857 | 0.1225 | 0.484112 | 0.8967 | 0.0618 | 0.1134 | 0.585991 | 0.9053 | 0.1109 | 0.2168 | 0.6089 | 0.9894 | NaN | -0.0057 | 0.1289 | 0.965042 | 0.9828 | -0.0576 | 0.1217 | 0.636044 | 0.83 | 0.0312 | 0.2259 | 0.890063 | 0.99 | NaN | 0.0714 | 0.1247 | 0.566864 | 0.8722 | 0.0261 | 0.1157 | 0.821426 | 0.9396 | 0.1215 | 0.2195 | 0.57998 | 0.9621 | NaN | 0.019 | 0.1282 | 0.882035 | 0.9588 | -0.0537 | 0.1196 | 0.653594 | 0.8652 | 0.0908 | 0.2241 | 0.685157 | 0.9459 |
| DG 38:5 | 664.5056 | 25.86453 | Lipid | Diacylglycerol | 0.3149 | 0.1371 | 0.021587 | 0.1953 | -0.0248 | 0.1401 | 0.85962 | 0.932 | 0.6617 | 0.2246 | 0.003214 | 0.1069 | NaN | 0.1682 | 0.1306 | 0.19765 | 0.7316 | -0.1335 | 0.1238 | 0.280919 | 0.7996 | 0.4861 | 0.2208 | 0.027671 | 0.5113 | NaN | 0.2168 | 0.1285 | 0.091518 | 0.5342 | -0.0637 | 0.1207 | 0.597492 | 0.9053 | 0.5132 | 0.2203 | 0.019814 | 0.3038 | NaN | 0.1677 | 0.1348 | 0.213304 | 0.6949 | -0.1676 | 0.1309 | 0.20035 | 0.5448 | 0.5115 | 0.2231 | 0.021846 | 0.4551 | NaN | 0.1984 | 0.1314 | 0.131243 | 0.6708 | -0.1147 | 0.1238 | 0.354012 | 0.7839 | 0.5311 | 0.2224 | 0.016957 | 0.423 | NaN | 0.1757 | 0.1348 | 0.192286 | 0.6472 | -0.1724 | 0.1285 | 0.179737 | 0.5692 | 0.5323 | 0.2244 | 0.017698 | 0.4132 |
| 15R-PGE2 methyl ester, 15-acetate | 408.2501 | 17.902542 | Lipid | Eicosanoid | -0.0726 | 0.1285 | 0.571963 | 0.8418 | -0.1481 | 0.1785 | 0.406622 | 0.674 | -0.0861 | 0.1819 | 0.636078 | 0.9104 | NaN | -0.0877 | 0.1188 | 0.460288 | 0.8498 | -0.2142 | 0.1562 | 0.170325 | 0.6773 | -0.0743 | 0.1706 | 0.663206 | 0.954 | NaN | -0.0707 | 0.1186 | 0.551262 | 0.9125 | -0.1114 | 0.154 | 0.469682 | 0.901 | -0.0714 | 0.1718 | 0.677815 | 0.9894 | NaN | -0.0664 | 0.1215 | 0.584777 | 0.8473 | -0.2725 | 0.1638 | 0.096215 | 0.4318 | -0.0282 | 0.1739 | 0.871012 | 0.9856 | NaN | -0.0709 | 0.1204 | 0.556067 | 0.872 | -0.2477 | 0.1566 | 0.113704 | 0.5706 | -0.0419 | 0.1743 | 0.810129 | 0.9621 | NaN | -0.072 | 0.1217 | 0.554122 | 0.8616 | -0.2792 | 0.1611 | 0.083017 | 0.3967 | -0.0393 | 0.1753 | 0.822816 | 0.9641 |
| leukotriene B4 | 336.2348 | 22.004122 | Lipid | Eicosanoid | 0.0004 | 0.1333 | 0.997338 | 0.9973 | 0.257 | 0.1596 | 0.107337 | 0.3922 | -0.1094 | 0.1971 | 0.578914 | 0.8849 | NaN | 0.0424 | 0.1234 | 0.731337 | 0.9367 | 0.159 | 0.1423 | 0.263748 | 0.7853 | 0.0208 | 0.1883 | 0.911926 | 0.9793 | NaN | 0.0206 | 0.1231 | 0.867374 | 0.9714 | 0.112 | 0.1413 | 0.428133 | 0.8947 | -0.0116 | 0.1884 | 0.950735 | 0.9976 | NaN | 0.0127 | 0.1261 | 0.919473 | 0.9828 | 0.1262 | 0.1508 | 0.402888 | 0.6937 | 0.0068 | 0.1908 | 0.971497 | 0.99 | NaN | 0.0075 | 0.1249 | 0.951889 | 0.9796 | 0.1469 | 0.1431 | 0.304386 | 0.7544 | -0.0444 | 0.1895 | 0.814883 | 0.9621 | NaN | 0.0176 | 0.1263 | 0.888993 | 0.9591 | 0.1409 | 0.1473 | 0.338808 | 0.6758 | -0.0139 | 0.1921 | 0.942246 | 0.9869 |
| FA 9:0 | 158.1307 | 18.327808 | Lipid | Fatty Acid | 0.1411 | 0.1352 | 0.296523 | 0.6742 | 0.2594 | 0.1467 | 0.076987 | 0.3571 | 0.0539 | 0.2115 | 0.798704 | 0.9647 | NaN | 0.1164 | 0.1251 | 0.352325 | 0.8419 | 0.1648 | 0.131 | 0.20845 | 0.7304 | 0.0921 | 0.1985 | 0.642469 | 0.954 | NaN | 0.0311 | 0.1265 | 0.806079 | 0.9673 | 0.1452 | 0.1292 | 0.2609 | 0.8057 | -0.0509 | 0.2018 | 0.800966 | 0.9935 | NaN | 0.1524 | 0.1277 | 0.232698 | 0.7062 | 0.2328 | 0.1344 | 0.083172 | 0.4089 | 0.0998 | 0.2013 | 0.62024 | 0.9375 | NaN | 0.1138 | 0.1269 | 0.369583 | 0.7978 | 0.1601 | 0.1315 | 0.223399 | 0.7047 | 0.0806 | 0.202 | 0.689927 | 0.9621 | NaN | 0.1517 | 0.128 | 0.235996 | 0.7013 | 0.1962 | 0.1335 | 0.141577 | 0.5193 | 0.1233 | 0.2039 | 0.545396 | 0.9041 |
| FA 12:0 | 200.1775 | 21.715498 | Lipid | Fatty Acid | -0.2203 | 0.1302 | 0.090546 | 0.4349 | -0.1579 | 0.1412 | 0.263306 | 0.5505 | -0.2615 | 0.2059 | 0.203917 | 0.7107 | NaN | -0.2061 | 0.1204 | 0.086955 | 0.6076 | -0.1339 | 0.124 | 0.280287 | 0.7996 | -0.2651 | 0.1928 | 0.169165 | 0.879 | NaN | -0.2571 | 0.1198 | 0.031952 | 0.2852 | -0.0699 | 0.1232 | 0.570391 | 0.9053 | -0.4303 | 0.196 | 0.028147 | 0.3487 | NaN | -0.2406 | 0.1228 | 0.050201 | 0.4263 | -0.1936 | 0.1287 | 0.132547 | 0.4784 | -0.2764 | 0.1954 | 0.157223 | 0.8679 | NaN | -0.1849 | 0.1223 | 0.130792 | 0.6708 | -0.1116 | 0.1247 | 0.371043 | 0.7999 | -0.2412 | 0.1968 | 0.220258 | 0.8892 | NaN | -0.2126 | 0.1233 | 0.084706 | 0.5441 | -0.1815 | 0.1267 | 0.152064 | 0.5214 | -0.2366 | 0.1979 | 0.231937 | 0.8424 |
| FA 14:0 | 228.2091 | 22.407074 | Lipid | Fatty Acid | -0.0169 | 0.1306 | 0.896968 | 0.9809 | -0.101 | 0.1402 | 0.471387 | 0.7413 | 0.0546 | 0.2072 | 0.79214 | 0.9647 | NaN | -0.0948 | 0.1213 | 0.434412 | 0.8498 | -0.106 | 0.1229 | 0.388258 | 0.8339 | -0.0889 | 0.1977 | 0.653166 | 0.954 | NaN | -0.0613 | 0.1207 | 0.611473 | 0.9125 | -0.011 | 0.1221 | 0.928509 | 0.9733 | -0.1049 | 0.2003 | 0.600433 | 0.9894 | NaN | -0.1113 | 0.1246 | 0.3717 | 0.7571 | -0.1579 | 0.1282 | 0.218013 | 0.5546 | -0.0727 | 0.2004 | 0.716958 | 0.9477 | NaN | -0.0778 | 0.1227 | 0.526326 | 0.8625 | -0.0941 | 0.1233 | 0.44515 | 0.8218 | -0.0566 | 0.2008 | 0.777862 | 0.9621 | NaN | -0.0946 | 0.1245 | 0.447535 | 0.801 | -0.1431 | 0.1261 | 0.256406 | 0.6316 | -0.0493 | 0.2017 | 0.807105 | 0.9623 |
| FA 15:0 | 242.2245 | 22.619587 | Lipid | Fatty Acid | -0.0697 | 0.1273 | 0.583951 | 0.8423 | -0.1497 | 0.129 | 0.245839 | 0.538 | 0.0158 | 0.2125 | 0.940607 | 0.9887 | NaN | -0.1168 | 0.1178 | 0.321686 | 0.7963 | -0.1548 | 0.1129 | 0.170542 | 0.6773 | -0.0709 | 0.2005 | 0.723443 | 0.954 | NaN | -0.0614 | 0.1176 | 0.601263 | 0.9125 | -0.0609 | 0.1128 | 0.589425 | 0.9053 | -0.056 | 0.2016 | 0.780984 | 0.9935 | NaN | -0.1452 | 0.121 | 0.230055 | 0.7062 | -0.211 | 0.1177 | 0.072969 | 0.3762 | -0.065 | 0.2033 | 0.749101 | 0.9572 | NaN | -0.1114 | 0.1194 | 0.350851 | 0.7873 | -0.1613 | 0.1131 | 0.153837 | 0.631 | -0.049 | 0.2038 | 0.809991 | 0.9621 | NaN | -0.1219 | 0.1209 | 0.313188 | 0.7485 | -0.1983 | 0.1157 | 0.08649 | 0.4044 | -0.0318 | 0.2045 | 0.876416 | 0.9695 |
| FA 16:0 | 256.2406 | 22.803902 | Lipid | Fatty Acid | 0.041 | 0.1321 | 0.756578 | 0.9343 | -0.1308 | 0.1404 | 0.351251 | 0.6332 | 0.1884 | 0.2107 | 0.371226 | 0.7534 | NaN | -0.0461 | 0.1231 | 0.70817 | 0.9314 | -0.1227 | 0.1231 | 0.319078 | 0.8095 | 0.0131 | 0.2038 | 0.948815 | 0.9911 | NaN | 0.0103 | 0.1221 | 0.932505 | 0.9728 | -0.0289 | 0.1227 | 0.814121 | 0.9402 | 0.0418 | 0.204 | 0.837654 | 0.9935 | NaN | -0.0644 | 0.1267 | 0.610986 | 0.8573 | -0.1773 | 0.1281 | 0.166359 | 0.5102 | 0.0295 | 0.2068 | 0.886666 | 0.99 | NaN | -0.0414 | 0.1248 | 0.739765 | 0.9289 | -0.1232 | 0.1234 | 0.317951 | 0.7579 | 0.0379 | 0.2076 | 0.855223 | 0.9621 | NaN | -0.0496 | 0.1266 | 0.695344 | 0.9035 | -0.1657 | 0.1261 | 0.188681 | 0.5692 | 0.0555 | 0.2079 | 0.789358 | 0.9525 |
| FA 17:0 | 270.256 | 22.96632 | Lipid | Fatty Acid | 0.0752 | 0.1299 | 0.562853 | 0.8352 | 0.1288 | 0.1374 | 0.348726 | 0.6332 | 0.0394 | 0.2096 | 0.850975 | 0.9732 | NaN | -0.054 | 0.1222 | 0.658238 | 0.9185 | 0.0165 | 0.123 | 0.893634 | 0.9729 | -0.0958 | 0.1995 | 0.631114 | 0.954 | NaN | 0.0165 | 0.1204 | 0.891117 | 0.9714 | 0.1145 | 0.1184 | 0.333401 | 0.8587 | -0.0512 | 0.1994 | 0.79745 | 0.9935 | NaN | -0.036 | 0.1249 | 0.773496 | 0.936 | 0.0199 | 0.1289 | 0.877393 | 0.961 | -0.0626 | 0.2014 | 0.755848 | 0.9586 | NaN | -0.0324 | 0.1235 | 0.79321 | 0.9477 | 0.021 | 0.1232 | 0.864557 | 0.9614 | -0.0604 | 0.2024 | 0.765228 | 0.9621 | NaN | -0.036 | 0.1253 | 0.774162 | 0.9371 | 0.0104 | 0.127 | 0.93445 | 0.9823 | -0.0571 | 0.2035 | 0.778906 | 0.9525 |
| FA 18:0 | 284.2719 | 23.144428 | Lipid | Fatty Acid | 0.0897 | 0.1301 | 0.490404 | 0.8041 | 0.0264 | 0.1428 | 0.853022 | 0.932 | 0.1423 | 0.2034 | 0.484389 | 0.8356 | NaN | 0.0002 | 0.1214 | 0.998433 | 0.9999 | 0.0011 | 0.1254 | 0.993056 | 0.9953 | -0.0037 | 0.1951 | 0.984765 | 0.9964 | NaN | 0.062 | 0.1203 | 0.606377 | 0.9125 | 0.1039 | 0.1233 | 0.399312 | 0.8818 | 0.0318 | 0.195 | 0.870615 | 0.9935 | NaN | -0.0076 | 0.1248 | 0.951606 | 0.9828 | -0.0331 | 0.1313 | 0.801022 | 0.9172 | 0.0092 | 0.1979 | 0.963007 | 0.99 | NaN | 0.0067 | 0.1231 | 0.956684 | 0.9796 | -0.0081 | 0.1257 | 0.948854 | 0.9923 | 0.0247 | 0.1982 | 0.900714 | 0.9681 | NaN | 0.0043 | 0.1247 | 0.972732 | 0.9893 | -0.0265 | 0.1291 | 0.837239 | 0.9451 | 0.0313 | 0.1992 | 0.875184 | 0.9695 |
| FA 19:0 | 298.2865 | 23.328478 | Lipid | Fatty Acid | -0.0462 | 0.1314 | 0.724994 | 0.9287 | -0.0753 | 0.14 | 0.590556 | 0.8109 | -0.0141 | 0.2119 | 0.947013 | 0.9887 | NaN | -0.069 | 0.1215 | 0.57015 | 0.9079 | -0.0632 | 0.1229 | 0.607287 | 0.9043 | -0.0889 | 0.1995 | 0.65607 | 0.954 | NaN | -0.0685 | 0.1213 | 0.572364 | 0.9125 | -0.0252 | 0.1211 | 0.835003 | 0.9475 | -0.125 | 0.202 | 0.535955 | 0.9894 | NaN | -0.0621 | 0.1242 | 0.617047 | 0.8606 | -0.0957 | 0.128 | 0.454418 | 0.7319 | -0.0421 | 0.2016 | 0.834505 | 0.9726 | NaN | -0.0298 | 0.1231 | 0.808598 | 0.952 | -0.0172 | 0.1238 | 0.889207 | 0.9727 | -0.0448 | 0.2025 | 0.825098 | 0.9621 | NaN | -0.0572 | 0.1245 | 0.645569 | 0.8907 | -0.0857 | 0.126 | 0.496283 | 0.7792 | -0.0409 | 0.2035 | 0.840905 | 0.9641 |
| FA 20:0 | 312.303 | 23.478868 | Lipid | Fatty Acid | 0.0281 | 0.1327 | 0.832376 | 0.9746 | -0.2252 | 0.1407 | 0.109419 | 0.3922 | 0.2363 | 0.2102 | 0.260817 | 0.7397 | NaN | 0.0227 | 0.1227 | 0.853229 | 0.9705 | -0.1201 | 0.1262 | 0.34129 | 0.8095 | 0.1201 | 0.2004 | 0.549111 | 0.954 | NaN | 0.0601 | 0.1226 | 0.623954 | 0.9185 | -0.0446 | 0.1271 | 0.725866 | 0.9241 | 0.1315 | 0.2015 | 0.513891 | 0.9894 | NaN | -0.0296 | 0.126 | 0.81447 | 0.9445 | -0.1983 | 0.129 | 0.124129 | 0.463 | 0.0938 | 0.2056 | 0.648234 | 0.9375 | NaN | 0.0267 | 0.1244 | 0.830217 | 0.9564 | -0.128 | 0.1261 | 0.310332 | 0.7544 | 0.1525 | 0.2031 | 0.452844 | 0.9359 | NaN | -0.0009 | 0.1259 | 0.994015 | 0.9956 | -0.1789 | 0.1275 | 0.160566 | 0.5372 | 0.1422 | 0.205 | 0.487797 | 0.8887 |
| FA 22:0 | 340.3339 | 24.054163 | Lipid | Fatty Acid | 0.2224 | 0.1364 | 0.102943 | 0.462 | 0.2402 | 0.1457 | 0.099244 | 0.3816 | 0.2379 | 0.2179 | 0.274967 | 0.744 | NaN | 0.2447 | 0.1258 | 0.05184 | 0.4443 | 0.2731 | 0.1268 | 0.031282 | 0.3133 | 0.2413 | 0.2042 | 0.237279 | 0.9223 | NaN | 0.2301 | 0.1257 | 0.067218 | 0.4638 | 0.2945 | 0.124 | 0.01758 | 0.2556 | 0.1861 | 0.2066 | 0.367771 | 0.9578 | NaN | 0.2463 | 0.1287 | 0.055622 | 0.445 | 0.2762 | 0.1324 | 0.037043 | 0.2538 | 0.25 | 0.2069 | 0.226895 | 0.8705 | NaN | 0.2467 | 0.1275 | 0.053071 | 0.4507 | 0.326 | 0.1266 | 0.009995 | 0.1672 | 0.2095 | 0.2084 | 0.314766 | 0.9106 | NaN | 0.2478 | 0.129 | 0.054679 | 0.4439 | 0.2799 | 0.1303 | 0.031637 | 0.2495 | 0.2492 | 0.2089 | 0.23284 | 0.8424 |
| FA 24:0 | 368.3658 | 24.705492 | Lipid | Fatty Acid | -0.0029 | 0.1361 | 0.982723 | 0.9936 | 0.1465 | 0.1355 | 0.279909 | 0.5701 | -0.1239 | 0.2377 | 0.602021 | 0.8909 | NaN | -0.0317 | 0.126 | 0.801039 | 0.9571 | 0.1656 | 0.1185 | 0.162331 | 0.6638 | -0.1982 | 0.2232 | 0.374414 | 0.9312 | NaN | -0.0166 | 0.1257 | 0.895183 | 0.9714 | 0.161 | 0.1163 | 0.166402 | 0.7308 | -0.1695 | 0.2245 | 0.450146 | 0.9816 | NaN | -0.0065 | 0.1287 | 0.959801 | 0.9828 | 0.1687 | 0.1236 | 0.172477 | 0.5146 | -0.1274 | 0.2259 | 0.57271 | 0.9375 | NaN | -0.0326 | 0.1277 | 0.798408 | 0.9498 | 0.168 | 0.1188 | 0.157239 | 0.631 | -0.1994 | 0.2276 | 0.380779 | 0.9106 | NaN | -0.0147 | 0.129 | 0.909462 | 0.971 | 0.163 | 0.1218 | 0.180711 | 0.5692 | -0.1421 | 0.228 | 0.533077 | 0.8971 |
| FA 25:0 | 382.3813 | 24.61329 | Lipid | Fatty Acid | 0.097 | 0.1354 | 0.473654 | 0.7972 | -0.0391 | 0.1355 | 0.773118 | 0.9217 | 0.2288 | 0.2297 | 0.319257 | 0.7534 | NaN | 0.0828 | 0.1252 | 0.508503 | 0.8786 | 0.0451 | 0.1199 | 0.706953 | 0.934 | 0.0843 | 0.2198 | 0.701214 | 0.954 | NaN | 0.1278 | 0.1249 | 0.306496 | 0.7943 | 0.1961 | 0.1216 | 0.10682 | 0.6422 | 0.0522 | 0.2237 | 0.815515 | 0.9935 | NaN | 0.0595 | 0.1283 | 0.643102 | 0.8652 | -0.0308 | 0.124 | 0.803751 | 0.9172 | 0.1163 | 0.2218 | 0.600106 | 0.9375 | NaN | 0.0731 | 0.127 | 0.565049 | 0.8722 | 0.0265 | 0.1198 | 0.824675 | 0.9397 | 0.1072 | 0.2236 | 0.631514 | 0.9621 | NaN | 0.0748 | 0.1284 | 0.560141 | 0.8661 | -0.0195 | 0.1222 | 0.873237 | 0.961 | 0.148 | 0.2227 | 0.506268 | 0.8946 |
| FA 26:0 | 396.3969 | 25.627758 | Lipid | Fatty Acid | 0.1774 | 0.1294 | 0.170489 | 0.531 | 0.1174 | 0.1211 | 0.332084 | 0.6193 | 0.301 | 0.2393 | 0.208568 | 0.7107 | NaN | 0.1799 | 0.1196 | 0.1325 | 0.6772 | 0.2173 | 0.1059 | 0.040233 | 0.3602 | 0.1611 | 0.2288 | 0.481252 | 0.954 | NaN | 0.1501 | 0.1197 | 0.209925 | 0.7361 | 0.1668 | 0.1037 | 0.107835 | 0.6422 | 0.1554 | 0.231 | 0.501086 | 0.9894 | NaN | 0.1906 | 0.1222 | 0.118962 | 0.579 | 0.1993 | 0.1109 | 0.072125 | 0.3762 | 0.2237 | 0.2294 | 0.329449 | 0.9044 | NaN | 0.1852 | 0.1212 | 0.126311 | 0.6708 | 0.234 | 0.1063 | 0.02775 | 0.2645 | 0.1786 | 0.233 | 0.443352 | 0.9359 | NaN | 0.2011 | 0.1225 | 0.100592 | 0.5529 | 0.2077 | 0.109 | 0.056836 | 0.3201 | 0.2503 | 0.2307 | 0.277994 | 0.8424 |
| FA 28:0 | 424.39 | 23.17103 | Lipid | Fatty Acid | 0.1952 | 0.1293 | 0.131172 | 0.5013 | -0.1532 | 0.1536 | 0.318667 | 0.6107 | 0.416 | 0.1914 | 0.029738 | 0.3084 | NaN | 0.2553 | 0.1193 | 0.032416 | 0.3509 | 0.0139 | 0.1392 | 0.920574 | 0.9729 | 0.39 | 0.1796 | 0.029948 | 0.5113 | NaN | 0.2526 | 0.1191 | 0.033979 | 0.2852 | 0.0699 | 0.1385 | 0.613544 | 0.9053 | 0.3538 | 0.1824 | 0.052392 | 0.477 | NaN | 0.193 | 0.1222 | 0.114278 | 0.5709 | -0.0703 | 0.1424 | 0.621573 | 0.8228 | 0.3478 | 0.1841 | 0.058849 | 0.5801 | NaN | 0.2538 | 0.121 | 0.035935 | 0.3542 | 0.0166 | 0.1396 | 0.905597 | 0.9744 | 0.3988 | 0.1828 | 0.029118 | 0.4772 | NaN | 0.2183 | 0.1223 | 0.074412 | 0.5189 | -0.052 | 0.1407 | 0.711879 | 0.8887 | 0.3842 | 0.1843 | 0.037077 | 0.4663 |
| FA 14:1 | 226.1935 | 22.031717 | Lipid | Fatty Acid | -0.2442 | 0.1321 | 0.064645 | 0.3641 | -0.1697 | 0.1321 | 0.198748 | 0.4993 | -0.3243 | 0.2247 | 0.148963 | 0.6229 | NaN | -0.3588 | 0.122 | 0.003275 | 0.0791 | -0.2391 | 0.115 | 0.037627 | 0.3462 | -0.4792 | 0.211 | 0.02314 | 0.4888 | NaN | -0.332 | 0.1216 | 0.00635 | 0.0974 | -0.1195 | 0.1144 | 0.296167 | 0.8336 | -0.583 | 0.2157 | 0.006875 | 0.1518 | NaN | -0.3901 | 0.1259 | 0.00194 | 0.0446 | -0.3005 | 0.1211 | 0.013052 | 0.14 | -0.4718 | 0.2145 | 0.027829 | 0.4788 | NaN | -0.3346 | 0.1237 | 0.006822 | 0.1299 | -0.2252 | 0.1153 | 0.050841 | 0.3844 | -0.4413 | 0.215 | 0.040119 | 0.4772 | NaN | -0.3703 | 0.1258 | 0.003255 | 0.0642 | -0.3029 | 0.1188 | 0.010788 | 0.1267 | -0.4309 | 0.2161 | 0.046175 | 0.4743 |
| FA 16:1 | 254.225 | 22.542202 | Lipid | Fatty Acid | -0.1104 | 0.1332 | 0.407362 | 0.734 | -0.2825 | 0.139 | 0.042123 | 0.2929 | 0.0391 | 0.214 | 0.854898 | 0.9732 | NaN | -0.1956 | 0.1234 | 0.112992 | 0.6749 | -0.2731 | 0.1214 | 0.024519 | 0.2806 | -0.1372 | 0.2054 | 0.504222 | 0.954 | NaN | -0.1489 | 0.1229 | 0.22579 | 0.7361 | -0.148 | 0.1238 | 0.232141 | 0.8003 | -0.1674 | 0.2091 | 0.423192 | 0.9816 | NaN | -0.2291 | 0.1272 | 0.071695 | 0.4947 | -0.3518 | 0.1257 | 0.005112 | 0.0822 | -0.1225 | 0.2085 | 0.556875 | 0.9375 | NaN | -0.1833 | 0.1251 | 0.142849 | 0.6708 | -0.268 | 0.1218 | 0.027793 | 0.2645 | -0.1037 | 0.2088 | 0.619558 | 0.9621 | NaN | -0.2074 | 0.1271 | 0.102618 | 0.5529 | -0.3313 | 0.1237 | 0.007402 | 0.1135 | -0.094 | 0.2097 | 0.653981 | 0.9459 |
| FA 17:1 | 268.2396 | 22.72618 | Lipid | Fatty Acid | 0.0637 | 0.1305 | 0.625287 | 0.8678 | -0.183 | 0.1314 | 0.163771 | 0.479 | 0.3248 | 0.2165 | 0.133632 | 0.6043 | NaN | -0.0644 | 0.1226 | 0.599802 | 0.9079 | -0.2883 | 0.1143 | 0.011638 | 0.1836 | 0.171 | 0.2089 | 0.41315 | 0.9419 | NaN | -0.0249 | 0.1215 | 0.837836 | 0.9714 | -0.1601 | 0.1133 | 0.15746 | 0.7183 | 0.1146 | 0.2158 | 0.595515 | 0.9894 | NaN | -0.054 | 0.1257 | 0.667657 | 0.8697 | -0.315 | 0.1203 | 0.008828 | 0.1189 | 0.218 | 0.2096 | 0.298158 | 0.8823 | NaN | -0.0299 | 0.1236 | 0.809104 | 0.952 | -0.2701 | 0.1145 | 0.018331 | 0.2263 | 0.2221 | 0.2105 | 0.291449 | 0.9039 | NaN | -0.0271 | 0.1252 | 0.828653 | 0.9491 | -0.3028 | 0.1179 | 0.010198 | 0.1267 | 0.2552 | 0.2099 | 0.223914 | 0.8424 |
| FA 18:1 | 282.2566 | 22.883368 | Lipid | Fatty Acid | -0.0898 | 0.1345 | 0.504099 | 0.8067 | -0.2585 | 0.1428 | 0.070346 | 0.3377 | 0.0493 | 0.2133 | 0.817031 | 0.9713 | NaN | -0.1528 | 0.1245 | 0.219418 | 0.7495 | -0.2453 | 0.125 | 0.049752 | 0.4099 | -0.088 | 0.203 | 0.664608 | 0.954 | NaN | -0.1131 | 0.1241 | 0.361868 | 0.8259 | -0.1383 | 0.1262 | 0.273196 | 0.806 | -0.108 | 0.2057 | 0.599517 | 0.9894 | NaN | -0.1889 | 0.128 | 0.140194 | 0.6148 | -0.3152 | 0.1295 | 0.014944 | 0.1422 | -0.0917 | 0.2067 | 0.657267 | 0.9375 | NaN | -0.1498 | 0.1262 | 0.235281 | 0.7108 | -0.2368 | 0.1255 | 0.05917 | 0.4149 | -0.0768 | 0.2072 | 0.710965 | 0.9621 | NaN | -0.1688 | 0.128 | 0.187102 | 0.6463 | -0.2982 | 0.1275 | 0.019357 | 0.1781 | -0.0631 | 0.2079 | 0.761609 | 0.9525 |
| FA 19:1 | 296.2718 | 23.05411 | Lipid | Fatty Acid | 0.0374 | 0.1296 | 0.772931 | 0.9439 | -0.0009 | 0.1332 | 0.994525 | 0.9963 | 0.0979 | 0.2147 | 0.648565 | 0.911 | NaN | -0.0256 | 0.1204 | 0.831672 | 0.967 | -0.1082 | 0.1181 | 0.359266 | 0.8161 | 0.0743 | 0.2016 | 0.71222 | 0.954 | NaN | -0.009 | 0.12 | 0.940295 | 0.9728 | -0.0138 | 0.1148 | 0.904062 | 0.973 | -0.0024 | 0.2049 | 0.99077 | 0.9976 | NaN | -0.0317 | 0.1234 | 0.79704 | 0.9381 | -0.1357 | 0.1248 | 0.276846 | 0.6088 | 0.096 | 0.2041 | 0.638009 | 0.9375 | NaN | -0.0174 | 0.1219 | 0.886196 | 0.9672 | -0.1046 | 0.1182 | 0.376455 | 0.7999 | 0.0781 | 0.2052 | 0.703476 | 0.9621 | NaN | -0.0281 | 0.1236 | 0.820328 | 0.9491 | -0.1452 | 0.1227 | 0.236593 | 0.6121 | 0.098 | 0.206 | 0.634497 | 0.9459 |
| FA 20:1 | 310.2876 | 23.21554 | Lipid | Fatty Acid | -0.1133 | 0.1362 | 0.405299 | 0.734 | -0.3305 | 0.1403 | 0.018453 | 0.2054 | 0.0767 | 0.2195 | 0.726641 | 0.9635 | NaN | -0.1708 | 0.1259 | 0.174975 | 0.7251 | -0.2949 | 0.1232 | 0.016649 | 0.2189 | -0.0789 | 0.2098 | 0.707041 | 0.954 | NaN | -0.1298 | 0.1256 | 0.301621 | 0.7865 | -0.1701 | 0.1267 | 0.179375 | 0.7308 | -0.1218 | 0.2141 | 0.569353 | 0.9894 | NaN | -0.2234 | 0.1298 | 0.085185 | 0.5283 | -0.39 | 0.1265 | 0.00204 | 0.055 | -0.0849 | 0.214 | 0.691428 | 0.9476 | NaN | -0.175 | 0.1277 | 0.170552 | 0.6753 | -0.3174 | 0.1227 | 0.009676 | 0.1669 | -0.0497 | 0.2133 | 0.815712 | 0.9621 | NaN | -0.1976 | 0.1296 | 0.127245 | 0.605 | -0.3793 | 0.1244 | 0.002304 | 0.0553 | -0.0395 | 0.2142 | 0.853702 | 0.9641 |
| FA 22:1 | 338.319 | 23.61596 | Lipid | Fatty Acid | -0.0587 | 0.1354 | 0.664513 | 0.886 | -0.2854 | 0.1316 | 0.03008 | 0.2636 | 0.1879 | 0.2308 | 0.415446 | 0.7762 | NaN | -0.0674 | 0.1252 | 0.590497 | 0.9079 | -0.2239 | 0.1167 | 0.054991 | 0.4399 | 0.0768 | 0.219 | 0.725913 | 0.954 | NaN | -0.0274 | 0.1252 | 0.827 | 0.9714 | -0.1385 | 0.1184 | 0.242252 | 0.8037 | 0.0641 | 0.2213 | 0.772184 | 0.9935 | NaN | -0.1046 | 0.1282 | 0.414834 | 0.7815 | -0.281 | 0.1199 | 0.019104 | 0.1701 | 0.0683 | 0.2229 | 0.759361 | 0.9586 | NaN | -0.0574 | 0.1269 | 0.651015 | 0.9029 | -0.2076 | 0.1176 | 0.077585 | 0.4639 | 0.0969 | 0.2227 | 0.663418 | 0.9621 | NaN | -0.0852 | 0.1284 | 0.506853 | 0.8285 | -0.2659 | 0.1184 | 0.024709 | 0.2033 | 0.1013 | 0.2238 | 0.650739 | 0.9459 |
| FA 24:1 | 366.3504 | 24.114376 | Lipid | Fatty Acid | -0.0811 | 0.132 | 0.538974 | 0.825 | -0.1547 | 0.1377 | 0.261285 | 0.5505 | -0.0142 | 0.2138 | 0.947196 | 0.9887 | NaN | -0.0853 | 0.122 | 0.484743 | 0.8576 | -0.1224 | 0.1212 | 0.312504 | 0.8095 | -0.0595 | 0.2008 | 0.767 | 0.954 | NaN | -0.0714 | 0.1219 | 0.558034 | 0.9125 | -0.0479 | 0.1208 | 0.691844 | 0.9195 | -0.1003 | 0.203 | 0.62122 | 0.9894 | NaN | -0.1186 | 0.1248 | 0.342024 | 0.741 | -0.1779 | 0.1256 | 0.156696 | 0.5021 | -0.07 | 0.2037 | 0.731132 | 0.9551 | NaN | -0.0811 | 0.1237 | 0.511992 | 0.8625 | -0.0993 | 0.122 | 0.41541 | 0.8188 | -0.0647 | 0.2046 | 0.751698 | 0.9621 | NaN | -0.1048 | 0.125 | 0.402047 | 0.787 | -0.1576 | 0.1238 | 0.203242 | 0.5756 | -0.0596 | 0.2056 | 0.771777 | 0.9525 |
| FA 25:1 | 380.3652 | 24.144978 | Lipid | Fatty Acid | -0.0097 | 0.137 | 0.943287 | 0.9855 | 0.0356 | 0.1362 | 0.793771 | 0.932 | -0.0562 | 0.236 | 0.811822 | 0.9713 | NaN | 0.0174 | 0.1268 | 0.890609 | 0.9705 | 0.1405 | 0.1203 | 0.24284 | 0.7677 | -0.1454 | 0.2222 | 0.512953 | 0.954 | NaN | 0.0626 | 0.127 | 0.622284 | 0.9185 | 0.2683 | 0.1202 | 0.025647 | 0.3319 | -0.1598 | 0.2242 | 0.475954 | 0.984 | NaN | -0.0312 | 0.1296 | 0.81005 | 0.9433 | 0.0417 | 0.1246 | 0.737581 | 0.8832 | -0.139 | 0.2253 | 0.537335 | 0.9375 | NaN | -0.0101 | 0.1284 | 0.937424 | 0.9796 | 0.1221 | 0.1203 | 0.309923 | 0.7544 | -0.1648 | 0.2272 | 0.468204 | 0.9359 | NaN | -0.0173 | 0.1299 | 0.894107 | 0.9621 | 0.0496 | 0.1227 | 0.686133 | 0.8747 | -0.1084 | 0.2269 | 0.633006 | 0.9459 |
| FA 26:1 | 394.3815 | 24.47697 | Lipid | Fatty Acid | 0.095 | 0.1318 | 0.47092 | 0.7972 | -0.0764 | 0.137 | 0.577235 | 0.8019 | 0.2552 | 0.217 | 0.239665 | 0.735 | NaN | 0.0945 | 0.1219 | 0.437858 | 0.8498 | 0.0198 | 0.1218 | 0.87094 | 0.9729 | 0.134 | 0.207 | 0.517387 | 0.954 | NaN | 0.1471 | 0.1217 | 0.226926 | 0.7361 | 0.1134 | 0.1221 | 0.35321 | 0.8722 | 0.1623 | 0.2073 | 0.433828 | 0.9816 | NaN | 0.0517 | 0.125 | 0.679448 | 0.8746 | -0.0552 | 0.1255 | 0.660289 | 0.8438 | 0.1191 | 0.2115 | 0.573371 | 0.9375 | NaN | 0.0789 | 0.1236 | 0.523025 | 0.8625 | 0.0073 | 0.1217 | 0.952149 | 0.9923 | 0.1382 | 0.2116 | 0.51374 | 0.9516 | NaN | 0.0682 | 0.1251 | 0.5855 | 0.8765 | -0.0394 | 0.1238 | 0.750505 | 0.9096 | 0.151 | 0.2121 | 0.476571 | 0.8887 |
| FA 16:2 | 252.2091 | 22.278397 | Lipid | Fatty Acid | -0.1165 | 0.1297 | 0.368754 | 0.7161 | -0.2591 | 0.1363 | 0.057337 | 0.3054 | -0.0034 | 0.2083 | 0.987131 | 0.9935 | NaN | -0.2043 | 0.1202 | 0.089141 | 0.6151 | -0.2764 | 0.1186 | 0.019743 | 0.2369 | -0.1482 | 0.1983 | 0.454796 | 0.9478 | NaN | -0.1815 | 0.1198 | 0.129635 | 0.6333 | -0.1597 | 0.1198 | 0.182705 | 0.7308 | -0.2139 | 0.2034 | 0.292978 | 0.9294 | NaN | -0.2352 | 0.1238 | 0.057514 | 0.4535 | -0.3599 | 0.1234 | 0.003542 | 0.0688 | -0.1303 | 0.201 | 0.516676 | 0.9375 | NaN | -0.1883 | 0.1217 | 0.121881 | 0.6708 | -0.268 | 0.119 | 0.024316 | 0.2532 | -0.117 | 0.2015 | 0.561576 | 0.9621 | NaN | -0.2106 | 0.1236 | 0.088466 | 0.5441 | -0.3482 | 0.1212 | 0.004065 | 0.0793 | -0.0932 | 0.2018 | 0.644149 | 0.9459 |
| FA 18:2 | 280.2409 | 22.678688 | Lipid | Fatty Acid | -0.009 | 0.1357 | 0.947295 | 0.9855 | -0.2254 | 0.1427 | 0.11422 | 0.3941 | 0.1749 | 0.2166 | 0.419375 | 0.7762 | NaN | -0.0745 | 0.1259 | 0.553883 | 0.9073 | -0.1933 | 0.1255 | 0.123484 | 0.6118 | 0.015 | 0.2081 | 0.942608 | 0.9911 | NaN | -0.033 | 0.1253 | 0.792576 | 0.9641 | -0.0879 | 0.1267 | 0.487804 | 0.9053 | 0.0027 | 0.2109 | 0.989678 | 0.9976 | NaN | -0.1072 | 0.1296 | 0.408102 | 0.7795 | -0.2676 | 0.1297 | 0.039123 | 0.2571 | 0.024 | 0.2115 | 0.909675 | 0.99 | NaN | -0.0676 | 0.1275 | 0.595872 | 0.8924 | -0.1901 | 0.1258 | 0.130841 | 0.5974 | 0.0415 | 0.2117 | 0.844589 | 0.9621 | NaN | -0.0853 | 0.1294 | 0.509847 | 0.8285 | -0.2513 | 0.1278 | 0.049218 | 0.289 | 0.0583 | 0.2121 | 0.783421 | 0.9525 |
| FA 20:2 | 308.2719 | 22.989353 | Lipid | Fatty Acid | -0.0727 | 0.1322 | 0.582451 | 0.8423 | -0.1952 | 0.138 | 0.15737 | 0.4721 | 0.0424 | 0.2137 | 0.842576 | 0.9732 | NaN | -0.1764 | 0.1229 | 0.151217 | 0.6956 | -0.2637 | 0.12 | 0.028039 | 0.292 | -0.0967 | 0.2034 | 0.634494 | 0.954 | NaN | -0.1213 | 0.1221 | 0.320695 | 0.8008 | -0.1364 | 0.1198 | 0.254809 | 0.8037 | -0.1154 | 0.206 | 0.575493 | 0.9894 | NaN | -0.204 | 0.1268 | 0.107717 | 0.5709 | -0.3244 | 0.1261 | 0.010125 | 0.127 | -0.093 | 0.2068 | 0.652777 | 0.9375 | NaN | -0.1632 | 0.1246 | 0.18997 | 0.6753 | -0.271 | 0.1203 | 0.024244 | 0.2532 | -0.0615 | 0.2065 | 0.765646 | 0.9621 | NaN | -0.1811 | 0.1266 | 0.152568 | 0.6269 | -0.3154 | 0.1237 | 0.010791 | 0.1267 | -0.0584 | 0.2076 | 0.778427 | 0.9525 |
| FA 22:2 | 336.3035 | 23.333275 | Lipid | Fatty Acid | -0.0417 | 0.1361 | 0.759474 | 0.9358 | -0.2564 | 0.1401 | 0.067179 | 0.3282 | 0.166 | 0.222 | 0.45459 | 0.8098 | NaN | -0.0563 | 0.1258 | 0.654721 | 0.918 | -0.2013 | 0.1238 | 0.103997 | 0.6118 | 0.0647 | 0.2104 | 0.758495 | 0.954 | NaN | -0.0392 | 0.1256 | 0.755308 | 0.96 | -0.1238 | 0.1245 | 0.319732 | 0.8445 | 0.0181 | 0.2143 | 0.932597 | 0.9935 | NaN | -0.099 | 0.129 | 0.442932 | 0.7844 | -0.2787 | 0.1273 | 0.028539 | 0.2205 | 0.064 | 0.2137 | 0.764773 | 0.9594 | NaN | -0.0495 | 0.1275 | 0.698101 | 0.9116 | -0.1981 | 0.1242 | 0.110697 | 0.5606 | 0.089 | 0.2137 | 0.677098 | 0.9621 | NaN | -0.0722 | 0.129 | 0.575542 | 0.8765 | -0.2608 | 0.1256 | 0.037804 | 0.2692 | 0.1033 | 0.2144 | 0.630068 | 0.9459 |
| FA 24:2 | 364.335 | 23.7592 | Lipid | Fatty Acid | -0.0871 | 0.1344 | 0.516793 | 0.8151 | -0.2484 | 0.1427 | 0.081821 | 0.3594 | 0.0671 | 0.2155 | 0.755605 | 0.9647 | NaN | -0.1124 | 0.1243 | 0.365863 | 0.8459 | -0.1802 | 0.1266 | 0.154466 | 0.6459 | -0.0614 | 0.2048 | 0.764269 | 0.954 | NaN | -0.0669 | 0.1242 | 0.590302 | 0.9125 | -0.0838 | 0.1282 | 0.51303 | 0.9053 | -0.0662 | 0.2068 | 0.74896 | 0.9935 | NaN | -0.1509 | 0.1274 | 0.236401 | 0.7062 | -0.2526 | 0.1301 | 0.052142 | 0.3062 | -0.0603 | 0.2083 | 0.772043 | 0.9598 | NaN | -0.1049 | 0.1259 | 0.404953 | 0.8263 | -0.1775 | 0.1269 | 0.162093 | 0.631 | -0.033 | 0.2081 | 0.874191 | 0.9621 | NaN | -0.1273 | 0.1274 | 0.318028 | 0.7485 | -0.2356 | 0.1284 | 0.066439 | 0.3536 | -0.0234 | 0.209 | 0.910957 | 0.9783 |
| FA 25:2 | 378.3497 | 23.828726 | Lipid | Fatty Acid | 0.1182 | 0.1306 | 0.36524 | 0.7161 | -0.1508 | 0.1345 | 0.262458 | 0.5505 | 0.3971 | 0.2168 | 0.06704 | 0.4459 | NaN | 0.1454 | 0.1207 | 0.228278 | 0.7495 | -0.0139 | 0.1217 | 0.909373 | 0.9729 | 0.279 | 0.2074 | 0.178551 | 0.879 | NaN | 0.1941 | 0.1207 | 0.107888 | 0.5672 | 0.082 | 0.1234 | 0.506399 | 0.9053 | 0.29 | 0.2084 | 0.164107 | 0.7677 | NaN | 0.0896 | 0.1237 | 0.468683 | 0.7888 | -0.1095 | 0.1237 | 0.37601 | 0.6783 | 0.2684 | 0.2118 | 0.205145 | 0.8705 | NaN | 0.128 | 0.1223 | 0.295248 | 0.7529 | -0.0386 | 0.121 | 0.749904 | 0.9098 | 0.2951 | 0.2111 | 0.16223 | 0.8292 | NaN | 0.1091 | 0.1238 | 0.37798 | 0.7638 | -0.0865 | 0.1225 | 0.480196 | 0.7728 | 0.2982 | 0.2123 | 0.160242 | 0.8041 |
| FA 26:2 | 392.3645 | 23.924543 | Lipid | Fatty Acid | 0.0136 | 0.1324 | 0.918112 | 0.9809 | -0.2035 | 0.1328 | 0.125454 | 0.4166 | 0.2539 | 0.2239 | 0.25683 | 0.7397 | NaN | 0.0641 | 0.1226 | 0.601239 | 0.9079 | -0.0375 | 0.1224 | 0.759368 | 0.9527 | 0.1408 | 0.213 | 0.508599 | 0.954 | NaN | 0.0913 | 0.1227 | 0.457005 | 0.8914 | 0.0572 | 0.1249 | 0.646924 | 0.9053 | 0.1116 | 0.2163 | 0.606038 | 0.9894 | NaN | -0.0087 | 0.1252 | 0.944709 | 0.9828 | -0.1487 | 0.1227 | 0.225754 | 0.5613 | 0.1161 | 0.218 | 0.594435 | 0.9375 | NaN | 0.0479 | 0.1242 | 0.699534 | 0.9116 | -0.0608 | 0.1214 | 0.616412 | 0.8623 | 0.1608 | 0.2166 | 0.457886 | 0.9359 | NaN | 0.0147 | 0.1254 | 0.906518 | 0.9698 | -0.128 | 0.1215 | 0.292282 | 0.6559 | 0.1582 | 0.2181 | 0.468159 | 0.8887 |
| FA 18:3 | 278.2229 | 22.803661 | Lipid | Fatty Acid | 0.0451 | 0.1297 | 0.728339 | 0.9287 | -0.057 | 0.1365 | 0.676362 | 0.8622 | 0.1437 | 0.21 | 0.493827 | 0.8401 | NaN | -0.0987 | 0.1222 | 0.419444 | 0.8498 | -0.1433 | 0.12 | 0.232628 | 0.7643 | -0.0505 | 0.2039 | 0.804324 | 0.9617 | NaN | -0.0158 | 0.1203 | 0.895725 | 0.9714 | -0.017 | 0.1178 | 0.885073 | 0.9694 | -0.0084 | 0.2033 | 0.967197 | 0.9976 | NaN | -0.1046 | 0.1261 | 0.406984 | 0.7795 | -0.1888 | 0.1268 | 0.136379 | 0.4784 | -0.0177 | 0.2059 | 0.931632 | 0.99 | NaN | -0.0797 | 0.1237 | 0.519144 | 0.8625 | -0.1371 | 0.1202 | 0.254202 | 0.7315 | -0.0128 | 0.207 | 0.950643 | 0.9854 | NaN | -0.0889 | 0.1259 | 0.480123 | 0.8278 | -0.1783 | 0.1242 | 0.151041 | 0.5211 | 0.0041 | 0.2074 | 0.984243 | 0.9987 |
| FA 20:3 | 306.2562 | 22.806253 | Lipid | Fatty Acid | 0.0518 | 0.1346 | 0.70017 | 0.9136 | -0.198 | 0.1427 | 0.165248 | 0.479 | 0.2591 | 0.2134 | 0.224627 | 0.7251 | NaN | -0.0135 | 0.125 | 0.913798 | 0.9776 | -0.1828 | 0.1251 | 0.143899 | 0.6288 | 0.1167 | 0.2049 | 0.568951 | 0.954 | NaN | 0.0118 | 0.1245 | 0.924717 | 0.9728 | -0.0961 | 0.125 | 0.442226 | 0.8947 | 0.0915 | 0.2085 | 0.660742 | 0.9894 | NaN | -0.0524 | 0.129 | 0.684798 | 0.877 | -0.2512 | 0.1298 | 0.052947 | 0.3076 | 0.1057 | 0.2095 | 0.613955 | 0.9375 | NaN | -0.0124 | 0.1267 | 0.922254 | 0.9796 | -0.187 | 0.1253 | 0.135559 | 0.5986 | 0.1366 | 0.2086 | 0.512625 | 0.9516 | NaN | -0.0235 | 0.1285 | 0.854955 | 0.9543 | -0.2338 | 0.1278 | 0.067351 | 0.3541 | 0.1509 | 0.2091 | 0.470286 | 0.8887 |
| FA 22:3 | 334.2871 | 23.009287 | Lipid | Fatty Acid | 0.089 | 0.1337 | 0.50573 | 0.8068 | -0.1885 | 0.1354 | 0.163658 | 0.479 | 0.3598 | 0.2196 | 0.101355 | 0.5278 | NaN | 0.0436 | 0.124 | 0.725229 | 0.9353 | -0.1795 | 0.1186 | 0.130125 | 0.6118 | 0.2607 | 0.2088 | 0.211706 | 0.9223 | NaN | 0.0935 | 0.1234 | 0.44876 | 0.8815 | -0.0515 | 0.1202 | 0.668564 | 0.9112 | 0.2341 | 0.212 | 0.269511 | 0.9016 | NaN | 0.0075 | 0.1276 | 0.953201 | 0.9828 | -0.249 | 0.1232 | 0.043207 | 0.2719 | 0.2622 | 0.212 | 0.216153 | 0.8705 | NaN | 0.0642 | 0.1254 | 0.608934 | 0.8964 | -0.1795 | 0.1188 | 0.130954 | 0.5974 | 0.3067 | 0.2109 | 0.145849 | 0.8056 | NaN | 0.027 | 0.1274 | 0.832223 | 0.9491 | -0.2413 | 0.1211 | 0.04642 | 0.2877 | 0.2937 | 0.2127 | 0.16735 | 0.8194 |
| FA 26:3 | 390.3503 | 23.76976 | Lipid | Fatty Acid | 0.1368 | 0.1309 | 0.295964 | 0.6742 | -0.1425 | 0.143 | 0.319161 | 0.6107 | 0.36 | 0.205 | 0.079075 | 0.4744 | NaN | 0.1281 | 0.121 | 0.289766 | 0.7802 | -0.0107 | 0.1287 | 0.933683 | 0.973 | 0.2167 | 0.198 | 0.273935 | 0.9223 | NaN | 0.1534 | 0.1207 | 0.203878 | 0.7361 | 0.1071 | 0.1309 | 0.413196 | 0.8818 | 0.1888 | 0.2024 | 0.350791 | 0.9578 | NaN | 0.0862 | 0.1243 | 0.48827 | 0.8037 | -0.1311 | 0.1309 | 0.316488 | 0.6447 | 0.2406 | 0.2 | 0.229042 | 0.8705 | NaN | 0.1176 | 0.1227 | 0.338052 | 0.7711 | -0.0605 | 0.1273 | 0.634736 | 0.8623 | 0.2577 | 0.1999 | 0.197342 | 0.8608 | NaN | 0.1053 | 0.1243 | 0.396905 | 0.7825 | -0.1085 | 0.1292 | 0.400992 | 0.721 | 0.2673 | 0.2006 | 0.182641 | 0.8197 |
| FA 13:4 | 206.0786 | 1.517414 | Lipid | Fatty Acid | 0.0951 | 0.1455 | 0.513265 | 0.8137 | 0.1809 | 0.1407 | 0.198549 | 0.4993 | -0.0219 | 0.254 | 0.931359 | 0.9887 | NaN | 0.0048 | 0.1356 | 0.971482 | 0.9952 | 0.0725 | 0.126 | 0.564933 | 0.9016 | -0.0723 | 0.2384 | 0.761852 | 0.954 | NaN | -0.0363 | 0.1363 | 0.789834 | 0.9641 | 0.0668 | 0.1237 | 0.589452 | 0.9053 | -0.1514 | 0.2419 | 0.531389 | 0.9894 | NaN | 0.0796 | 0.1376 | 0.562808 | 0.846 | 0.1349 | 0.1295 | 0.297594 | 0.627 | 0.011 | 0.2416 | 0.963729 | 0.99 | NaN | 0.0413 | 0.1368 | 0.762945 | 0.938 | 0.1193 | 0.1247 | 0.339077 | 0.7831 | -0.0579 | 0.2427 | 0.81157 | 0.9621 | NaN | 0.0689 | 0.138 | 0.617377 | 0.8808 | 0.1043 | 0.1285 | 0.416977 | 0.7354 | 0.0186 | 0.2441 | 0.939165 | 0.9869 |
| FA 15:4 | 234.1102 | 4.254336 | Lipid | Fatty Acid | 0.1903 | 0.1438 | 0.185843 | 0.5527 | 0.1582 | 0.1457 | 0.277409 | 0.5701 | 0.2217 | 0.2397 | 0.355198 | 0.7534 | NaN | 0.1697 | 0.1331 | 0.202255 | 0.7394 | 0.0987 | 0.1287 | 0.443348 | 0.8547 | 0.2436 | 0.2246 | 0.278131 | 0.9223 | NaN | 0.1037 | 0.134 | 0.439006 | 0.8792 | 0.0638 | 0.1272 | 0.615997 | 0.9053 | 0.1386 | 0.2281 | 0.543409 | 0.9894 | NaN | 0.2287 | 0.1358 | 0.092232 | 0.5372 | 0.1697 | 0.133 | 0.201788 | 0.546 | 0.29 | 0.2279 | 0.203164 | 0.8705 | NaN | 0.196 | 0.1346 | 0.145462 | 0.6708 | 0.1123 | 0.1287 | 0.382781 | 0.8065 | 0.2755 | 0.2289 | 0.228737 | 0.8892 | NaN | 0.221 | 0.1361 | 0.1044 | 0.5529 | 0.1283 | 0.1315 | 0.329488 | 0.6739 | 0.3161 | 0.2308 | 0.170839 | 0.8194 |
| FA 16:4 | 248.1258 | 4.832441 | Lipid | Fatty Acid | 0.1443 | 0.1413 | 0.306898 | 0.6742 | 0.2485 | 0.1343 | 0.06434 | 0.3256 | -0.0046 | 0.2505 | 0.985305 | 0.9935 | NaN | 0.1399 | 0.1306 | 0.283938 | 0.7683 | 0.183 | 0.1192 | 0.124775 | 0.6118 | 0.0807 | 0.2359 | 0.73222 | 0.954 | NaN | 0.049 | 0.1317 | 0.710005 | 0.9481 | 0.1777 | 0.117 | 0.128945 | 0.6741 | -0.1192 | 0.2384 | 0.616947 | 0.9894 | NaN | 0.1852 | 0.1335 | 0.165447 | 0.6495 | 0.2216 | 0.1231 | 0.071856 | 0.3762 | 0.1284 | 0.241 | 0.594266 | 0.9375 | NaN | 0.1512 | 0.1323 | 0.253002 | 0.735 | 0.1942 | 0.119 | 0.102724 | 0.5299 | 0.0777 | 0.2404 | 0.746666 | 0.9621 | NaN | 0.1832 | 0.1338 | 0.170839 | 0.6372 | 0.1901 | 0.1223 | 0.120029 | 0.4801 | 0.1594 | 0.2456 | 0.516512 | 0.8946 |
| FA 18:4 | 276.1573 | 10.004185 | Lipid | Fatty Acid | -0.0656 | 0.1344 | 0.6257 | 0.8678 | 0.133 | 0.1365 | 0.329659 | 0.619 | -0.3172 | 0.2299 | 0.167742 | 0.6614 | NaN | -0.0531 | 0.1243 | 0.669637 | 0.9208 | 0.0357 | 0.1217 | 0.769524 | 0.961 | -0.1872 | 0.2197 | 0.393988 | 0.9398 | NaN | -0.0233 | 0.1244 | 0.85171 | 0.9714 | 0.0811 | 0.1182 | 0.492429 | 0.9053 | -0.1663 | 0.2229 | 0.455684 | 0.9816 | NaN | -0.0579 | 0.1271 | 0.648929 | 0.8652 | 0.06 | 0.1265 | 0.635408 | 0.83 | -0.2388 | 0.2206 | 0.278887 | 0.8705 | NaN | -0.0483 | 0.126 | 0.701776 | 0.9116 | 0.0363 | 0.122 | 0.766162 | 0.9234 | -0.1966 | 0.2242 | 0.380463 | 0.9106 | NaN | -0.0662 | 0.1274 | 0.603379 | 0.8765 | 0.0328 | 0.1254 | 0.793885 | 0.9226 | -0.2368 | 0.2231 | 0.288611 | 0.8424 |
| FA 20:4 | 304.241 | 22.665243 | Lipid | Fatty Acid | 0.0803 | 0.1326 | 0.544759 | 0.8252 | -0.1851 | 0.1439 | 0.19845 | 0.4993 | 0.295 | 0.2075 | 0.155137 | 0.6351 | NaN | 0.0613 | 0.1227 | 0.61712 | 0.9079 | -0.1235 | 0.1273 | 0.332051 | 0.8095 | 0.1942 | 0.1975 | 0.325434 | 0.9223 | NaN | 0.1089 | 0.1224 | 0.37366 | 0.8283 | -0.0395 | 0.1277 | 0.757278 | 0.9266 | 0.2101 | 0.1983 | 0.289343 | 0.9294 | NaN | 0.0102 | 0.1262 | 0.935355 | 0.9828 | -0.1954 | 0.1313 | 0.136618 | 0.4784 | 0.1644 | 0.2027 | 0.417307 | 0.9375 | NaN | 0.0668 | 0.1243 | 0.590846 | 0.8924 | -0.1133 | 0.1279 | 0.375489 | 0.7999 | 0.2107 | 0.2008 | 0.29407 | 0.9039 | NaN | 0.0327 | 0.1261 | 0.795477 | 0.9471 | -0.1705 | 0.1296 | 0.188578 | 0.5692 | 0.1937 | 0.2033 | 0.340707 | 0.8785 |
| FA 22:4 | 332.2713 | 22.904213 | Lipid | Fatty Acid | -0.0472 | 0.1291 | 0.714419 | 0.9246 | -0.0362 | 0.1554 | 0.815808 | 0.932 | -0.0269 | 0.1943 | 0.890052 | 0.9826 | NaN | -0.033 | 0.1194 | 0.782334 | 0.9571 | -0.0915 | 0.1365 | 0.502905 | 0.8931 | 0.0155 | 0.1825 | 0.932412 | 0.9911 | NaN | -0.0357 | 0.1192 | 0.764466 | 0.96 | -0.0647 | 0.1339 | 0.628932 | 0.9053 | -0.0262 | 0.1834 | 0.886222 | 0.9935 | NaN | -0.0252 | 0.1222 | 0.836357 | 0.9598 | -0.0709 | 0.1422 | 0.618229 | 0.8228 | 0.0259 | 0.1853 | 0.888856 | 0.99 | NaN | -0.047 | 0.121 | 0.697424 | 0.9116 | -0.1065 | 0.1369 | 0.436536 | 0.8205 | -0.0046 | 0.1856 | 0.980435 | 0.9969 | NaN | -0.0209 | 0.1225 | 0.864202 | 0.9576 | -0.0965 | 0.1403 | 0.491524 | 0.7774 | 0.04 | 0.1877 | 0.831021 | 0.9641 |
| FA 24:4 | 360.3031 | 23.212015 | Lipid | Fatty Acid | -0.0293 | 0.1287 | 0.820076 | 0.9693 | -0.1598 | 0.1337 | 0.232165 | 0.5274 | 0.1426 | 0.2149 | 0.507085 | 0.856 | NaN | -0.0354 | 0.119 | 0.766072 | 0.9524 | -0.1344 | 0.1176 | 0.252808 | 0.7821 | 0.0899 | 0.2023 | 0.656564 | 0.954 | NaN | -0.0175 | 0.1188 | 0.882827 | 0.9714 | -0.0591 | 0.1173 | 0.614497 | 0.9053 | 0.027 | 0.2059 | 0.895794 | 0.9935 | NaN | -0.0697 | 0.1218 | 0.567426 | 0.846 | -0.1722 | 0.122 | 0.158208 | 0.5021 | 0.0743 | 0.2056 | 0.717646 | 0.9477 | NaN | -0.0459 | 0.1206 | 0.703304 | 0.9116 | -0.1498 | 0.1175 | 0.202345 | 0.6801 | 0.089 | 0.2061 | 0.665893 | 0.9621 | NaN | -0.0466 | 0.1219 | 0.702273 | 0.9035 | -0.1765 | 0.1201 | 0.14156 | 0.5193 | 0.1236 | 0.2064 | 0.549291 | 0.9078 |
| FA 26:4 | 388.3348 | 23.58473 | Lipid | Fatty Acid | 0.0365 | 0.1292 | 0.777629 | 0.9476 | -0.1874 | 0.1407 | 0.18284 | 0.4964 | 0.2284 | 0.2031 | 0.260821 | 0.7397 | NaN | 0.0444 | 0.1195 | 0.710345 | 0.9314 | -0.1332 | 0.1243 | 0.283935 | 0.7996 | 0.1824 | 0.1912 | 0.340138 | 0.9223 | NaN | 0.0643 | 0.1194 | 0.59024 | 0.9125 | -0.062 | 0.1242 | 0.617599 | 0.9053 | 0.1522 | 0.1936 | 0.431757 | 0.9816 | NaN | 0.0055 | 0.1224 | 0.964396 | 0.9828 | -0.1862 | 0.1285 | 0.147145 | 0.4863 | 0.1624 | 0.1946 | 0.404001 | 0.9375 | NaN | 0.0464 | 0.1211 | 0.701591 | 0.9116 | -0.1239 | 0.1248 | 0.320674 | 0.7579 | 0.1876 | 0.1947 | 0.33529 | 0.9106 | NaN | 0.0275 | 0.1225 | 0.82239 | 0.9491 | -0.1688 | 0.1268 | 0.183138 | 0.5692 | 0.1913 | 0.1956 | 0.327981 | 0.8727 |
| FA 20:5 | 302.2251 | 22.461945 | Lipid | Fatty Acid | 0.1932 | 0.1372 | 0.159252 | 0.5264 | -0.0698 | 0.1529 | 0.647776 | 0.8471 | 0.3895 | 0.2111 | 0.064951 | 0.4426 | NaN | 0.1069 | 0.1282 | 0.404496 | 0.8498 | -0.1514 | 0.1343 | 0.259418 | 0.7828 | 0.2954 | 0.2007 | 0.141144 | 0.8611 | NaN | 0.1248 | 0.1276 | 0.327765 | 0.8017 | -0.0227 | 0.1321 | 0.863302 | 0.9569 | 0.2343 | 0.2067 | 0.256933 | 0.9 | NaN | 0.1018 | 0.1316 | 0.438926 | 0.7844 | -0.1836 | 0.141 | 0.192999 | 0.5441 | 0.3104 | 0.2031 | 0.126463 | 0.8047 | NaN | 0.1176 | 0.1298 | 0.364884 | 0.7978 | -0.1415 | 0.1345 | 0.292704 | 0.7544 | 0.3094 | 0.2042 | 0.129858 | 0.772 | NaN | 0.119 | 0.1313 | 0.365055 | 0.7576 | -0.1733 | 0.1384 | 0.210432 | 0.5756 | 0.3314 | 0.2042 | 0.104635 | 0.6959 |
| FA 21:5 | 316.2604 | 21.114538 | Lipid | Fatty Acid | -0.0624 | 0.1303 | 0.632188 | 0.8678 | -0.2289 | 0.1448 | 0.113911 | 0.3941 | 0.0622 | 0.2053 | 0.761986 | 0.9647 | NaN | -0.0947 | 0.1205 | 0.431981 | 0.8498 | -0.1717 | 0.128 | 0.179703 | 0.6937 | -0.0288 | 0.194 | 0.881984 | 0.977 | NaN | -0.1567 | 0.1209 | 0.194854 | 0.7268 | -0.1694 | 0.1256 | 0.17741 | 0.7308 | -0.1444 | 0.2014 | 0.473512 | 0.9826 | NaN | -0.1235 | 0.1235 | 0.317388 | 0.741 | -0.2171 | 0.1323 | 0.100756 | 0.4326 | -0.0412 | 0.1975 | 0.834775 | 0.9726 | NaN | -0.0821 | 0.1221 | 0.501183 | 0.8625 | -0.1539 | 0.1288 | 0.232361 | 0.7214 | -0.0111 | 0.1974 | 0.955058 | 0.9854 | NaN | -0.104 | 0.1236 | 0.400039 | 0.7858 | -0.2061 | 0.1305 | 0.114347 | 0.4676 | -0.008 | 0.1984 | 0.967784 | 0.9896 |
| FA 22:5 | 330.2556 | 22.778202 | Lipid | Fatty Acid | 0.0246 | 0.1326 | 0.853072 | 0.9778 | -0.0747 | 0.1442 | 0.604408 | 0.8198 | 0.1213 | 0.2102 | 0.564012 | 0.8721 | NaN | -0.0052 | 0.1227 | 0.966472 | 0.9952 | -0.1267 | 0.1264 | 0.316381 | 0.8095 | 0.0954 | 0.1974 | 0.628736 | 0.954 | NaN | 0.0072 | 0.1225 | 0.95341 | 0.9728 | -0.0466 | 0.1244 | 0.708064 | 0.9195 | 0.0397 | 0.2001 | 0.842774 | 0.9935 | NaN | -0.0475 | 0.1262 | 0.706763 | 0.8887 | -0.1711 | 0.1327 | 0.197154 | 0.5441 | 0.0566 | 0.201 | 0.778223 | 0.961 | NaN | -0.0061 | 0.1244 | 0.960954 | 0.9796 | -0.1244 | 0.1267 | 0.326259 | 0.7631 | 0.0911 | 0.2011 | 0.650345 | 0.9621 | NaN | -0.0307 | 0.1261 | 0.807774 | 0.9477 | -0.1651 | 0.1303 | 0.205137 | 0.5756 | 0.0795 | 0.2024 | 0.694468 | 0.9459 |
| FA 24:5 | 358.2875 | 23.041843 | Lipid | Fatty Acid | -0.0509 | 0.1286 | 0.692352 | 0.9084 | -0.2853 | 0.1342 | 0.03351 | 0.2761 | 0.1715 | 0.2077 | 0.408952 | 0.7758 | NaN | -0.0997 | 0.1191 | 0.402537 | 0.8498 | -0.3128 | 0.1163 | 0.007168 | 0.154 | 0.0991 | 0.1962 | 0.613448 | 0.954 | NaN | -0.0803 | 0.1188 | 0.498861 | 0.9053 | -0.2132 | 0.117 | 0.068381 | 0.5719 | 0.0315 | 0.2007 | 0.875317 | 0.9935 | NaN | -0.1253 | 0.1223 | 0.305448 | 0.741 | -0.3659 | 0.1211 | 0.002528 | 0.0558 | 0.1063 | 0.1988 | 0.59269 | 0.9375 | NaN | -0.1061 | 0.1208 | 0.379832 | 0.7993 | -0.3407 | 0.1161 | 0.003331 | 0.1082 | 0.1114 | 0.1996 | 0.576669 | 0.9621 | NaN | -0.1115 | 0.1223 | 0.362165 | 0.7576 | -0.3677 | 0.119 | 0.002 | 0.0531 | 0.1287 | 0.2001 | 0.520232 | 0.8946 |
| FA 26:5 | 386.3387 | 22.630043 | Lipid | Fatty Acid | 0.0796 | 0.1342 | 0.553215 | 0.8298 | -0.0189 | 0.136 | 0.889231 | 0.9513 | 0.2188 | 0.2283 | 0.337861 | 0.7534 | NaN | 0.1635 | 0.1245 | 0.18916 | 0.7251 | 0.1059 | 0.1211 | 0.381577 | 0.8325 | 0.2311 | 0.2139 | 0.279963 | 0.9223 | NaN | 0.1335 | 0.124 | 0.281707 | 0.7865 | 0.112 | 0.1187 | 0.345294 | 0.8633 | 0.1519 | 0.2169 | 0.483688 | 0.9848 | NaN | 0.1147 | 0.127 | 0.366288 | 0.7543 | 0.0434 | 0.1251 | 0.728618 | 0.8801 | 0.2075 | 0.2171 | 0.339154 | 0.9044 | NaN | 0.1522 | 0.1262 | 0.22755 | 0.7057 | 0.0966 | 0.1211 | 0.425186 | 0.8205 | 0.2307 | 0.2178 | 0.289675 | 0.9039 | NaN | 0.126 | 0.1273 | 0.322341 | 0.7485 | 0.0543 | 0.1233 | 0.659965 | 0.8674 | 0.2243 | 0.219 | 0.305802 | 0.8671 |
| FA 28:5 | 414.3696 | 22.880224 | Lipid | Fatty Acid | -0.1016 | 0.1298 | 0.433568 | 0.7622 | -0.3616 | 0.1354 | 0.007595 | 0.1497 | 0.1213 | 0.2081 | 0.559988 | 0.8707 | NaN | -0.0592 | 0.1203 | 0.622873 | 0.9079 | -0.239 | 0.1234 | 0.052746 | 0.4282 | 0.0638 | 0.196 | 0.744783 | 0.954 | NaN | -0.0154 | 0.1209 | 0.898758 | 0.9717 | -0.1379 | 0.128 | 0.28127 | 0.8127 | 0.0521 | 0.1977 | 0.792092 | 0.9935 | NaN | -0.1353 | 0.1227 | 0.269994 | 0.7313 | -0.3454 | 0.1235 | 0.005166 | 0.0822 | 0.0261 | 0.2002 | 0.896259 | 0.99 | NaN | -0.087 | 0.1217 | 0.474388 | 0.8625 | -0.2817 | 0.1211 | 0.020041 | 0.2314 | 0.0673 | 0.1996 | 0.735968 | 0.9621 | NaN | -0.1115 | 0.1229 | 0.364414 | 0.7576 | -0.3211 | 0.1225 | 0.008734 | 0.1236 | 0.0566 | 0.2011 | 0.778319 | 0.9525 |
| FA 30:5 | 442.3994 | 22.915 | Lipid | Fatty Acid | -0.0612 | 0.1351 | 0.650689 | 0.8739 | -0.3447 | 0.1357 | 0.011066 | 0.1697 | 0.2226 | 0.2257 | 0.324016 | 0.7534 | NaN | 0.0251 | 0.1259 | 0.841833 | 0.9694 | -0.1719 | 0.1271 | 0.176182 | 0.6897 | 0.1722 | 0.2124 | 0.417425 | 0.9419 | NaN | 0.0191 | 0.1255 | 0.879015 | 0.9714 | -0.1177 | 0.1281 | 0.358202 | 0.873 | 0.1068 | 0.2163 | 0.621547 | 0.9894 | NaN | -0.0552 | 0.1278 | 0.665913 | 0.8697 | -0.2751 | 0.1263 | 0.029353 | 0.222 | 0.1289 | 0.217 | 0.552673 | 0.9375 | NaN | 0.0097 | 0.1274 | 0.939536 | 0.9796 | -0.1807 | 0.1267 | 0.153946 | 0.631 | 0.1761 | 0.2163 | 0.415569 | 0.9359 | NaN | -0.0307 | 0.1282 | 0.810658 | 0.9477 | -0.252 | 0.1255 | 0.044611 | 0.283 | 0.167 | 0.2177 | 0.443025 | 0.8887 |
| FA 20:6 | 300.235 | 21.899794 | Lipid | Fatty Acid | -0.1685 | 0.1327 | 0.204048 | 0.5717 | -0.1067 | 0.1304 | 0.413266 | 0.6809 | -0.2594 | 0.2343 | 0.268416 | 0.7397 | NaN | -0.0984 | 0.1236 | 0.426085 | 0.8498 | -0.0194 | 0.116 | 0.867244 | 0.9729 | -0.2354 | 0.22 | 0.284541 | 0.9223 | NaN | -0.1033 | 0.1233 | 0.40196 | 0.8501 | 0.0399 | 0.1155 | 0.729602 | 0.9241 | -0.3079 | 0.2209 | 0.163501 | 0.7677 | NaN | -0.1434 | 0.1256 | 0.253534 | 0.714 | -0.0887 | 0.1194 | 0.457718 | 0.7319 | -0.2551 | 0.2227 | 0.251855 | 0.8705 | NaN | -0.1337 | 0.1246 | 0.283395 | 0.7504 | -0.0544 | 0.1153 | 0.637138 | 0.8623 | -0.2612 | 0.2236 | 0.242855 | 0.9039 | NaN | -0.1361 | 0.126 | 0.279991 | 0.7337 | -0.0875 | 0.1176 | 0.456727 | 0.7516 | -0.2351 | 0.2252 | 0.296463 | 0.8568 |
| FA 22:6 | 328.2413 | 22.651737 | Lipid | Fatty Acid | -0.1499 | 0.1354 | 0.268142 | 0.6376 | -0.3167 | 0.149 | 0.033516 | 0.2761 | -0.0278 | 0.2095 | 0.894493 | 0.9826 | NaN | -0.1344 | 0.1253 | 0.28333 | 0.7683 | -0.2443 | 0.1322 | 0.064603 | 0.4801 | -0.0652 | 0.1966 | 0.740296 | 0.954 | NaN | -0.1496 | 0.125 | 0.231272 | 0.7361 | -0.1671 | 0.1331 | 0.209349 | 0.7942 | -0.1548 | 0.2002 | 0.439383 | 0.9816 | NaN | -0.1777 | 0.1279 | 0.16471 | 0.6495 | -0.3326 | 0.1353 | 0.013949 | 0.14 | -0.0683 | 0.1994 | 0.731898 | 0.9551 | NaN | -0.1471 | 0.1268 | 0.24612 | 0.7211 | -0.2559 | 0.132 | 0.052556 | 0.392 | -0.0699 | 0.2003 | 0.727192 | 0.9621 | NaN | -0.1585 | 0.1282 | 0.216411 | 0.676 | -0.3177 | 0.1334 | 0.017276 | 0.1644 | -0.0444 | 0.201 | 0.825322 | 0.9641 |
| FA 28:6 | 412.356 | 22.890285 | Lipid | Fatty Acid | 0.0917 | 0.1406 | 0.514432 | 0.8137 | -0.0287 | 0.1408 | 0.838372 | 0.932 | 0.2131 | 0.241 | 0.376557 | 0.7534 | NaN | 0.1431 | 0.1301 | 0.271117 | 0.7625 | 0.0965 | 0.1254 | 0.44137 | 0.8547 | 0.1538 | 0.2269 | 0.49792 | 0.954 | NaN | 0.1611 | 0.13 | 0.215154 | 0.7361 | 0.2276 | 0.1264 | 0.071841 | 0.5732 | 0.0847 | 0.2312 | 0.713965 | 0.99 | NaN | 0.1011 | 0.1329 | 0.446579 | 0.7844 | -0.0045 | 0.129 | 0.972453 | 0.9926 | 0.1768 | 0.2296 | 0.441321 | 0.9375 | NaN | 0.1192 | 0.1317 | 0.365438 | 0.7978 | 0.049 | 0.1246 | 0.694436 | 0.8748 | 0.1737 | 0.2307 | 0.451466 | 0.9359 | NaN | 0.091 | 0.1332 | 0.494663 | 0.8278 | -0.0032 | 0.127 | 0.979821 | 0.9946 | 0.1613 | 0.2322 | 0.487287 | 0.8887 |
| FA 29:6 | 426.3724 | 22.978584 | Lipid | Fatty Acid | 0.0864 | 0.1372 | 0.529051 | 0.8226 | -0.1042 | 0.141 | 0.459951 | 0.7289 | 0.2743 | 0.2285 | 0.229928 | 0.7298 | NaN | 0.151 | 0.127 | 0.234609 | 0.7495 | 0.0223 | 0.1264 | 0.86001 | 0.9729 | 0.2457 | 0.2145 | 0.252099 | 0.9223 | NaN | 0.1583 | 0.1269 | 0.212317 | 0.7361 | 0.0953 | 0.1263 | 0.450359 | 0.8947 | 0.1985 | 0.2174 | 0.361203 | 0.9578 | NaN | 0.0907 | 0.1297 | 0.484584 | 0.8009 | -0.0556 | 0.1297 | 0.667995 | 0.8438 | 0.2038 | 0.2188 | 0.351573 | 0.9133 | NaN | 0.1425 | 0.1287 | 0.268365 | 0.7442 | -0.0021 | 0.1259 | 0.986936 | 0.9923 | 0.2687 | 0.2181 | 0.217859 | 0.8892 | NaN | 0.1103 | 0.13 | 0.396068 | 0.7825 | -0.036 | 0.1282 | 0.778842 | 0.9173 | 0.2343 | 0.2199 | 0.286636 | 0.8424 |
| FA 30:6 | 440.3876 | 23.740631 | Lipid | Fatty Acid | 0.0793 | 0.135 | 0.556957 | 0.8309 | -0.1493 | 0.1398 | 0.285501 | 0.5742 | 0.3195 | 0.2265 | 0.158413 | 0.6354 | NaN | 0.0953 | 0.1248 | 0.445233 | 0.8498 | -0.0115 | 0.1262 | 0.927359 | 0.9729 | 0.17 | 0.2177 | 0.434861 | 0.9478 | NaN | 0.103 | 0.1246 | 0.408436 | 0.8508 | 0.0122 | 0.1245 | 0.922021 | 0.973 | 0.1664 | 0.2199 | 0.449201 | 0.9816 | NaN | 0.0557 | 0.1278 | 0.663159 | 0.8697 | -0.0844 | 0.1293 | 0.513965 | 0.7647 | 0.1634 | 0.2223 | 0.462481 | 0.9375 | NaN | 0.0819 | 0.1265 | 0.517139 | 0.8625 | -0.0159 | 0.1263 | 0.90002 | 0.9741 | 0.1796 | 0.2225 | 0.419569 | 0.9359 | NaN | 0.0669 | 0.128 | 0.601418 | 0.8765 | -0.0603 | 0.128 | 0.637821 | 0.8546 | 0.1825 | 0.2241 | 0.415317 | 0.8887 |
| AC 3:0 | 217.1321 | 1.629795 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.276 | 0.1364 | 0.042982 | 0.3003 | 0.3381 | 0.167 | 0.042841 | 0.2929 | 0.2526 | 0.1997 | 0.205888 | 0.7107 | NaN | 0.1314 | 0.1297 | 0.310796 | 0.7898 | 0.0191 | 0.1634 | 0.907183 | 0.9729 | 0.1926 | 0.1884 | 0.306705 | 0.9223 | NaN | 0.2089 | 0.1269 | 0.099642 | 0.55 | 0.1665 | 0.1493 | 0.264567 | 0.806 | 0.2287 | 0.1888 | 0.225619 | 0.8771 | NaN | 0.171 | 0.1316 | 0.19384 | 0.6616 | 0.1194 | 0.1657 | 0.471223 | 0.7332 | 0.2048 | 0.1907 | 0.282896 | 0.8705 | NaN | 0.1401 | 0.1315 | 0.286855 | 0.7504 | 0.0484 | 0.1615 | 0.764298 | 0.9232 | 0.1821 | 0.1926 | 0.344513 | 0.9106 | NaN | 0.1833 | 0.1315 | 0.163144 | 0.6278 | 0.082 | 0.165 | 0.619406 | 0.8372 | 0.2342 | 0.1918 | 0.22197 | 0.8424 |
| AC 4:0 | 231.1476 | 2.899889 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.045 | 0.1391 | 0.746219 | 0.9321 | 0.2061 | 0.1538 | 0.180405 | 0.4964 | -0.0504 | 0.2159 | 0.815409 | 0.9713 | NaN | -0.1151 | 0.1312 | 0.380297 | 0.8465 | -0.0192 | 0.1432 | 0.89331 | 0.9729 | -0.1492 | 0.2036 | 0.463598 | 0.9478 | NaN | -0.1223 | 0.1312 | 0.351142 | 0.8224 | -0.0131 | 0.1394 | 0.924987 | 0.973 | -0.1798 | 0.2061 | 0.382926 | 0.9793 | NaN | -0.0759 | 0.1337 | 0.570159 | 0.846 | 0.0262 | 0.1487 | 0.860302 | 0.95 | -0.1099 | 0.2057 | 0.593197 | 0.9375 | NaN | -0.089 | 0.1326 | 0.501933 | 0.8625 | 0.0169 | 0.1415 | 0.904721 | 0.9744 | -0.1404 | 0.2075 | 0.498756 | 0.9436 | NaN | -0.0733 | 0.134 | 0.584478 | 0.8765 | 0.0146 | 0.1462 | 0.920677 | 0.979 | -0.1077 | 0.2078 | 0.604353 | 0.9371 |
| AC 11:0 | 329.2544 | 16.329609 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0718 | 0.1498 | 0.631651 | 0.8678 | -0.2096 | 0.1642 | 0.201769 | 0.5003 | 0.0005 | 0.2345 | 0.998461 | 0.9985 | NaN | -0.159 | 0.1389 | 0.252473 | 0.7495 | -0.2214 | 0.1436 | 0.123076 | 0.6118 | -0.1552 | 0.223 | 0.486444 | 0.954 | NaN | -0.1876 | 0.1391 | 0.177426 | 0.6946 | -0.2654 | 0.1404 | 0.058668 | 0.5223 | -0.1514 | 0.2247 | 0.500436 | 0.9894 | NaN | -0.1188 | 0.1418 | 0.402036 | 0.7795 | -0.1949 | 0.1502 | 0.194484 | 0.5441 | -0.1155 | 0.2251 | 0.607893 | 0.9375 | NaN | -0.1207 | 0.1405 | 0.390384 | 0.8071 | -0.1953 | 0.1443 | 0.175855 | 0.6515 | -0.0934 | 0.2255 | 0.678766 | 0.9621 | NaN | -0.1009 | 0.142 | 0.47711 | 0.8278 | -0.1819 | 0.1481 | 0.219485 | 0.5853 | -0.0796 | 0.2264 | 0.725056 | 0.9459 |
| AC 14:0 | 371.3022 | 19.886253 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.3001 | 0.132 | 0.023007 | 0.2027 | -0.292 | 0.1353 | 0.030923 | 0.2667 | -0.2779 | 0.2202 | 0.206986 | 0.7107 | NaN | -0.3086 | 0.1217 | 0.011223 | 0.1674 | -0.3125 | 0.1174 | 0.007776 | 0.1553 | -0.2754 | 0.2064 | 0.182062 | 0.8816 | NaN | -0.3582 | 0.1212 | 0.003119 | 0.0615 | -0.3237 | 0.1148 | 0.004811 | 0.1328 | -0.3888 | 0.2081 | 0.061763 | 0.4941 | NaN | -0.3392 | 0.1243 | 0.006365 | 0.1004 | -0.3549 | 0.1222 | 0.003687 | 0.0688 | -0.2818 | 0.2091 | 0.177879 | 0.8705 | NaN | -0.2907 | 0.1236 | 0.01868 | 0.2578 | -0.2799 | 0.1185 | 0.018166 | 0.2263 | -0.2741 | 0.2102 | 0.192224 | 0.8608 | NaN | -0.3169 | 0.1247 | 0.011054 | 0.1606 | -0.3409 | 0.1203 | 0.004596 | 0.0793 | -0.2598 | 0.2115 | 0.219344 | 0.8424 |
| AC 16:0 | 399.335 | 21.273067 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1256 | 0.1381 | 0.363158 | 0.7161 | -0.2881 | 0.1437 | 0.045028 | 0.2929 | 0.0432 | 0.2254 | 0.848063 | 0.9732 | NaN | -0.1883 | 0.1277 | 0.140383 | 0.6828 | -0.3101 | 0.1249 | 0.013025 | 0.1892 | -0.0627 | 0.2132 | 0.768738 | 0.954 | NaN | -0.1599 | 0.1274 | 0.209499 | 0.7361 | -0.2463 | 0.1241 | 0.047096 | 0.4581 | -0.0837 | 0.2156 | 0.697785 | 0.9894 | NaN | -0.2076 | 0.131 | 0.113129 | 0.5709 | -0.3528 | 0.13 | 0.006657 | 0.1015 | -0.0485 | 0.216 | 0.82242 | 0.97 | NaN | -0.1658 | 0.1294 | 0.200174 | 0.6855 | -0.284 | 0.1257 | 0.023858 | 0.2532 | -0.0378 | 0.2167 | 0.861523 | 0.9621 | NaN | -0.1782 | 0.131 | 0.173687 | 0.6392 | -0.3322 | 0.128 | 0.009485 | 0.1247 | -0.0126 | 0.2171 | 0.953655 | 0.9877 |
| AC 18:0 | 427.3648 | 21.812096 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0869 | 0.1154 | 0.451521 | 0.7813 | -0.1385 | 0.1107 | 0.210914 | 0.5065 | -0.0015 | 0.2047 | 0.994068 | 0.9959 | NaN | -0.0528 | 0.107 | 0.621948 | 0.9079 | -0.0788 | 0.0983 | 0.422658 | 0.847 | -0.0066 | 0.192 | 0.972768 | 0.9911 | NaN | -0.0671 | 0.1067 | 0.529248 | 0.9101 | -0.0581 | 0.097 | 0.549094 | 0.9053 | -0.0739 | 0.1941 | 0.703578 | 0.9894 | NaN | -0.0822 | 0.1091 | 0.45141 | 0.7844 | -0.1146 | 0.1015 | 0.25889 | 0.5881 | -0.0171 | 0.1946 | 0.929849 | 0.99 | NaN | -0.0681 | 0.1083 | 0.529514 | 0.8625 | -0.0714 | 0.0987 | 0.469661 | 0.8272 | -0.0428 | 0.1958 | 0.82698 | 0.9621 | NaN | -0.0672 | 0.1095 | 0.539585 | 0.851 | -0.1095 | 0.1001 | 0.274033 | 0.648 | 0.0124 | 0.1964 | 0.949713 | 0.9869 |
| AC 5:1 | 243.1468 | 4.074276 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.2613 | 0.1386 | 0.059512 | 0.3473 | 0.1752 | 0.152 | 0.249142 | 0.5393 | 0.3217 | 0.2183 | 0.140583 | 0.6043 | NaN | 0.1921 | 0.1292 | 0.136914 | 0.6828 | 0.0268 | 0.1373 | 0.844993 | 0.9729 | 0.3076 | 0.2047 | 0.133003 | 0.8611 | NaN | 0.2026 | 0.1287 | 0.115462 | 0.6 | 0.0725 | 0.1329 | 0.585422 | 0.9053 | 0.2856 | 0.2066 | 0.166988 | 0.7746 | NaN | 0.2267 | 0.1314 | 0.084596 | 0.5283 | 0.0837 | 0.1414 | 0.553877 | 0.786 | 0.3235 | 0.2073 | 0.11863 | 0.7964 | NaN | 0.2417 | 0.13 | 0.063018 | 0.4979 | 0.064 | 0.1361 | 0.638247 | 0.8623 | 0.3621 | 0.208 | 0.08174 | 0.6055 | NaN | 0.2282 | 0.1317 | 0.083114 | 0.5441 | 0.043 | 0.1408 | 0.759927 | 0.9096 | 0.3529 | 0.2091 | 0.091413 | 0.6639 |
| AC 7:1 | 271.1774 | 7.654182 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.0488 | 0.1404 | 0.728078 | 0.9287 | 0.1961 | 0.1608 | 0.222472 | 0.5117 | -0.0379 | 0.2125 | 0.858535 | 0.9732 | NaN | -0.0586 | 0.1311 | 0.654916 | 0.918 | 0.1065 | 0.1428 | 0.455842 | 0.8559 | -0.1606 | 0.2012 | 0.424749 | 0.9419 | NaN | -0.0179 | 0.1302 | 0.890481 | 0.9714 | 0.1651 | 0.1386 | 0.233639 | 0.8003 | -0.1303 | 0.2019 | 0.518789 | 0.9894 | NaN | -0.104 | 0.1361 | 0.44491 | 0.7844 | 0.0148 | 0.1546 | 0.923547 | 0.9748 | -0.1716 | 0.205 | 0.402427 | 0.9375 | NaN | -0.0709 | 0.1334 | 0.595203 | 0.8924 | 0.0771 | 0.1441 | 0.59274 | 0.8623 | -0.1579 | 0.2056 | 0.442551 | 0.9359 | NaN | -0.1068 | 0.1367 | 0.434428 | 0.795 | -0.0042 | 0.1525 | 0.977935 | 0.9946 | -0.166 | 0.2074 | 0.423426 | 0.8887 |
| AC 8:1 | 285.1943 | 9.563584 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0065 | 0.1394 | 0.963014 | 0.9911 | 0.0535 | 0.1468 | 0.715536 | 0.8876 | -0.0267 | 0.2272 | 0.906409 | 0.9838 | NaN | -0.2298 | 0.133 | 0.084093 | 0.6028 | -0.2326 | 0.1367 | 0.088733 | 0.5442 | -0.2115 | 0.2172 | 0.330063 | 0.9223 | NaN | -0.1379 | 0.1302 | 0.289591 | 0.7865 | -0.0954 | 0.1288 | 0.458544 | 0.8952 | -0.1799 | 0.2178 | 0.408739 | 0.9816 | NaN | -0.2458 | 0.1385 | 0.075863 | 0.4957 | -0.2261 | 0.1458 | 0.120938 | 0.4541 | -0.2448 | 0.2232 | 0.272776 | 0.8705 | NaN | -0.2215 | 0.1354 | 0.101708 | 0.6358 | -0.189 | 0.1352 | 0.162284 | 0.631 | -0.2375 | 0.2245 | 0.289978 | 0.9039 | NaN | -0.2375 | 0.1386 | 0.086605 | 0.5441 | -0.2327 | 0.1424 | 0.102059 | 0.4543 | -0.2316 | 0.2261 | 0.305682 | 0.8671 |
| AC 11:1 | 327.24 | 15.28524 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.2225 | 0.1369 | 0.10397 | 0.4628 | -0.337 | 0.1345 | 0.012191 | 0.1771 | -0.1281 | 0.2316 | 0.580065 | 0.8849 | NaN | -0.2611 | 0.1262 | 0.038551 | 0.3941 | -0.4076 | 0.1152 | 0.000401 | 0.0277 | -0.1362 | 0.2171 | 0.530639 | 0.954 | NaN | -0.2982 | 0.1261 | 0.017996 | 0.216 | -0.4141 | 0.1125 | 0.000234 | 0.0129 | -0.2008 | 0.219 | 0.359355 | 0.9578 | NaN | -0.2336 | 0.1292 | 0.070636 | 0.4947 | -0.3558 | 0.1217 | 0.003456 | 0.0688 | -0.1405 | 0.2201 | 0.52314 | 0.9375 | NaN | -0.2569 | 0.128 | 0.0447 | 0.4112 | -0.3847 | 0.1159 | 0.0009 | 0.0574 | -0.153 | 0.2211 | 0.48888 | 0.9403 | NaN | -0.2369 | 0.1295 | 0.067287 | 0.4832 | -0.3569 | 0.1197 | 0.00286 | 0.0631 | -0.1453 | 0.2222 | 0.513262 | 0.8946 |
| AC 13:1 | 355.2707 | 17.844881 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.2587 | 0.1425 | 0.069457 | 0.3759 | -0.3443 | 0.1451 | 0.01763 | 0.2037 | -0.1609 | 0.235 | 0.493579 | 0.8401 | NaN | -0.2574 | 0.1316 | 0.050414 | 0.4443 | -0.3137 | 0.1272 | 0.013642 | 0.1911 | -0.1973 | 0.2203 | 0.370569 | 0.9312 | NaN | -0.2802 | 0.1312 | 0.032697 | 0.2852 | -0.3261 | 0.1242 | 0.008663 | 0.1839 | -0.2412 | 0.2223 | 0.27783 | 0.9183 | NaN | -0.2258 | 0.135 | 0.094408 | 0.5372 | -0.2977 | 0.1336 | 0.025827 | 0.2147 | -0.1402 | 0.2236 | 0.530503 | 0.9375 | NaN | -0.2531 | 0.1334 | 0.057791 | 0.4833 | -0.3014 | 0.1279 | 0.018448 | 0.2263 | -0.1952 | 0.2244 | 0.384361 | 0.9106 | NaN | -0.2281 | 0.1353 | 0.091764 | 0.5459 | -0.3028 | 0.1312 | 0.021002 | 0.187 | -0.1394 | 0.2257 | 0.536896 | 0.8971 |
| AC 18:1 | 425.35 | 21.472305 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.2815 | 0.1329 | 0.034185 | 0.2621 | -0.3327 | 0.1378 | 0.015753 | 0.2 | -0.218 | 0.2166 | 0.31424 | 0.7534 | NaN | -0.3212 | 0.1224 | 0.008673 | 0.1451 | -0.3424 | 0.1196 | 0.004187 | 0.1179 | -0.2905 | 0.203 | 0.15238 | 0.879 | NaN | -0.3359 | 0.1221 | 0.005959 | 0.094 | -0.3034 | 0.1184 | 0.010376 | 0.2019 | -0.3726 | 0.2062 | 0.070725 | 0.5348 | NaN | -0.3528 | 0.1253 | 0.004879 | 0.0842 | -0.3902 | 0.1242 | 0.001672 | 0.0513 | -0.2989 | 0.2061 | 0.146993 | 0.828 | NaN | -0.3047 | 0.1242 | 0.014127 | 0.2166 | -0.3068 | 0.1209 | 0.011167 | 0.1792 | -0.2875 | 0.207 | 0.164789 | 0.8292 | NaN | -0.3151 | 0.1256 | 0.012079 | 0.1667 | -0.359 | 0.1226 | 0.003401 | 0.0722 | -0.2556 | 0.2077 | 0.218449 | 0.8424 |
| AC 8:2 | 283.1773 | 7.484311 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1328 | 0.1395 | 0.341227 | 0.7042 | 0.0334 | 0.1504 | 0.824187 | 0.932 | -0.2341 | 0.2228 | 0.293212 | 0.7534 | NaN | -0.2143 | 0.1291 | 0.096965 | 0.6297 | -0.0312 | 0.1326 | 0.814152 | 0.965 | -0.3322 | 0.209 | 0.111895 | 0.7818 | NaN | -0.2191 | 0.1289 | 0.089336 | 0.5342 | 0.0375 | 0.1295 | 0.771949 | 0.9284 | -0.4282 | 0.213 | 0.044434 | 0.438 | NaN | -0.2021 | 0.1321 | 0.126026 | 0.5846 | -0.0675 | 0.1394 | 0.628242 | 0.8277 | -0.262 | 0.2115 | 0.215428 | 0.8705 | NaN | -0.2185 | 0.131 | 0.095471 | 0.6274 | -0.0444 | 0.133 | 0.738807 | 0.9043 | -0.3285 | 0.2132 | 0.123418 | 0.757 | NaN | -0.2097 | 0.1325 | 0.113671 | 0.5578 | -0.0873 | 0.1376 | 0.525658 | 0.7998 | -0.2687 | 0.2136 | 0.208271 | 0.8424 |
| AC 18:2 | 423.3342 | 20.982098 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1615 | 0.1367 | 0.237631 | 0.6073 | -0.1125 | 0.1475 | 0.445669 | 0.7172 | -0.1749 | 0.2199 | 0.42628 | 0.7818 | NaN | -0.2264 | 0.1263 | 0.073159 | 0.5384 | -0.1299 | 0.1292 | 0.314925 | 0.8095 | -0.281 | 0.2067 | 0.174059 | 0.879 | NaN | -0.229 | 0.1261 | 0.069464 | 0.4734 | -0.0944 | 0.1271 | 0.457796 | 0.8952 | -0.3323 | 0.2097 | 0.113081 | 0.6617 | NaN | -0.2361 | 0.1295 | 0.068209 | 0.4931 | -0.1666 | 0.1348 | 0.21665 | 0.5546 | -0.2546 | 0.2094 | 0.224066 | 0.8705 | NaN | -0.1973 | 0.128 | 0.123155 | 0.6708 | -0.0923 | 0.1299 | 0.477226 | 0.8272 | -0.2538 | 0.2104 | 0.227778 | 0.8892 | NaN | -0.1962 | 0.1295 | 0.129697 | 0.605 | -0.1475 | 0.1327 | 0.266349 | 0.6386 | -0.1975 | 0.2109 | 0.348852 | 0.8785 |
| AC 10:3 | 309.194 | 11.500111 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.015 | 0.1392 | 0.914265 | 0.9809 | -0.1027 | 0.1559 | 0.509829 | 0.7648 | 0.0745 | 0.2163 | 0.730558 | 0.9647 | NaN | -0.0728 | 0.129 | 0.572448 | 0.9079 | -0.2137 | 0.1369 | 0.118494 | 0.6118 | 0.0445 | 0.2031 | 0.826701 | 0.9669 | NaN | -0.0331 | 0.1285 | 0.796873 | 0.9641 | -0.1386 | 0.134 | 0.300954 | 0.8336 | 0.0408 | 0.2046 | 0.841857 | 0.9935 | NaN | -0.1075 | 0.1327 | 0.417597 | 0.7841 | -0.2479 | 0.1441 | 0.085422 | 0.4123 | 0.0136 | 0.2065 | 0.947597 | 0.99 | NaN | -0.0788 | 0.1309 | 0.546858 | 0.867 | -0.2101 | 0.1371 | 0.125481 | 0.5933 | 0.0272 | 0.2072 | 0.895723 | 0.9681 | NaN | -0.1063 | 0.133 | 0.424028 | 0.795 | -0.2553 | 0.1416 | 0.071491 | 0.3687 | 0.0139 | 0.2087 | 0.946715 | 0.9869 |
| AC 17:3 | 407.3014 | 22.77926 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0338 | 0.1303 | 0.794987 | 0.9602 | 0.0272 | 0.1309 | 0.835617 | 0.932 | -0.0456 | 0.225 | 0.839374 | 0.9732 | NaN | -0.0304 | 0.1205 | 0.800559 | 0.9571 | 0.0646 | 0.1149 | 0.57421 | 0.904 | -0.0883 | 0.2112 | 0.675859 | 0.954 | NaN | -0.0854 | 0.1204 | 0.478441 | 0.8967 | -0.0555 | 0.1135 | 0.624781 | 0.9053 | -0.0967 | 0.2128 | 0.649409 | 0.9894 | NaN | 0.0008 | 0.1234 | 0.994923 | 0.9985 | 0.1443 | 0.1217 | 0.235558 | 0.5767 | -0.0953 | 0.2143 | 0.656433 | 0.9375 | NaN | -0.0076 | 0.1222 | 0.950202 | 0.9796 | 0.0921 | 0.1154 | 0.424837 | 0.8205 | -0.0629 | 0.2149 | 0.7698 | 0.9621 | NaN | -0.0025 | 0.1236 | 0.984143 | 0.995 | 0.1559 | 0.1198 | 0.193125 | 0.5731 | -0.1045 | 0.2166 | 0.629611 | 0.9459 |
| AC 19:3 | 435.335 | 23.046375 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1502 | 0.1344 | 0.26371 | 0.6341 | -0.1677 | 0.1293 | 0.194812 | 0.4993 | -0.1262 | 0.2367 | 0.593779 | 0.8909 | NaN | -0.1677 | 0.1241 | 0.176667 | 0.7251 | -0.1682 | 0.1132 | 0.137407 | 0.6175 | -0.18 | 0.222 | 0.417434 | 0.9419 | NaN | -0.1837 | 0.1239 | 0.138326 | 0.6531 | -0.193 | 0.1107 | 0.081228 | 0.59 | -0.1867 | 0.2237 | 0.403856 | 0.9816 | NaN | -0.2177 | 0.1272 | 0.087098 | 0.5308 | -0.2232 | 0.1178 | 0.058012 | 0.3268 | -0.2242 | 0.226 | 0.321123 | 0.9044 | NaN | -0.1679 | 0.1258 | 0.182018 | 0.6753 | -0.1776 | 0.1133 | 0.116999 | 0.5766 | -0.1633 | 0.226 | 0.469993 | 0.9359 | NaN | -0.2012 | 0.1274 | 0.114185 | 0.5578 | -0.2041 | 0.1159 | 0.078196 | 0.3854 | -0.2089 | 0.228 | 0.359554 | 0.8785 |
| 3-dehydroxycarnitine | 145.1097 | 0.670247 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.0536 | 0.135 | 0.691332 | 0.9084 | -0.2625 | 0.1508 | 0.081722 | 0.3594 | 0.0812 | 0.2132 | 0.703449 | 0.9541 | NaN | -0.0601 | 0.1248 | 0.630114 | 0.9079 | -0.2851 | 0.1313 | 0.029857 | 0.3052 | 0.06 | 0.2001 | 0.764206 | 0.954 | NaN | -0.0538 | 0.1246 | 0.665856 | 0.935 | -0.3059 | 0.1284 | 0.017194 | 0.2556 | 0.0833 | 0.2013 | 0.679083 | 0.9894 | NaN | -0.0094 | 0.128 | 0.941495 | 0.9828 | -0.2348 | 0.1382 | 0.089198 | 0.4173 | 0.113 | 0.2027 | 0.57719 | 0.9375 | NaN | 0.0061 | 0.127 | 0.961833 | 0.9796 | -0.2213 | 0.133 | 0.096082 | 0.52 | 0.1368 | 0.204 | 0.50258 | 0.9436 | NaN | -0.0082 | 0.1283 | 0.949331 | 0.9794 | -0.2394 | 0.1359 | 0.078076 | 0.3854 | 0.1205 | 0.2048 | 0.556414 | 0.9114 |
| L-carnitine | 161.105 | 0.668089 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | 0.191 | 0.1349 | 0.157021 | 0.5264 | 0.1405 | 0.1435 | 0.32771 | 0.6183 | 0.2083 | 0.2184 | 0.340343 | 0.7534 | NaN | 0.0925 | 0.1264 | 0.464426 | 0.8498 | 0.0119 | 0.129 | 0.926426 | 0.9729 | 0.1507 | 0.2058 | 0.463763 | 0.9478 | NaN | 0.0745 | 0.1267 | 0.556445 | 0.9125 | 0.0524 | 0.1251 | 0.67561 | 0.9163 | 0.0943 | 0.2094 | 0.65257 | 0.9894 | NaN | 0.1155 | 0.1289 | 0.370299 | 0.7571 | 0.0123 | 0.1354 | 0.927744 | 0.9755 | 0.1883 | 0.2078 | 0.364765 | 0.9223 | NaN | 0.0827 | 0.1287 | 0.52058 | 0.8625 | 0.0028 | 0.1296 | 0.982868 | 0.9923 | 0.133 | 0.2104 | 0.527402 | 0.9583 | NaN | 0.1175 | 0.1292 | 0.362923 | 0.7576 | 0.0051 | 0.1332 | 0.969731 | 0.9946 | 0.191 | 0.2097 | 0.362463 | 0.8814 |
| O-adipoylcarnitine | 289.153 | 2.560197 | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.1652 | 0.1392 | 0.235583 | 0.6073 | -0.0543 | 0.1697 | 0.748926 | 0.9087 | -0.212 | 0.2046 | 0.300193 | 0.7534 | NaN | -0.2164 | 0.1286 | 0.092377 | 0.622 | -0.1429 | 0.1492 | 0.338199 | 0.8095 | -0.2434 | 0.1916 | 0.203877 | 0.9223 | NaN | -0.2253 | 0.1284 | 0.079414 | 0.5097 | -0.1805 | 0.1467 | 0.218531 | 0.7942 | -0.2447 | 0.1929 | 0.204736 | 0.8462 | NaN | -0.2349 | 0.1318 | 0.07469 | 0.4957 | -0.1681 | 0.1565 | 0.282816 | 0.6122 | -0.256 | 0.1943 | 0.187693 | 0.8705 | NaN | -0.1845 | 0.1303 | 0.156826 | 0.6753 | -0.0657 | 0.1492 | 0.659794 | 0.8623 | -0.2376 | 0.1951 | 0.223288 | 0.8892 | NaN | -0.2342 | 0.1321 | 0.076261 | 0.5197 | -0.1601 | 0.1537 | 0.297498 | 0.6559 | -0.2626 | 0.1963 | 0.181097 | 0.8194 |
| AC 4:0 (OH) | 247.1422 | 1.145753 | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.2627 | 0.1344 | 0.050621 | 0.3212 | 0.0112 | 0.141 | 0.936425 | 0.9724 | -0.4827 | 0.217 | 0.026076 | 0.2999 | NaN | -0.2635 | 0.1241 | 0.033639 | 0.3571 | -0.0958 | 0.125 | 0.443276 | 0.8547 | -0.381 | 0.2068 | 0.06541 | 0.6334 | NaN | -0.264 | 0.1239 | 0.033015 | 0.2852 | -0.1002 | 0.1225 | 0.413342 | 0.8818 | -0.3989 | 0.2075 | 0.054486 | 0.477 | NaN | -0.3213 | 0.1267 | 0.01125 | 0.1515 | -0.1782 | 0.1344 | 0.184859 | 0.5328 | -0.4093 | 0.2085 | 0.049624 | 0.559 | NaN | -0.2844 | 0.1256 | 0.023533 | 0.2887 | -0.1014 | 0.1253 | 0.418725 | 0.8188 | -0.4309 | 0.2084 | 0.038726 | 0.4772 | NaN | -0.3202 | 0.127 | 0.011732 | 0.1661 | -0.1743 | 0.1313 | 0.184488 | 0.5692 | -0.4302 | 0.2096 | 0.040148 | 0.4663 |
| AC 5:0 (OH) | 261.1578 | 1.981441 | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.1757 | 0.1397 | 0.208439 | 0.5782 | 0.2522 | 0.1531 | 0.099496 | 0.3816 | 0.1391 | 0.2184 | 0.524357 | 0.8655 | NaN | 0.0052 | 0.133 | 0.968644 | 0.9952 | 0.0398 | 0.1426 | 0.77991 | 0.9615 | 0.0091 | 0.2081 | 0.965138 | 0.9911 | NaN | 0.0801 | 0.1304 | 0.538812 | 0.9125 | 0.1662 | 0.1335 | 0.213124 | 0.7942 | 0.0332 | 0.2088 | 0.87376 | 0.9935 | NaN | 0.0728 | 0.1342 | 0.587419 | 0.8473 | 0.0919 | 0.1472 | 0.532314 | 0.7819 | 0.0959 | 0.2082 | 0.64512 | 0.9375 | NaN | 0.0381 | 0.134 | 0.776101 | 0.938 | 0.0542 | 0.1421 | 0.702748 | 0.8781 | 0.0475 | 0.2109 | 0.821898 | 0.9621 | NaN | 0.0711 | 0.1346 | 0.597414 | 0.8765 | 0.0704 | 0.1457 | 0.629111 | 0.8449 | 0.0975 | 0.2102 | 0.642825 | 0.9459 |
| N-undecanoylglycine | 243.1826 | 15.799677 | Lipid | Fatty Acid, acylglycine | 0.0059 | 0.1275 | 0.963077 | 0.9911 | 0.1189 | 0.1918 | 0.535395 | 0.7813 | -0.003 | 0.1744 | 0.986142 | 0.9935 | NaN | 0.0355 | 0.118 | 0.763366 | 0.9512 | 0.0625 | 0.1689 | 0.711071 | 0.934 | 0.0595 | 0.1643 | 0.71699 | 0.954 | NaN | 0.0599 | 0.118 | 0.611604 | 0.9125 | -0.0109 | 0.1671 | 0.948115 | 0.9765 | 0.1002 | 0.1668 | 0.547886 | 0.9894 | NaN | 0.0331 | 0.1207 | 0.783833 | 0.936 | 0.1279 | 0.1753 | 0.465416 | 0.7319 | 0.0426 | 0.1663 | 0.797713 | 0.9662 | NaN | 0.0182 | 0.1195 | 0.878953 | 0.9672 | 0.0938 | 0.1688 | 0.578379 | 0.8623 | 0.019 | 0.1667 | 0.909244 | 0.9693 | NaN | 0.0145 | 0.1208 | 0.904311 | 0.9693 | 0.1066 | 0.1728 | 0.537385 | 0.8003 | 0.0176 | 0.1675 | 0.91618 | 0.9801 |
| 3-aminoisobutanoate | 103.0638 | 1.812905 | Lipid | Fatty Acid, Amino | 0.0833 | 0.1342 | 0.535034 | 0.825 | 0.1571 | 0.132 | 0.234198 | 0.5274 | 0.0339 | 0.2308 | 0.883277 | 0.9791 | NaN | 0.1394 | 0.1242 | 0.261727 | 0.7604 | 0.2055 | 0.1152 | 0.0744 | 0.4865 | 0.095 | 0.2169 | 0.661419 | 0.954 | NaN | 0.0976 | 0.1239 | 0.430985 | 0.8779 | 0.1756 | 0.1132 | 0.120952 | 0.6704 | 0.0257 | 0.218 | 0.906077 | 0.9935 | NaN | 0.1144 | 0.1269 | 0.367566 | 0.7543 | 0.179 | 0.1204 | 0.136937 | 0.4784 | 0.0829 | 0.2198 | 0.706134 | 0.9477 | NaN | 0.1684 | 0.1263 | 0.182576 | 0.6753 | 0.2346 | 0.1154 | 0.041989 | 0.3563 | 0.1233 | 0.2218 | 0.57811 | 0.9621 | NaN | 0.1317 | 0.1274 | 0.301188 | 0.7481 | 0.1889 | 0.1184 | 0.11076 | 0.4635 | 0.105 | 0.2225 | 0.637013 | 0.9459 |
| C8 H14 O2 | 142.099 | 8.877983 | Lipid | Fatty acid, branched chain fatty acid | 0.1409 | 0.1266 | 0.265867 | 0.6353 | 0.0958 | 0.1396 | 0.492357 | 0.7545 | 0.1611 | 0.1984 | 0.416593 | 0.7762 | NaN | 0.1141 | 0.1172 | 0.330661 | 0.8078 | 0.0467 | 0.123 | 0.704509 | 0.934 | 0.1474 | 0.1861 | 0.428282 | 0.9419 | NaN | 0.0989 | 0.1173 | 0.39891 | 0.8469 | 0.1096 | 0.12 | 0.360933 | 0.873 | 0.0773 | 0.1892 | 0.682938 | 0.9894 | NaN | 0.1034 | 0.1201 | 0.389321 | 0.773 | -0.0086 | 0.1303 | 0.947626 | 0.987 | 0.1702 | 0.1885 | 0.366481 | 0.9223 | NaN | 0.123 | 0.1187 | 0.300072 | 0.7529 | 0.0584 | 0.1231 | 0.635205 | 0.8623 | 0.1535 | 0.1894 | 0.417892 | 0.9359 | NaN | 0.1071 | 0.1203 | 0.373398 | 0.7624 | -0.009 | 0.128 | 0.943992 | 0.9823 | 0.1707 | 0.1903 | 0.369553 | 0.8861 |
| C9 H16 O2 | 156.1147 | 11.847941 | Lipid | Fatty acid, branched chain fatty acid | 0.0813 | 0.1356 | 0.548633 | 0.8252 | 0.1122 | 0.1588 | 0.480025 | 0.7524 | 0.0522 | 0.2036 | 0.797738 | 0.9647 | NaN | 0.0207 | 0.1259 | 0.869594 | 0.9705 | 0.0192 | 0.1408 | 0.891442 | 0.9729 | 0.0114 | 0.1913 | 0.95239 | 0.9911 | NaN | -0.0239 | 0.1265 | 0.850151 | 0.9714 | 0.0804 | 0.137 | 0.557361 | 0.9053 | -0.0983 | 0.1965 | 0.617005 | 0.9894 | NaN | 0.0339 | 0.1286 | 0.79189 | 0.936 | -0.0038 | 0.1482 | 0.979349 | 0.9926 | 0.0463 | 0.1936 | 0.810925 | 0.9674 | NaN | 0.0303 | 0.1275 | 0.811968 | 0.952 | 0.0203 | 0.1411 | 0.885504 | 0.9727 | 0.0245 | 0.1947 | 0.899922 | 0.9681 | NaN | 0.0402 | 0.1288 | 0.755025 | 0.9321 | -0.0317 | 0.1467 | 0.82908 | 0.9397 | 0.068 | 0.1954 | 0.727707 | 0.9459 |
| FA 5:0 (DiC) | 132.0424 | 2.036774 | Lipid | Fatty Acid, Dicarboxylate | 0.1659 | 0.139 | 0.232499 | 0.6054 | 0.264 | 0.1377 | 0.055198 | 0.3047 | 0.0763 | 0.2359 | 0.746444 | 0.9647 | NaN | 0.1083 | 0.1291 | 0.401639 | 0.8498 | 0.1363 | 0.125 | 0.275481 | 0.798 | 0.1228 | 0.2214 | 0.57899 | 0.954 | NaN | 0.046 | 0.1304 | 0.724146 | 0.9552 | 0.1718 | 0.1207 | 0.154817 | 0.7183 | -0.0631 | 0.2261 | 0.78018 | 0.9935 | NaN | 0.1437 | 0.1316 | 0.274712 | 0.7361 | 0.1878 | 0.1283 | 0.14322 | 0.485 | 0.1447 | 0.2248 | 0.519712 | 0.9375 | NaN | 0.1174 | 0.1308 | 0.36945 | 0.7978 | 0.144 | 0.1248 | 0.248678 | 0.7302 | 0.1127 | 0.2254 | 0.61692 | 0.9621 | NaN | 0.1371 | 0.1319 | 0.298569 | 0.7481 | 0.1473 | 0.1283 | 0.250943 | 0.627 | 0.1626 | 0.2276 | 0.474923 | 0.8887 |
| FA 6:0 (DiC) | 146.0586 | 3.541705 | Lipid | Fatty Acid, Dicarboxylate | 0.1131 | 0.1427 | 0.428005 | 0.7581 | 0.2411 | 0.1565 | 0.12329 | 0.4125 | 0.0287 | 0.2229 | 0.897521 | 0.983 | NaN | 0.063 | 0.1323 | 0.633818 | 0.9087 | 0.1343 | 0.1399 | 0.337146 | 0.8095 | 0.0381 | 0.209 | 0.855404 | 0.9765 | NaN | -0.0714 | 0.1355 | 0.598421 | 0.9125 | 0.082 | 0.1392 | 0.555785 | 0.9053 | -0.169 | 0.2165 | 0.435091 | 0.9816 | NaN | 0.1041 | 0.1349 | 0.440241 | 0.7844 | 0.1915 | 0.144 | 0.183669 | 0.5328 | 0.0697 | 0.2121 | 0.742461 | 0.9572 | NaN | 0.0825 | 0.1339 | 0.537794 | 0.8632 | 0.1503 | 0.1396 | 0.281363 | 0.7544 | 0.0493 | 0.2129 | 0.816952 | 0.9621 | NaN | 0.1058 | 0.1352 | 0.43398 | 0.795 | 0.1596 | 0.1429 | 0.264091 | 0.6386 | 0.09 | 0.2146 | 0.674818 | 0.9459 |
| FA 7:0 (DiC) | 160.074 | 5.69702 | Lipid | Fatty Acid, Dicarboxylate | 0.1866 | 0.1353 | 0.16805 | 0.531 | 0.1966 | 0.1535 | 0.200168 | 0.5 | 0.1919 | 0.2071 | 0.354223 | 0.7534 | NaN | 0.063 | 0.1275 | 0.620975 | 0.9079 | 0.0392 | 0.1392 | 0.778307 | 0.9615 | 0.0951 | 0.1965 | 0.628479 | 0.954 | NaN | 0.0254 | 0.1286 | 0.843641 | 0.9714 | 0.0465 | 0.1359 | 0.732426 | 0.9241 | 0.0192 | 0.2025 | 0.924261 | 0.9935 | NaN | 0.0664 | 0.1309 | 0.611844 | 0.8573 | 0.041 | 0.1465 | 0.779568 | 0.9085 | 0.1006 | 0.1993 | 0.613745 | 0.9375 | NaN | 0.0662 | 0.1294 | 0.60923 | 0.8964 | 0.0316 | 0.1399 | 0.821118 | 0.9396 | 0.1012 | 0.2004 | 0.613608 | 0.9621 | NaN | 0.079 | 0.1308 | 0.545907 | 0.8553 | 0.0442 | 0.1434 | 0.757878 | 0.9096 | 0.1155 | 0.2009 | 0.565417 | 0.9205 |
| FA 9:0 (DiC) | 188.105 | 10.741281 | Lipid | Fatty Acid, Dicarboxylate | 0.2091 | 0.1292 | 0.105764 | 0.4671 | 0.2701 | 0.1446 | 0.061905 | 0.3164 | 0.179 | 0.1985 | 0.367367 | 0.7534 | NaN | 0.1082 | 0.1213 | 0.372373 | 0.8459 | 0.1059 | 0.1329 | 0.425693 | 0.847 | 0.1269 | 0.187 | 0.497311 | 0.954 | NaN | 0.0624 | 0.1227 | 0.611277 | 0.9125 | 0.1028 | 0.1301 | 0.429355 | 0.8947 | 0.0406 | 0.1922 | 0.832639 | 0.9935 | NaN | 0.1259 | 0.1239 | 0.309396 | 0.741 | 0.1316 | 0.1385 | 0.341881 | 0.67 | 0.1418 | 0.1893 | 0.453683 | 0.9375 | NaN | 0.1094 | 0.1232 | 0.374522 | 0.7993 | 0.1117 | 0.1329 | 0.400457 | 0.8162 | 0.1172 | 0.1909 | 0.5395 | 0.9621 | NaN | 0.135 | 0.1239 | 0.276075 | 0.7337 | 0.1374 | 0.1353 | 0.309875 | 0.6689 | 0.1452 | 0.191 | 0.447289 | 0.8887 |
| FA 10:0 (DiC) | 202.1208 | 13.31509 | Lipid | Fatty Acid, Dicarboxylate | -0.0185 | 0.135 | 0.891107 | 0.9809 | 0.0004 | 0.1613 | 0.998096 | 0.9981 | -0.0456 | 0.2009 | 0.820531 | 0.9713 | NaN | -0.0523 | 0.1249 | 0.675593 | 0.9208 | -0.0482 | 0.1417 | 0.733981 | 0.94 | -0.0702 | 0.1884 | 0.709298 | 0.954 | NaN | -0.0571 | 0.1247 | 0.64689 | 0.9331 | 0.0346 | 0.139 | 0.803319 | 0.9363 | -0.1192 | 0.1904 | 0.531176 | 0.9894 | NaN | -0.0623 | 0.1278 | 0.625964 | 0.8606 | -0.1358 | 0.15 | 0.365366 | 0.6762 | -0.0371 | 0.191 | 0.846075 | 0.975 | NaN | -0.0479 | 0.1266 | 0.705189 | 0.9116 | -0.0691 | 0.1422 | 0.627288 | 0.8623 | -0.0521 | 0.1918 | 0.78589 | 0.9621 | NaN | -0.0566 | 0.1281 | 0.65857 | 0.8998 | -0.1539 | 0.1479 | 0.298232 | 0.6559 | -0.0244 | 0.1929 | 0.899141 | 0.9769 |
| FA 11:0 (DiC) | 216.1365 | 14.872025 | Lipid | Fatty Acid, Dicarboxylate | 0.2059 | 0.131 | 0.115956 | 0.4809 | 0.2493 | 0.1426 | 0.080447 | 0.3594 | 0.1803 | 0.205 | 0.379281 | 0.7534 | NaN | 0.0903 | 0.1234 | 0.46443 | 0.8498 | 0.0787 | 0.1314 | 0.549244 | 0.9009 | 0.111 | 0.1936 | 0.566429 | 0.954 | NaN | 0.046 | 0.1248 | 0.712768 | 0.9481 | 0.0939 | 0.1276 | 0.462074 | 0.8956 | 0.0121 | 0.2001 | 0.951924 | 0.9976 | NaN | 0.1108 | 0.126 | 0.379027 | 0.7664 | 0.1004 | 0.1373 | 0.464905 | 0.7319 | 0.1323 | 0.1957 | 0.49909 | 0.9375 | NaN | 0.1038 | 0.1249 | 0.405678 | 0.8263 | 0.093 | 0.1309 | 0.477407 | 0.8272 | 0.1164 | 0.1972 | 0.555074 | 0.9621 | NaN | 0.1225 | 0.1259 | 0.330181 | 0.7485 | 0.1006 | 0.1344 | 0.4545 | 0.7516 | 0.1447 | 0.1973 | 0.463282 | 0.8887 |
| FA 12:0 (DiC) | 230.1519 | 16.474684 | Lipid | Fatty Acid, Dicarboxylate | 0.0027 | 0.1356 | 0.984096 | 0.9936 | 0.1652 | 0.1395 | 0.236241 | 0.528 | -0.1295 | 0.2217 | 0.559134 | 0.8707 | NaN | -0.0163 | 0.1254 | 0.896673 | 0.9705 | 0.076 | 0.1242 | 0.540451 | 0.8967 | -0.0705 | 0.2087 | 0.735676 | 0.954 | NaN | -0.1163 | 0.1265 | 0.357919 | 0.8251 | 0.0892 | 0.1214 | 0.462419 | 0.8956 | -0.2976 | 0.2123 | 0.160847 | 0.7677 | NaN | -0.0129 | 0.1282 | 0.919936 | 0.9828 | 0.0884 | 0.1295 | 0.494545 | 0.752 | -0.0697 | 0.2117 | 0.741808 | 0.9572 | NaN | -0.0039 | 0.1271 | 0.975536 | 0.9861 | 0.0961 | 0.1239 | 0.437658 | 0.8205 | -0.0796 | 0.2124 | 0.708019 | 0.9621 | NaN | 0.0064 | 0.1285 | 0.960412 | 0.9855 | 0.0737 | 0.1279 | 0.564696 | 0.8092 | -0.0312 | 0.2155 | 0.88507 | 0.9702 |
| FA 13:0 (DiC) | 244.1675 | 17.88523 | Lipid | Fatty Acid, Dicarboxylate | 0.1457 | 0.1393 | 0.295574 | 0.6742 | 0.2379 | 0.1382 | 0.085123 | 0.3625 | 0.0663 | 0.2355 | 0.778237 | 0.9647 | NaN | 0.0845 | 0.1295 | 0.514153 | 0.8827 | 0.1498 | 0.1234 | 0.224827 | 0.7475 | 0.0454 | 0.221 | 0.837153 | 0.9721 | NaN | -0.0052 | 0.1316 | 0.968625 | 0.9794 | 0.1416 | 0.1212 | 0.242835 | 0.8037 | -0.1495 | 0.2297 | 0.51524 | 0.9894 | NaN | 0.1253 | 0.1318 | 0.34189 | 0.741 | 0.2004 | 0.127 | 0.114473 | 0.445 | 0.077 | 0.2239 | 0.730934 | 0.9551 | NaN | 0.1055 | 0.1309 | 0.42026 | 0.8375 | 0.1745 | 0.1227 | 0.155056 | 0.631 | 0.053 | 0.225 | 0.813756 | 0.9621 | NaN | 0.1373 | 0.132 | 0.298271 | 0.7481 | 0.1806 | 0.1257 | 0.150744 | 0.5211 | 0.1188 | 0.2265 | 0.60001 | 0.9357 |
| FA 14:0 (DiC) | 258.1833 | 19.113493 | Lipid | Fatty Acid, Dicarboxylate | -0.2618 | 0.1327 | 0.048585 | 0.316 | -0.0546 | 0.1409 | 0.698217 | 0.8759 | -0.4315 | 0.2145 | 0.044272 | 0.3491 | NaN | -0.224 | 0.1231 | 0.0688 | 0.5202 | -0.101 | 0.1236 | 0.41373 | 0.847 | -0.3021 | 0.2062 | 0.142828 | 0.8611 | NaN | -0.2723 | 0.1222 | 0.025931 | 0.27 | -0.0536 | 0.1213 | 0.658759 | 0.9087 | -0.4425 | 0.2019 | 0.028428 | 0.3487 | NaN | -0.2671 | 0.1253 | 0.032987 | 0.3436 | -0.1729 | 0.1304 | 0.185006 | 0.5328 | -0.3142 | 0.209 | 0.132767 | 0.8047 | NaN | -0.2279 | 0.1247 | 0.067582 | 0.511 | -0.1145 | 0.124 | 0.355495 | 0.7839 | -0.3182 | 0.21 | 0.129815 | 0.772 | NaN | -0.2546 | 0.1257 | 0.042828 | 0.3876 | -0.1918 | 0.1286 | 0.135645 | 0.5164 | -0.3014 | 0.2134 | 0.157783 | 0.799 |
| FA 16:0 (DiC) | 286.2147 | 21.107553 | Lipid | Fatty Acid, Dicarboxylate | -0.3138 | 0.1323 | 0.017703 | 0.1685 | -0.0124 | 0.1431 | 0.93095 | 0.9696 | -0.5555 | 0.2096 | 0.008033 | 0.1612 | NaN | -0.2831 | 0.1225 | 0.020851 | 0.2807 | -0.0802 | 0.126 | 0.524093 | 0.8967 | -0.4277 | 0.2022 | 0.034375 | 0.5144 | NaN | -0.326 | 0.1217 | 0.007402 | 0.1075 | -0.0358 | 0.1233 | 0.771291 | 0.9284 | -0.5448 | 0.1974 | 0.005786 | 0.1494 | NaN | -0.3338 | 0.1247 | 0.007416 | 0.1106 | -0.1577 | 0.1339 | 0.238877 | 0.5767 | -0.451 | 0.204 | 0.027058 | 0.4788 | NaN | -0.2945 | 0.124 | 0.017571 | 0.2552 | -0.1069 | 0.1266 | 0.398401 | 0.8162 | -0.4492 | 0.2055 | 0.028846 | 0.4772 | NaN | -0.3272 | 0.125 | 0.008849 | 0.1357 | -0.1736 | 0.1319 | 0.188133 | 0.5692 | -0.452 | 0.2068 | 0.028871 | 0.4663 |
| FA 18:0 (DiC) | 314.2461 | 22.242228 | Lipid | Fatty Acid, Dicarboxylate | 0.267 | 0.1389 | 0.054651 | 0.3387 | 0.2464 | 0.1514 | 0.103528 | 0.3835 | 0.3249 | 0.223 | 0.145188 | 0.6118 | NaN | 0.1939 | 0.1296 | 0.134429 | 0.6808 | 0.1838 | 0.1339 | 0.169832 | 0.6773 | 0.2123 | 0.2125 | 0.317768 | 0.9223 | NaN | 0.1669 | 0.1301 | 0.199609 | 0.7361 | 0.1709 | 0.1317 | 0.194328 | 0.7683 | 0.158 | 0.2178 | 0.468248 | 0.9816 | NaN | 0.2038 | 0.1324 | 0.123764 | 0.579 | 0.1975 | 0.1394 | 0.156517 | 0.5021 | 0.2222 | 0.2154 | 0.302241 | 0.8827 | NaN | 0.1974 | 0.1313 | 0.132721 | 0.6708 | 0.1997 | 0.1337 | 0.135232 | 0.5986 | 0.2144 | 0.2171 | 0.3234 | 0.9106 | NaN | 0.2204 | 0.1323 | 0.095667 | 0.55 | 0.2009 | 0.137 | 0.142593 | 0.5193 | 0.2538 | 0.2161 | 0.24021 | 0.8424 |
| FA 19:0 (DiC) | 328.2614 | 22.461948 | Lipid | Fatty Acid, Dicarboxylate | -0.214 | 0.128 | 0.094437 | 0.4455 | -0.1285 | 0.1495 | 0.390187 | 0.6593 | -0.2623 | 0.1931 | 0.174329 | 0.6772 | NaN | -0.1476 | 0.1193 | 0.21567 | 0.7487 | -0.0673 | 0.1321 | 0.610642 | 0.9043 | -0.1999 | 0.1824 | 0.272878 | 0.9223 | NaN | -0.1918 | 0.1183 | 0.104812 | 0.5628 | -0.1966 | 0.1283 | 0.125387 | 0.6704 | -0.1985 | 0.1838 | 0.280112 | 0.9204 | NaN | -0.1279 | 0.1228 | 0.297638 | 0.7401 | -0.0034 | 0.1405 | 0.980721 | 0.9926 | -0.2065 | 0.1848 | 0.263708 | 0.8705 | NaN | -0.1615 | 0.1206 | 0.180492 | 0.6753 | -0.1101 | 0.1316 | 0.402713 | 0.8162 | -0.198 | 0.1861 | 0.287296 | 0.9039 | NaN | -0.1194 | 0.1235 | 0.333553 | 0.7485 | 0.0193 | 0.1389 | 0.889294 | 0.9667 | -0.2025 | 0.1869 | 0.278737 | 0.8424 |
| FA 20:0 (DiC) | 342.2767 | 22.332983 | Lipid | Fatty Acid, Dicarboxylate | 0.0758 | 0.1323 | 0.566528 | 0.8382 | -0.0591 | 0.1382 | 0.668956 | 0.8568 | 0.2082 | 0.2154 | 0.333877 | 0.7534 | NaN | 0.1616 | 0.1228 | 0.188061 | 0.7251 | 0.1125 | 0.1249 | 0.368044 | 0.824 | 0.1951 | 0.2021 | 0.334219 | 0.9223 | NaN | 0.127 | 0.1222 | 0.298931 | 0.7865 | 0.1094 | 0.1221 | 0.370243 | 0.8809 | 0.1363 | 0.2049 | 0.505799 | 0.9894 | NaN | 0.1092 | 0.1251 | 0.382739 | 0.7683 | 0.0284 | 0.1281 | 0.824638 | 0.9271 | 0.1752 | 0.2052 | 0.393196 | 0.9375 | NaN | 0.1379 | 0.1242 | 0.266876 | 0.7442 | 0.0936 | 0.1246 | 0.452263 | 0.8246 | 0.1844 | 0.206 | 0.370711 | 0.9106 | NaN | 0.1114 | 0.1254 | 0.374319 | 0.7624 | 0.0344 | 0.1261 | 0.785282 | 0.9203 | 0.1833 | 0.207 | 0.375876 | 0.8875 |
| FA 24:0 (DiC) | 398.3392 | 23.17186 | Lipid | Fatty Acid, Dicarboxylate | 0.1108 | 0.1337 | 0.407193 | 0.734 | -0.1523 | 0.1382 | 0.270393 | 0.5632 | 0.3952 | 0.2215 | 0.074483 | 0.462 | NaN | 0.1402 | 0.1236 | 0.256452 | 0.7495 | 0.0106 | 0.126 | 0.932634 | 0.973 | 0.2582 | 0.2128 | 0.225016 | 0.9223 | NaN | 0.1488 | 0.1234 | 0.227751 | 0.7361 | 0.0256 | 0.1238 | 0.835904 | 0.9475 | 0.2591 | 0.2147 | 0.227435 | 0.8779 | NaN | 0.0857 | 0.1266 | 0.498217 | 0.8089 | -0.0776 | 0.1282 | 0.545015 | 0.7845 | 0.2436 | 0.2181 | 0.264087 | 0.8705 | NaN | 0.1377 | 0.1252 | 0.271622 | 0.7442 | 0.0074 | 0.1261 | 0.953291 | 0.9923 | 0.286 | 0.216 | 0.185569 | 0.8608 | NaN | 0.1137 | 0.1266 | 0.369128 | 0.7603 | -0.0551 | 0.1269 | 0.664122 | 0.8681 | 0.2934 | 0.217 | 0.176313 | 0.8194 |
| FA 7:1 (DiC) | 158.0578 | 2.836201 | Lipid | Fatty Acid, Dicarboxylate | 0.0828 | 0.1355 | 0.541058 | 0.825 | 0.2094 | 0.1296 | 0.106218 | 0.3909 | -0.0936 | 0.2408 | 0.69752 | 0.9492 | NaN | 0.0469 | 0.1255 | 0.708666 | 0.9314 | 0.1012 | 0.1168 | 0.386141 | 0.8339 | -0.0315 | 0.2266 | 0.889602 | 0.977 | NaN | 0.0231 | 0.1256 | 0.854258 | 0.9714 | 0.1065 | 0.1142 | 0.350943 | 0.8722 | -0.0929 | 0.2274 | 0.682983 | 0.9894 | NaN | 0.0715 | 0.1281 | 0.57673 | 0.8473 | 0.1458 | 0.1202 | 0.225151 | 0.5613 | -0.0456 | 0.2295 | 0.842456 | 0.9736 | NaN | 0.073 | 0.127 | 0.565361 | 0.8722 | 0.1217 | 0.1162 | 0.294723 | 0.7544 | -0.0149 | 0.2314 | 0.948809 | 0.9854 | NaN | 0.0627 | 0.1285 | 0.625507 | 0.8808 | 0.1112 | 0.1198 | 0.353579 | 0.6867 | -0.0285 | 0.2322 | 0.902272 | 0.9769 |
| FA 8:1 (DiC) | 172.074 | 4.380399 | Lipid | Fatty Acid, Dicarboxylate | 0.1634 | 0.1364 | 0.230964 | 0.6042 | 0.2291 | 0.1731 | 0.185618 | 0.4974 | 0.1256 | 0.1965 | 0.522666 | 0.8655 | NaN | 0.0526 | 0.128 | 0.681042 | 0.9237 | -0.0308 | 0.1614 | 0.848746 | 0.9729 | 0.0901 | 0.1846 | 0.625691 | 0.954 | NaN | 0.0243 | 0.1286 | 0.849927 | 0.9714 | 0.0497 | 0.1537 | 0.746677 | 0.9241 | 0.0103 | 0.1887 | 0.956265 | 0.9976 | NaN | 0.0816 | 0.1304 | 0.531299 | 0.8308 | 0.008 | 0.1686 | 0.962189 | 0.9926 | 0.1144 | 0.1868 | 0.540279 | 0.9375 | NaN | 0.0844 | 0.129 | 0.513062 | 0.8625 | 0.0317 | 0.1584 | 0.841368 | 0.946 | 0.1012 | 0.1878 | 0.590063 | 0.9621 | NaN | 0.087 | 0.1306 | 0.505181 | 0.8285 | -0.0338 | 0.1678 | 0.84017 | 0.9451 | 0.1317 | 0.1885 | 0.484542 | 0.8887 |
| FA 9:1 (DiC) | 186.0894 | 6.299434 | Lipid | Fatty Acid, Dicarboxylate | 0.202 | 0.1318 | 0.125274 | 0.4924 | 0.2833 | 0.1457 | 0.05184 | 0.3003 | 0.1264 | 0.2052 | 0.537783 | 0.8655 | NaN | 0.0673 | 0.1248 | 0.589533 | 0.9079 | 0.0278 | 0.1404 | 0.843054 | 0.9729 | 0.0879 | 0.1929 | 0.648599 | 0.954 | NaN | 0.0492 | 0.1252 | 0.694373 | 0.9481 | 0.0649 | 0.1341 | 0.628602 | 0.9053 | 0.0327 | 0.1958 | 0.867328 | 0.9935 | NaN | 0.1253 | 0.126 | 0.320226 | 0.741 | 0.1107 | 0.1425 | 0.437435 | 0.7301 | 0.1266 | 0.195 | 0.516329 | 0.9375 | NaN | 0.1163 | 0.125 | 0.352304 | 0.7873 | 0.1017 | 0.1354 | 0.452612 | 0.8246 | 0.1092 | 0.196 | 0.577539 | 0.9621 | NaN | 0.1236 | 0.1264 | 0.328081 | 0.7485 | 0.0779 | 0.142 | 0.583098 | 0.8128 | 0.1354 | 0.1968 | 0.4914 | 0.8887 |
| FA 12:1 (DiC) | 228.1364 | 15.499843 | Lipid | Fatty Acid, Dicarboxylate | -0.2947 | 0.1279 | 0.021252 | 0.1953 | -0.303 | 0.1425 | 0.033419 | 0.2761 | -0.313 | 0.1983 | 0.114505 | 0.5694 | NaN | -0.1609 | 0.1218 | 0.186316 | 0.7251 | -0.1867 | 0.1286 | 0.146614 | 0.6288 | -0.1657 | 0.192 | 0.388009 | 0.9389 | NaN | -0.2102 | 0.1197 | 0.078983 | 0.5097 | -0.1955 | 0.1255 | 0.119454 | 0.6704 | -0.2376 | 0.1893 | 0.209511 | 0.8462 | NaN | -0.1648 | 0.1253 | 0.188606 | 0.6616 | -0.2239 | 0.1328 | 0.091894 | 0.4192 | -0.1411 | 0.1983 | 0.476832 | 0.9375 | NaN | -0.1479 | 0.1247 | 0.235639 | 0.7108 | -0.192 | 0.1286 | 0.135529 | 0.5986 | -0.1439 | 0.1998 | 0.47133 | 0.9359 | NaN | -0.1657 | 0.1257 | 0.187415 | 0.6463 | -0.2382 | 0.1299 | 0.066612 | 0.3536 | -0.1401 | 0.2027 | 0.489217 | 0.8887 |
| FA 14:1 (DiC) | 256.1678 | 18.092892 | Lipid | Fatty Acid, Dicarboxylate | -0.1907 | 0.1325 | 0.150042 | 0.5192 | -0.2559 | 0.1474 | 0.082553 | 0.3594 | -0.1814 | 0.2075 | 0.38187 | 0.7534 | NaN | -0.1214 | 0.1234 | 0.325066 | 0.8011 | -0.238 | 0.1292 | 0.065318 | 0.4801 | -0.0742 | 0.1972 | 0.706753 | 0.954 | NaN | -0.1315 | 0.123 | 0.285103 | 0.7865 | -0.1977 | 0.1278 | 0.1218 | 0.6704 | -0.1137 | 0.1972 | 0.564207 | 0.9894 | NaN | -0.1017 | 0.127 | 0.423475 | 0.7844 | -0.2564 | 0.1344 | 0.05642 | 0.3211 | -0.0233 | 0.2037 | 0.909058 | 0.99 | NaN | -0.1087 | 0.1255 | 0.386583 | 0.8025 | -0.2577 | 0.129 | 0.045759 | 0.3608 | -0.0436 | 0.2036 | 0.830371 | 0.9621 | NaN | -0.1057 | 0.1272 | 0.406067 | 0.7874 | -0.2777 | 0.1319 | 0.035265 | 0.2595 | -0.0249 | 0.2069 | 0.904382 | 0.9769 |
| FA 18:1 (DiC) | 312.2305 | 21.571661 | Lipid | Fatty Acid, Dicarboxylate | -0.1208 | 0.144 | 0.401501 | 0.7322 | -0.0297 | 0.1503 | 0.843458 | 0.932 | -0.2093 | 0.2348 | 0.372756 | 0.7534 | NaN | -0.0206 | 0.1345 | 0.878364 | 0.9705 | 0.0168 | 0.1322 | 0.899147 | 0.9729 | -0.042 | 0.2255 | 0.852231 | 0.9765 | NaN | -0.1157 | 0.1329 | 0.384132 | 0.8414 | 0.0014 | 0.1296 | 0.991316 | 0.9931 | -0.2101 | 0.2216 | 0.343102 | 0.957 | NaN | -0.0545 | 0.137 | 0.691021 | 0.883 | -0.0384 | 0.1374 | 0.780137 | 0.9085 | -0.0488 | 0.2293 | 0.831545 | 0.9726 | NaN | -0.0394 | 0.136 | 0.771819 | 0.938 | -0.0175 | 0.1322 | 0.894402 | 0.9727 | -0.0595 | 0.2301 | 0.796019 | 0.9621 | NaN | -0.0464 | 0.1375 | 0.73578 | 0.918 | -0.0424 | 0.1354 | 0.754248 | 0.9096 | -0.043 | 0.2332 | 0.853618 | 0.9641 |
| FA 20:1 (DiC) | 340.2575 | 22.070116 | Lipid | Fatty Acid, Dicarboxylate | 0.1402 | 0.1334 | 0.293114 | 0.6742 | 0.1435 | 0.1386 | 0.300497 | 0.5924 | 0.1512 | 0.2174 | 0.486686 | 0.8369 | NaN | 0.249 | 0.1237 | 0.044177 | 0.4204 | 0.2908 | 0.1215 | 0.016657 | 0.2189 | 0.2206 | 0.204 | 0.279571 | 0.9223 | NaN | 0.2062 | 0.1231 | 0.093952 | 0.5363 | 0.2819 | 0.1188 | 0.017597 | 0.2556 | 0.1476 | 0.2052 | 0.471951 | 0.9826 | NaN | 0.1792 | 0.126 | 0.155003 | 0.6367 | 0.2247 | 0.1267 | 0.076181 | 0.3823 | 0.1501 | 0.2066 | 0.467441 | 0.9375 | NaN | 0.2326 | 0.1254 | 0.063564 | 0.4979 | 0.272 | 0.1216 | 0.025258 | 0.2579 | 0.2117 | 0.2078 | 0.30847 | 0.9106 | NaN | 0.1918 | 0.1264 | 0.129297 | 0.605 | 0.2186 | 0.1245 | 0.07912 | 0.3865 | 0.184 | 0.2086 | 0.377815 | 0.8875 |
| FA 21:1 (DiC) | 354.2763 | 22.34594 | Lipid | Fatty Acid, Dicarboxylate | 0.1551 | 0.1346 | 0.249235 | 0.6174 | 0.0709 | 0.14 | 0.61245 | 0.8251 | 0.2236 | 0.2205 | 0.310563 | 0.7534 | NaN | 0.1882 | 0.1243 | 0.129859 | 0.6772 | 0.1098 | 0.1227 | 0.370869 | 0.824 | 0.2403 | 0.2065 | 0.244576 | 0.9223 | NaN | 0.1456 | 0.1242 | 0.24134 | 0.7381 | 0.1314 | 0.1205 | 0.275326 | 0.806 | 0.1435 | 0.2099 | 0.494183 | 0.9848 | NaN | 0.2142 | 0.1273 | 0.092394 | 0.5372 | 0.074 | 0.128 | 0.563159 | 0.789 | 0.3374 | 0.2104 | 0.108919 | 0.7851 | NaN | 0.2121 | 0.1261 | 0.092541 | 0.6195 | 0.1426 | 0.1231 | 0.246799 | 0.7302 | 0.2601 | 0.2103 | 0.216165 | 0.8892 | NaN | 0.2248 | 0.1277 | 0.078379 | 0.5276 | 0.0913 | 0.126 | 0.468677 | 0.7618 | 0.3344 | 0.2129 | 0.116199 | 0.7458 |
| FA 24:1 (DiC) | 396.3218 | 22.667086 | Lipid | Fatty Acid, Dicarboxylate | 0.0415 | 0.1418 | 0.769905 | 0.9439 | -0.0106 | 0.1214 | 0.930701 | 0.9696 | 0.19 | 0.306 | 0.534637 | 0.8655 | NaN | 0.1067 | 0.1314 | 0.416716 | 0.8498 | 0.0585 | 0.1072 | 0.5852 | 0.904 | 0.2009 | 0.2868 | 0.483704 | 0.954 | NaN | 0.1007 | 0.1312 | 0.442529 | 0.8792 | 0.1061 | 0.1059 | 0.316476 | 0.8439 | 0.0664 | 0.2914 | 0.819833 | 0.9935 | NaN | 0.0558 | 0.1341 | 0.677027 | 0.8746 | 0.0148 | 0.1112 | 0.894314 | 0.9695 | 0.1431 | 0.2914 | 0.623433 | 0.9375 | NaN | 0.1021 | 0.1332 | 0.4434 | 0.8528 | 0.0683 | 0.1076 | 0.525335 | 0.8496 | 0.1833 | 0.2921 | 0.530261 | 0.9597 | NaN | 0.0773 | 0.1345 | 0.565375 | 0.8718 | 0.0222 | 0.1096 | 0.83977 | 0.9451 | 0.2066 | 0.2935 | 0.481506 | 0.8887 |
| FA 26:1 (DiC) | 424.355 | 22.844032 | Lipid | Fatty Acid, Dicarboxylate | -0.0962 | 0.1351 | 0.476576 | 0.7972 | -0.1307 | 0.1353 | 0.334129 | 0.621 | -0.0777 | 0.2334 | 0.739248 | 0.9647 | NaN | -0.0189 | 0.1258 | 0.880364 | 0.9705 | -0.0379 | 0.1206 | 0.753558 | 0.9514 | -0.0429 | 0.2192 | 0.844771 | 0.9765 | NaN | -0.03 | 0.1254 | 0.811033 | 0.9676 | 0.0133 | 0.1198 | 0.911889 | 0.973 | -0.1132 | 0.2205 | 0.607686 | 0.9894 | NaN | -0.0614 | 0.128 | 0.631492 | 0.8606 | -0.0691 | 0.125 | 0.580163 | 0.804 | -0.1092 | 0.2219 | 0.622823 | 0.9375 | NaN | -0.0117 | 0.1278 | 0.927152 | 0.9796 | -0.0274 | 0.1212 | 0.821225 | 0.9396 | -0.0272 | 0.2235 | 0.903216 | 0.9681 | NaN | -0.039 | 0.1287 | 0.76178 | 0.9324 | -0.0492 | 0.1236 | 0.690553 | 0.8763 | -0.0698 | 0.224 | 0.755379 | 0.9525 |
| FA 27:1 (DiC) | 438.3719 | 23.034887 | Lipid | Fatty Acid, Dicarboxylate | 0.1395 | 0.1348 | 0.300836 | 0.6742 | -0.0112 | 0.1289 | 0.930697 | 0.9696 | 0.3572 | 0.2414 | 0.138926 | 0.6043 | NaN | 0.1706 | 0.1245 | 0.17062 | 0.7251 | 0.0105 | 0.1132 | 0.926066 | 0.9729 | 0.3805 | 0.2258 | 0.091888 | 0.7567 | NaN | 0.1528 | 0.1244 | 0.219093 | 0.7361 | 0.0591 | 0.1115 | 0.595875 | 0.9053 | 0.263 | 0.2304 | 0.253604 | 0.9 | NaN | 0.1297 | 0.1275 | 0.308832 | 0.741 | -0.0405 | 0.118 | 0.731298 | 0.8813 | 0.3644 | 0.2291 | 0.111716 | 0.787 | NaN | 0.1962 | 0.1263 | 0.12047 | 0.6708 | 0.0405 | 0.1137 | 0.721498 | 0.887 | 0.4025 | 0.2299 | 0.080018 | 0.6055 | NaN | 0.1676 | 0.1277 | 0.189342 | 0.6463 | -0.0184 | 0.1161 | 0.873962 | 0.961 | 0.4216 | 0.2313 | 0.0683 | 0.6024 |
| FA 28:1 (DiC) | 452.3876 | 23.075253 | Lipid | Fatty Acid, Dicarboxylate | 0.013 | 0.1351 | 0.923161 | 0.9811 | -0.2229 | 0.1359 | 0.101032 | 0.3816 | 0.2503 | 0.2264 | 0.269062 | 0.7397 | NaN | 0.0896 | 0.1254 | 0.475195 | 0.8544 | -0.0801 | 0.1239 | 0.517837 | 0.8967 | 0.2214 | 0.2126 | 0.297778 | 0.9223 | NaN | 0.0839 | 0.1252 | 0.502474 | 0.9053 | -0.038 | 0.1234 | 0.758251 | 0.9266 | 0.1733 | 0.2155 | 0.421191 | 0.9816 | NaN | 0.0149 | 0.1277 | 0.907101 | 0.9828 | -0.1686 | 0.1256 | 0.17937 | 0.5323 | 0.1664 | 0.2174 | 0.443979 | 0.9375 | NaN | 0.0837 | 0.1271 | 0.510516 | 0.8625 | -0.0864 | 0.1239 | 0.485726 | 0.8301 | 0.2357 | 0.2163 | 0.275901 | 0.9039 | NaN | 0.0489 | 0.1282 | 0.702545 | 0.9035 | -0.1364 | 0.1249 | 0.274685 | 0.648 | 0.2136 | 0.2179 | 0.327027 | 0.8727 |
| FA 17:2 (DiC) | 296.1984 | 22.410254 | Lipid | Fatty Acid, Dicarboxylate | -0.0863 | 0.1285 | 0.502003 | 0.8067 | -0.3087 | 0.138 | 0.025259 | 0.2446 | 0.0787 | 0.2009 | 0.695052 | 0.9492 | NaN | -0.1251 | 0.1188 | 0.292442 | 0.7802 | -0.2871 | 0.1208 | 0.017439 | 0.2239 | -0.011 | 0.19 | 0.953763 | 0.9911 | NaN | -0.1114 | 0.1186 | 0.347826 | 0.8224 | -0.1848 | 0.1226 | 0.131834 | 0.6741 | -0.0701 | 0.1941 | 0.717877 | 0.99 | NaN | -0.1601 | 0.122 | 0.189262 | 0.6616 | -0.3613 | 0.1246 | 0.00374 | 0.0688 | -0.0117 | 0.1929 | 0.951491 | 0.99 | NaN | -0.1079 | 0.1204 | 0.369972 | 0.7978 | -0.2752 | 0.1214 | 0.023428 | 0.2532 | 0.0181 | 0.1928 | 0.92523 | 0.9774 | NaN | -0.1308 | 0.1219 | 0.283306 | 0.7342 | -0.3428 | 0.1228 | 0.005245 | 0.0852 | 0.0285 | 0.1936 | 0.88312 | 0.9702 |
| FA 18:2 (DiC) | 310.2144 | 21.042389 | Lipid | Fatty Acid, Dicarboxylate | -0.1004 | 0.1405 | 0.47512 | 0.7972 | -0.0873 | 0.1571 | 0.578188 | 0.8019 | -0.0855 | 0.219 | 0.696298 | 0.9492 | NaN | -0.0111 | 0.131 | 0.932486 | 0.9861 | -0.0557 | 0.1381 | 0.686601 | 0.9267 | 0.0598 | 0.209 | 0.77465 | 0.954 | NaN | -0.0983 | 0.1297 | 0.448505 | 0.8815 | -0.0668 | 0.1354 | 0.621777 | 0.9053 | -0.1062 | 0.2068 | 0.607626 | 0.9894 | NaN | -0.0299 | 0.1338 | 0.823195 | 0.9526 | -0.1041 | 0.1436 | 0.468486 | 0.7332 | 0.0842 | 0.2141 | 0.694311 | 0.9477 | NaN | -0.0291 | 0.1325 | 0.826164 | 0.9564 | -0.0947 | 0.138 | 0.492396 | 0.8363 | 0.0441 | 0.2131 | 0.836054 | 0.9621 | NaN | -0.0274 | 0.1342 | 0.838215 | 0.9501 | -0.1114 | 0.1414 | 0.43077 | 0.7453 | 0.0765 | 0.2169 | 0.724205 | 0.9459 |
| FA 22:2 (DiC) | 366.2777 | 22.203842 | Lipid | Fatty Acid, Dicarboxylate | -0.1578 | 0.1359 | 0.245494 | 0.616 | -0.0098 | 0.1438 | 0.945686 | 0.9739 | -0.2888 | 0.2179 | 0.184997 | 0.6943 | NaN | -0.05 | 0.1274 | 0.694728 | 0.9308 | 0.0878 | 0.1272 | 0.489938 | 0.8867 | -0.1687 | 0.208 | 0.417402 | 0.9419 | NaN | -0.1099 | 0.1259 | 0.382703 | 0.8414 | 0.0779 | 0.1246 | 0.531676 | 0.9053 | -0.265 | 0.206 | 0.198208 | 0.8462 | NaN | -0.0634 | 0.1303 | 0.626505 | 0.8606 | 0.054 | 0.1323 | 0.683013 | 0.853 | -0.1618 | 0.212 | 0.445267 | 0.9375 | NaN | -0.056 | 0.1292 | 0.664369 | 0.9055 | 0.0926 | 0.1276 | 0.46781 | 0.8272 | -0.1855 | 0.2117 | 0.380991 | 0.9106 | NaN | -0.0642 | 0.1306 | 0.623211 | 0.8808 | 0.0552 | 0.1302 | 0.671397 | 0.8694 | -0.1694 | 0.2143 | 0.429237 | 0.8887 |
| FA 26:2 (DiC) | 422.3414 | 22.776163 | Lipid | Fatty Acid, Dicarboxylate | -0.0168 | 0.1419 | 0.905865 | 0.9809 | -0.0925 | 0.1465 | 0.527796 | 0.7811 | 0.0743 | 0.2353 | 0.752315 | 0.9647 | NaN | 0.0885 | 0.1322 | 0.503475 | 0.8758 | 0.0107 | 0.1303 | 0.934822 | 0.973 | 0.1606 | 0.2214 | 0.468261 | 0.9478 | NaN | 0.0763 | 0.1318 | 0.562915 | 0.9125 | 0.0823 | 0.1298 | 0.525831 | 0.9053 | 0.0586 | 0.2223 | 0.792011 | 0.9935 | NaN | 0.0184 | 0.1343 | 0.890892 | 0.9771 | -0.0238 | 0.1352 | 0.860468 | 0.95 | 0.0563 | 0.2238 | 0.801513 | 0.9662 | NaN | 0.064 | 0.1337 | 0.632204 | 0.8971 | -0.0199 | 0.1298 | 0.877885 | 0.9692 | 0.1464 | 0.2254 | 0.516108 | 0.9524 | NaN | 0.0489 | 0.135 | 0.717175 | 0.9116 | -0.025 | 0.133 | 0.851066 | 0.9491 | 0.1256 | 0.2262 | 0.578671 | 0.9205 |
| FA 27:2 (DiC) | 436.3568 | 22.928392 | Lipid | Fatty Acid, Dicarboxylate | -0.1865 | 0.1339 | 0.163559 | 0.531 | -0.1453 | 0.1365 | 0.287103 | 0.5742 | -0.2223 | 0.2223 | 0.317322 | 0.7534 | NaN | -0.1409 | 0.1242 | 0.256609 | 0.7495 | -0.0134 | 0.1231 | 0.913332 | 0.9729 | -0.2834 | 0.2082 | 0.173476 | 0.879 | NaN | -0.1375 | 0.1241 | 0.267764 | 0.7779 | 0.0284 | 0.1221 | 0.816038 | 0.9404 | -0.3068 | 0.21 | 0.143969 | 0.7483 | NaN | -0.197 | 0.1264 | 0.119147 | 0.579 | -0.0871 | 0.126 | 0.489202 | 0.7494 | -0.3299 | 0.212 | 0.119753 | 0.7964 | NaN | -0.1681 | 0.1255 | 0.180551 | 0.6753 | -0.0323 | 0.1226 | 0.792264 | 0.929 | -0.3025 | 0.2126 | 0.154707 | 0.8056 | NaN | -0.1872 | 0.1268 | 0.139707 | 0.605 | -0.0717 | 0.1245 | 0.564809 | 0.8092 | -0.3102 | 0.214 | 0.147082 | 0.7588 |
| FA 28:2 (DiC) | 450.3724 | 22.945812 | Lipid | Fatty Acid, Dicarboxylate | 0.0223 | 0.137 | 0.870874 | 0.9809 | -0.1704 | 0.1373 | 0.214607 | 0.5076 | 0.2198 | 0.2308 | 0.340933 | 0.7534 | NaN | 0.1278 | 0.1276 | 0.316499 | 0.7898 | 0.0187 | 0.1269 | 0.882814 | 0.9729 | 0.2031 | 0.2166 | 0.348276 | 0.9223 | NaN | 0.102 | 0.127 | 0.422154 | 0.8695 | 0.049 | 0.1254 | 0.695682 | 0.9195 | 0.134 | 0.2199 | 0.542048 | 0.9894 | NaN | 0.0592 | 0.1297 | 0.648013 | 0.8652 | -0.0745 | 0.1285 | 0.561726 | 0.789 | 0.1629 | 0.2205 | 0.460004 | 0.9375 | NaN | 0.11 | 0.1292 | 0.394529 | 0.8103 | 0.0052 | 0.1265 | 0.967386 | 0.9923 | 0.2044 | 0.2205 | 0.353946 | 0.9106 | NaN | 0.0822 | 0.1303 | 0.528095 | 0.845 | -0.0477 | 0.1275 | 0.708605 | 0.8887 | 0.1961 | 0.2218 | 0.376483 | 0.8875 |
| Methyl 8-2-2-formyl-vinyl-3-hydroxy-5-oxo-cyclopentyl]-octanoate | 310.1761 | 17.698135 | Lipid | Fatty Acid, Dicarboxylate | -0.0941 | 0.1306 | 0.470993 | 0.7972 | 0.0015 | 0.1471 | 0.99211 | 0.9963 | -0.205 | 0.2046 | 0.316244 | 0.7534 | NaN | -0.1025 | 0.1207 | 0.395788 | 0.8498 | -0.0337 | 0.1292 | 0.794505 | 0.9639 | -0.1926 | 0.1919 | 0.31543 | 0.9223 | NaN | -0.082 | 0.1206 | 0.496761 | 0.9053 | 0.0289 | 0.1268 | 0.819667 | 0.9425 | -0.1831 | 0.1934 | 0.343549 | 0.957 | NaN | -0.0915 | 0.1234 | 0.458335 | 0.7844 | -0.0778 | 0.1355 | 0.566072 | 0.7911 | -0.1486 | 0.1956 | 0.447312 | 0.9375 | NaN | -0.092 | 0.1223 | 0.451839 | 0.8543 | -0.0463 | 0.1296 | 0.721164 | 0.887 | -0.1678 | 0.1959 | 0.391734 | 0.9163 | NaN | -0.1027 | 0.1237 | 0.406521 | 0.7874 | -0.1029 | 0.1339 | 0.442015 | 0.7458 | -0.1567 | 0.1973 | 0.426966 | 0.8887 |
| FA 11:3 (DiC, diOH) | 242.077 | 2.402914 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.1502 | 0.1343 | 0.26349 | 0.6341 | -0.0778 | 0.1564 | 0.618909 | 0.8272 | -0.2041 | 0.2054 | 0.320362 | 0.7534 | NaN | -0.1763 | 0.124 | 0.155284 | 0.7026 | -0.0871 | 0.1372 | 0.525359 | 0.8967 | -0.2237 | 0.1924 | 0.245005 | 0.9223 | NaN | -0.2392 | 0.1241 | 0.053865 | 0.3814 | -0.0081 | 0.1354 | 0.952261 | 0.9769 | -0.3924 | 0.1969 | 0.046285 | 0.4482 | NaN | -0.196 | 0.1269 | 0.122597 | 0.579 | -0.1781 | 0.1438 | 0.21578 | 0.5546 | -0.1921 | 0.1953 | 0.325255 | 0.9044 | NaN | -0.1826 | 0.1257 | 0.146303 | 0.6708 | -0.0919 | 0.1374 | 0.503912 | 0.848 | -0.2328 | 0.1959 | 0.23487 | 0.9039 | NaN | -0.176 | 0.1271 | 0.166243 | 0.6293 | -0.1797 | 0.1414 | 0.20392 | 0.5756 | -0.1659 | 0.1978 | 0.401557 | 0.8887 |
| FA 13:3 (DiC, diOH) | 270.1081 | 7.462934 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | 0.1895 | 0.1323 | 0.152106 | 0.5192 | 0.3015 | 0.147 | 0.040272 | 0.2925 | 0.1065 | 0.204 | 0.601645 | 0.8909 | NaN | 0.2246 | 0.1221 | 0.065889 | 0.5123 | 0.2872 | 0.1286 | 0.02548 | 0.2806 | 0.1846 | 0.1917 | 0.335784 | 0.9223 | NaN | 0.1349 | 0.1228 | 0.27203 | 0.7821 | 0.2278 | 0.128 | 0.075053 | 0.5751 | 0.0732 | 0.1929 | 0.704357 | 0.9894 | NaN | 0.2608 | 0.1252 | 0.03726 | 0.3473 | 0.2962 | 0.134 | 0.02709 | 0.2147 | 0.2476 | 0.1966 | 0.207983 | 0.8705 | NaN | 0.2195 | 0.1238 | 0.076293 | 0.5579 | 0.317 | 0.1281 | 0.013331 | 0.1989 | 0.1483 | 0.1949 | 0.446669 | 0.9359 | NaN | 0.2521 | 0.1254 | 0.044401 | 0.389 | 0.2956 | 0.1319 | 0.025041 | 0.2033 | 0.2219 | 0.1981 | 0.262595 | 0.8424 |
| FA 14:3 (DiC, diOH) | 284.1241 | 8.084486 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0156 | 0.1316 | 0.905669 | 0.9809 | 0.0027 | 0.1523 | 0.985763 | 0.9963 | -0.059 | 0.2048 | 0.773148 | 0.9647 | NaN | 0.039 | 0.122 | 0.748931 | 0.9484 | 0.0051 | 0.1337 | 0.969393 | 0.9891 | 0.0257 | 0.1934 | 0.894376 | 0.977 | NaN | 0.0237 | 0.1216 | 0.845831 | 0.9714 | 0.0594 | 0.1314 | 0.651466 | 0.9053 | -0.0287 | 0.1936 | 0.881996 | 0.9935 | NaN | 0.0691 | 0.1255 | 0.581611 | 0.8473 | 0.0083 | 0.1393 | 0.952278 | 0.987 | 0.0731 | 0.1984 | 0.712612 | 0.9477 | NaN | 0.0475 | 0.1238 | 0.701479 | 0.9116 | 0.0177 | 0.134 | 0.895137 | 0.9727 | 0.0286 | 0.1975 | 0.884764 | 0.9633 | NaN | 0.0571 | 0.1255 | 0.648863 | 0.8907 | -0.0276 | 0.1373 | 0.840696 | 0.9451 | 0.0718 | 0.2011 | 0.721201 | 0.9459 |
| FA 16:3 (DiC, diOH) | 312.1554 | 12.519212 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.1979 | 0.1265 | 0.117851 | 0.4809 | -0.0459 | 0.1283 | 0.720302 | 0.8908 | -0.3604 | 0.2125 | 0.089961 | 0.4966 | NaN | -0.2602 | 0.1167 | 0.02582 | 0.3185 | -0.0843 | 0.1126 | 0.453934 | 0.8559 | -0.4341 | 0.1985 | 0.028719 | 0.5113 | NaN | -0.2353 | 0.1165 | 0.043422 | 0.3329 | -0.0787 | 0.1104 | 0.476028 | 0.9053 | -0.3797 | 0.2001 | 0.057787 | 0.4797 | NaN | -0.2237 | 0.1194 | 0.061036 | 0.4615 | -0.0344 | 0.1174 | 0.769406 | 0.9036 | -0.4205 | 0.2014 | 0.036768 | 0.5138 | NaN | -0.2211 | 0.1183 | 0.061633 | 0.4979 | -0.0813 | 0.1128 | 0.470792 | 0.8272 | -0.3584 | 0.2027 | 0.077058 | 0.6055 | NaN | -0.213 | 0.1197 | 0.075197 | 0.5189 | -0.0177 | 0.1158 | 0.878552 | 0.9641 | -0.41 | 0.2034 | 0.043891 | 0.4743 |
| FA 17:3 (DiC, diOH) | 326.1711 | 14.668848 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.257 | 0.1303 | 0.048523 | 0.316 | -0.3154 | 0.1401 | 0.024366 | 0.2445 | -0.2448 | 0.2075 | 0.23822 | 0.735 | NaN | -0.1669 | 0.1221 | 0.171668 | 0.7251 | -0.1933 | 0.127 | 0.128023 | 0.6118 | -0.1899 | 0.1956 | 0.331577 | 0.9223 | NaN | -0.1811 | 0.1215 | 0.136123 | 0.6531 | -0.1557 | 0.1264 | 0.217935 | 0.7942 | -0.2311 | 0.196 | 0.238357 | 0.888 | NaN | -0.1773 | 0.1249 | 0.155712 | 0.6367 | -0.2558 | 0.1297 | 0.048503 | 0.2946 | -0.1566 | 0.1998 | 0.433189 | 0.9375 | NaN | -0.1518 | 0.1245 | 0.222974 | 0.7052 | -0.1942 | 0.1272 | 0.126824 | 0.5933 | -0.1543 | 0.201 | 0.442748 | 0.9359 | NaN | -0.1755 | 0.1253 | 0.161379 | 0.6278 | -0.2685 | 0.127 | 0.034439 | 0.2595 | -0.1424 | 0.2031 | 0.483285 | 0.8887 |
| FA 18:3 (DiC, diOH) | 340.186 | 14.15057 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.0083 | 0.1296 | 0.948833 | 0.9855 | -0.0597 | 0.1477 | 0.685879 | 0.8664 | -0.0062 | 0.2021 | 0.975492 | 0.9935 | NaN | 0.0538 | 0.1202 | 0.654425 | 0.918 | -0.0243 | 0.1299 | 0.851397 | 0.9729 | 0.071 | 0.1905 | 0.709565 | 0.954 | NaN | 0.0519 | 0.12 | 0.6654 | 0.935 | 0.0566 | 0.1288 | 0.660122 | 0.9087 | 0.0233 | 0.191 | 0.902757 | 0.9935 | NaN | 0.0807 | 0.1237 | 0.513774 | 0.8197 | -0.0532 | 0.1351 | 0.693643 | 0.8624 | 0.1422 | 0.1964 | 0.469004 | 0.9375 | NaN | 0.0571 | 0.1219 | 0.639448 | 0.8992 | -0.0363 | 0.13 | 0.780333 | 0.9247 | 0.0843 | 0.1948 | 0.665232 | 0.9621 | NaN | 0.0654 | 0.1236 | 0.596463 | 0.8765 | -0.0918 | 0.133 | 0.489922 | 0.7774 | 0.1367 | 0.1989 | 0.49176 | 0.8887 |
| FA 19:3 (DiC, diOH) | 354.2024 | 16.772755 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.2002 | 0.1312 | 0.127018 | 0.4938 | -0.1912 | 0.152 | 0.208416 | 0.5065 | -0.2362 | 0.2002 | 0.237988 | 0.735 | NaN | -0.1515 | 0.1219 | 0.213672 | 0.7484 | -0.1414 | 0.1341 | 0.291727 | 0.8051 | -0.1915 | 0.1884 | 0.309499 | 0.9223 | NaN | -0.1282 | 0.1222 | 0.294042 | 0.7865 | -0.0684 | 0.1336 | 0.608811 | 0.9053 | -0.1871 | 0.1899 | 0.324537 | 0.9479 | NaN | -0.1478 | 0.1248 | 0.236267 | 0.7062 | -0.2118 | 0.1386 | 0.126488 | 0.4686 | -0.1393 | 0.1933 | 0.471347 | 0.9375 | NaN | -0.1409 | 0.1238 | 0.255128 | 0.7358 | -0.1462 | 0.1342 | 0.275999 | 0.7544 | -0.17 | 0.1928 | 0.378057 | 0.9106 | NaN | -0.1636 | 0.1247 | 0.189686 | 0.6463 | -0.2408 | 0.1362 | 0.077184 | 0.3854 | -0.1551 | 0.1947 | 0.425899 | 0.8887 |
| FA 20:3 (DiC, diOH) | 368.2165 | 17.202263 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | 0.1854 | 0.1299 | 0.153304 | 0.5192 | 0.2363 | 0.1448 | 0.102651 | 0.3829 | 0.14 | 0.2028 | 0.489812 | 0.8397 | NaN | 0.1909 | 0.1199 | 0.111569 | 0.6749 | 0.1599 | 0.1286 | 0.213999 | 0.7304 | 0.2046 | 0.1903 | 0.282246 | 0.9223 | NaN | 0.1454 | 0.1203 | 0.226539 | 0.7361 | 0.1719 | 0.1257 | 0.171497 | 0.7308 | 0.1127 | 0.1917 | 0.556742 | 0.9894 | NaN | 0.2061 | 0.1226 | 0.09272 | 0.5372 | 0.1462 | 0.1352 | 0.27951 | 0.6088 | 0.248 | 0.1941 | 0.201296 | 0.8705 | NaN | 0.1851 | 0.1216 | 0.127862 | 0.6708 | 0.144 | 0.1295 | 0.26607 | 0.7359 | 0.1975 | 0.1939 | 0.308284 | 0.9106 | NaN | 0.1967 | 0.1229 | 0.109396 | 0.554 | 0.1183 | 0.1343 | 0.378399 | 0.6983 | 0.24 | 0.1961 | 0.220971 | 0.8424 |
| FA 21:3 (DiC, diOH) | 382.2322 | 19.090963 | Lipid | Fatty Acid, Dicarboxylate, dihydroxy | -0.1033 | 0.1134 | 0.362193 | 0.7161 | -0.0541 | 0.1219 | 0.656986 | 0.8482 | -0.1666 | 0.1819 | 0.359835 | 0.7534 | NaN | -0.0701 | 0.1051 | 0.504545 | 0.8758 | 0.0053 | 0.1076 | 0.960532 | 0.9874 | -0.1624 | 0.1706 | 0.340963 | 0.9223 | NaN | -0.0765 | 0.1048 | 0.465497 | 0.8953 | 0.082 | 0.1073 | 0.445052 | 0.8947 | -0.223 | 0.1718 | 0.194175 | 0.8462 | NaN | -0.0813 | 0.1073 | 0.448715 | 0.7844 | -0.0846 | 0.1115 | 0.447785 | 0.7319 | -0.1056 | 0.1743 | 0.544652 | 0.9375 | NaN | -0.0728 | 0.1065 | 0.494294 | 0.8625 | -0.0292 | 0.1073 | 0.785686 | 0.9267 | -0.1339 | 0.1742 | 0.442043 | 0.9359 | NaN | -0.0743 | 0.1077 | 0.490059 | 0.8278 | -0.0828 | 0.1097 | 0.450642 | 0.7515 | -0.0987 | 0.1765 | 0.575817 | 0.9205 |
| FA 8:0 (Dic, OH) | 190.0842 | 3.548903 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1012 | 0.1448 | 0.484565 | 0.8041 | 0.1302 | 0.1469 | 0.375449 | 0.6456 | 0.0724 | 0.2411 | 0.764034 | 0.9647 | NaN | 0.1116 | 0.1339 | 0.404334 | 0.8498 | 0.1169 | 0.1289 | 0.364302 | 0.824 | 0.1055 | 0.2262 | 0.640888 | 0.954 | NaN | 0.0356 | 0.1343 | 0.790744 | 0.9641 | 0.0733 | 0.1272 | 0.564331 | 0.9053 | -0.0056 | 0.2288 | 0.98043 | 0.9976 | NaN | 0.1629 | 0.1371 | 0.234956 | 0.7062 | 0.169 | 0.134 | 0.207431 | 0.5478 | 0.1564 | 0.2301 | 0.496558 | 0.9375 | NaN | 0.119 | 0.1356 | 0.380319 | 0.7993 | 0.1087 | 0.1293 | 0.400179 | 0.8162 | 0.1245 | 0.2306 | 0.589342 | 0.9621 | NaN | 0.1494 | 0.1373 | 0.276527 | 0.7337 | 0.1247 | 0.1322 | 0.34571 | 0.6824 | 0.1732 | 0.2331 | 0.45739 | 0.8887 |
| FA 9:0 (DiC,OH) | 204.1001 | 5.214559 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1205 | 0.1324 | 0.362728 | 0.7161 | 0.1049 | 0.152 | 0.490013 | 0.7545 | 0.1253 | 0.2009 | 0.532819 | 0.8655 | NaN | 0.0946 | 0.1226 | 0.440478 | 0.8498 | 0.0518 | 0.134 | 0.698986 | 0.9328 | 0.121 | 0.1884 | 0.520679 | 0.954 | NaN | 0.0582 | 0.1229 | 0.635946 | 0.9282 | 0.0817 | 0.1311 | 0.533167 | 0.9053 | 0.0412 | 0.1914 | 0.82952 | 0.9935 | NaN | 0.0923 | 0.1254 | 0.461425 | 0.7861 | 0.017 | 0.1409 | 0.904135 | 0.9695 | 0.143 | 0.1909 | 0.453871 | 0.9375 | NaN | 0.0869 | 0.1243 | 0.48467 | 0.8625 | 0.0363 | 0.1346 | 0.78763 | 0.927 | 0.1149 | 0.1919 | 0.54928 | 0.9621 | NaN | 0.1007 | 0.1256 | 0.422545 | 0.795 | 0.018 | 0.1385 | 0.896355 | 0.9683 | 0.1501 | 0.1927 | 0.436257 | 0.8887 |
| FA 10:0 (DiC,OH) | 218.1156 | 9.113856 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.2039 | 0.1304 | 0.117752 | 0.4809 | 0.2523 | 0.1506 | 0.093859 | 0.381 | 0.1654 | 0.1974 | 0.402203 | 0.7709 | NaN | 0.106 | 0.1223 | 0.38616 | 0.8498 | 0.0653 | 0.139 | 0.638445 | 0.9073 | 0.1241 | 0.1857 | 0.503899 | 0.954 | NaN | 0.0654 | 0.1234 | 0.596142 | 0.9125 | 0.1115 | 0.1336 | 0.403795 | 0.8818 | 0.0264 | 0.1911 | 0.890273 | 0.9935 | NaN | 0.1337 | 0.1245 | 0.282771 | 0.7388 | 0.0906 | 0.1452 | 0.53258 | 0.7819 | 0.1524 | 0.1877 | 0.41704 | 0.9375 | NaN | 0.1177 | 0.1238 | 0.341436 | 0.7724 | 0.0693 | 0.1391 | 0.618157 | 0.8623 | 0.1331 | 0.189 | 0.481225 | 0.9403 | NaN | 0.1383 | 0.1247 | 0.267304 | 0.7315 | 0.0655 | 0.1439 | 0.648955 | 0.8632 | 0.1675 | 0.1894 | 0.376431 | 0.8875 |
| FA 11:0 (DiC,OH) | 232.131 | 10.740578 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1169 | 0.1303 | 0.369751 | 0.7161 | 0.1159 | 0.1692 | 0.493437 | 0.7545 | 0.1013 | 0.1871 | 0.588118 | 0.887 | NaN | 0.0555 | 0.1211 | 0.646885 | 0.9179 | -0.0295 | 0.1513 | 0.845403 | 0.9729 | 0.0758 | 0.1757 | 0.665995 | 0.954 | NaN | 0.0206 | 0.1217 | 0.865796 | 0.9714 | 0.0478 | 0.1465 | 0.744129 | 0.9241 | -0.0062 | 0.1794 | 0.972535 | 0.9976 | NaN | 0.0778 | 0.1236 | 0.528683 | 0.8293 | -0.042 | 0.1594 | 0.792149 | 0.9148 | 0.1119 | 0.1778 | 0.52912 | 0.9375 | NaN | 0.0667 | 0.1226 | 0.586485 | 0.8918 | -0.0334 | 0.1518 | 0.825677 | 0.9397 | 0.0905 | 0.1787 | 0.612677 | 0.9621 | NaN | 0.0804 | 0.1238 | 0.516275 | 0.8333 | -0.0845 | 0.1584 | 0.593733 | 0.8199 | 0.1281 | 0.1795 | 0.475595 | 0.8887 |
| FA 12:0 (DiC,OH) | 246.1469 | 12.772049 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0075 | 0.1336 | 0.955255 | 0.9893 | -0.0274 | 0.1563 | 0.860835 | 0.932 | -0.033 | 0.2062 | 0.872837 | 0.9753 | NaN | 0.0013 | 0.1236 | 0.991663 | 0.9999 | -0.0728 | 0.1372 | 0.595776 | 0.904 | 0.0072 | 0.1937 | 0.970531 | 0.9911 | NaN | -0.002 | 0.1234 | 0.98736 | 0.9928 | 0.0233 | 0.1349 | 0.863041 | 0.9569 | -0.0476 | 0.1947 | 0.806938 | 0.9935 | NaN | 0.0173 | 0.1264 | 0.890932 | 0.9771 | -0.1051 | 0.1436 | 0.464352 | 0.7319 | 0.0506 | 0.1975 | 0.797761 | 0.9662 | NaN | 0.0179 | 0.1253 | 0.886568 | 0.9672 | -0.0749 | 0.1375 | 0.586176 | 0.8623 | 0.0333 | 0.1979 | 0.866325 | 0.9621 | NaN | 0.0094 | 0.1266 | 0.94104 | 0.9794 | -0.1531 | 0.1423 | 0.282053 | 0.652 | 0.0596 | 0.2001 | 0.765621 | 0.9525 |
| FA 13:0 (DiC,OH) | 260.1627 | 14.14954 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0021 | 0.1321 | 0.987407 | 0.9936 | -0.0247 | 0.1524 | 0.871132 | 0.9391 | -0.0215 | 0.2073 | 0.917479 | 0.9838 | NaN | 0.0107 | 0.1222 | 0.930119 | 0.9861 | -0.0819 | 0.1339 | 0.540922 | 0.8967 | 0.0279 | 0.1948 | 0.886132 | 0.977 | NaN | 0.0173 | 0.122 | 0.887495 | 0.9714 | 0.0086 | 0.1314 | 0.947608 | 0.9765 | -0.0093 | 0.1957 | 0.962259 | 0.9976 | NaN | 0.0398 | 0.1251 | 0.750444 | 0.9165 | -0.0915 | 0.1399 | 0.512847 | 0.7647 | 0.081 | 0.1991 | 0.68428 | 0.9476 | NaN | 0.0333 | 0.1239 | 0.78789 | 0.9455 | -0.0733 | 0.1341 | 0.584838 | 0.8623 | 0.0578 | 0.1993 | 0.772007 | 0.9621 | NaN | 0.0295 | 0.1253 | 0.813606 | 0.9477 | -0.1325 | 0.1384 | 0.33862 | 0.6758 | 0.0827 | 0.2016 | 0.681734 | 0.9459 |
| FA 14:0 (DiC,OH) | 274.1783 | 15.688103 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0578 | 0.127 | 0.649099 | 0.8739 | 0.0013 | 0.1628 | 0.993765 | 0.9963 | 0.0757 | 0.1862 | 0.684574 | 0.94 | NaN | 0.1176 | 0.1177 | 0.317637 | 0.7898 | -0.0189 | 0.1429 | 0.894851 | 0.9729 | 0.1698 | 0.1757 | 0.333685 | 0.9223 | NaN | 0.1286 | 0.1176 | 0.27404 | 0.7838 | 0.0345 | 0.1403 | 0.805984 | 0.9363 | 0.1567 | 0.1767 | 0.37528 | 0.9726 | NaN | 0.1149 | 0.1204 | 0.339785 | 0.741 | -0.0342 | 0.1491 | 0.818773 | 0.9271 | 0.1737 | 0.1786 | 0.33063 | 0.9044 | NaN | 0.1105 | 0.1192 | 0.354121 | 0.7882 | -0.0324 | 0.1433 | 0.820908 | 0.9396 | 0.1598 | 0.1791 | 0.372113 | 0.9106 | NaN | 0.0973 | 0.1205 | 0.419213 | 0.7925 | -0.0609 | 0.1471 | 0.678802 | 0.8734 | 0.1513 | 0.1799 | 0.400233 | 0.8887 |
| FA 15:0 (Dic, OH) | 288.1942 | 17.041286 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0835 | 0.1313 | 0.525033 | 0.8187 | 0.0385 | 0.1436 | 0.788382 | 0.9319 | -0.239 | 0.215 | 0.2662 | 0.7397 | NaN | -0.0318 | 0.1218 | 0.794358 | 0.9571 | 0.0162 | 0.1261 | 0.898104 | 0.9729 | -0.1264 | 0.2047 | 0.536959 | 0.954 | NaN | -0.0203 | 0.1218 | 0.867861 | 0.9714 | 0.0463 | 0.1236 | 0.708277 | 0.9195 | -0.1139 | 0.207 | 0.58222 | 0.9894 | NaN | -0.0167 | 0.125 | 0.893942 | 0.9771 | 0.0256 | 0.1314 | 0.845569 | 0.941 | -0.1183 | 0.2086 | 0.570474 | 0.9375 | NaN | -0.0189 | 0.1238 | 0.878504 | 0.9672 | 0.0141 | 0.1264 | 0.911366 | 0.9768 | -0.109 | 0.2105 | 0.604575 | 0.9621 | NaN | -0.0302 | 0.125 | 0.809186 | 0.9477 | -0.011 | 0.1298 | 0.932673 | 0.9823 | -0.1195 | 0.2113 | 0.571663 | 0.9205 |
| FA 16:0 (DiC,OH) | 302.2097 | 18.320814 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0712 | 0.1295 | 0.582311 | 0.8423 | 0.1342 | 0.143 | 0.347836 | 0.6332 | -0.0101 | 0.2094 | 0.961725 | 0.9887 | NaN | 0.066 | 0.1198 | 0.58167 | 0.9079 | 0.0356 | 0.1274 | 0.779936 | 0.9615 | 0.0553 | 0.1971 | 0.779071 | 0.954 | NaN | 0.0492 | 0.1197 | 0.681013 | 0.9406 | 0.1013 | 0.1234 | 0.411744 | 0.8818 | -0.0206 | 0.1978 | 0.917223 | 0.9935 | NaN | 0.1073 | 0.1225 | 0.381187 | 0.7679 | 0.044 | 0.133 | 0.740659 | 0.8849 | 0.1252 | 0.2025 | 0.536547 | 0.9375 | NaN | 0.0842 | 0.1213 | 0.48783 | 0.8625 | 0.0485 | 0.1273 | 0.703123 | 0.8781 | 0.0703 | 0.2014 | 0.727103 | 0.9621 | NaN | 0.0969 | 0.1227 | 0.429698 | 0.795 | 0.0098 | 0.1322 | 0.940874 | 0.9823 | 0.1207 | 0.205 | 0.556028 | 0.9114 |
| FA 17:0 (DiC,OH) | 316.2246 | 19.429361 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1979 | 0.1313 | 0.131676 | 0.5013 | 0.2364 | 0.1528 | 0.121773 | 0.412 | 0.1606 | 0.1994 | 0.4206 | 0.7762 | NaN | 0.1327 | 0.1223 | 0.277714 | 0.7644 | 0.0791 | 0.139 | 0.569462 | 0.904 | 0.1515 | 0.1871 | 0.418099 | 0.9419 | NaN | 0.0779 | 0.1236 | 0.528241 | 0.9101 | 0.121 | 0.1343 | 0.367342 | 0.8778 | 0.0345 | 0.1922 | 0.857535 | 0.9935 | NaN | 0.1717 | 0.1243 | 0.167427 | 0.6495 | 0.0882 | 0.1459 | 0.545267 | 0.7845 | 0.2133 | 0.1896 | 0.260624 | 0.8705 | NaN | 0.1508 | 0.1236 | 0.222399 | 0.7052 | 0.0951 | 0.1385 | 0.492357 | 0.8363 | 0.1643 | 0.1903 | 0.388093 | 0.9155 | NaN | 0.1743 | 0.1246 | 0.161873 | 0.6278 | 0.0631 | 0.1446 | 0.662792 | 0.8681 | 0.2232 | 0.1918 | 0.244541 | 0.8424 |
| FA 18:0 (DiC,OH) | 330.2409 | 20.418041 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1916 | 0.1305 | 0.142049 | 0.5159 | 0.2638 | 0.1518 | 0.082277 | 0.3594 | 0.1408 | 0.197 | 0.475 | 0.8245 | NaN | 0.1358 | 0.1214 | 0.263269 | 0.7609 | 0.1192 | 0.1378 | 0.386877 | 0.8339 | 0.1405 | 0.1847 | 0.44693 | 0.9478 | NaN | 0.0659 | 0.123 | 0.592141 | 0.9125 | 0.1557 | 0.1333 | 0.242872 | 0.8037 | -0.0013 | 0.1908 | 0.994436 | 0.9976 | NaN | 0.1706 | 0.1235 | 0.167251 | 0.6495 | 0.1304 | 0.1443 | 0.365986 | 0.6762 | 0.1954 | 0.1875 | 0.297143 | 0.8823 | NaN | 0.1553 | 0.1227 | 0.205504 | 0.6855 | 0.1419 | 0.137 | 0.300215 | 0.7544 | 0.1509 | 0.188 | 0.422225 | 0.9359 | NaN | 0.1767 | 0.1237 | 0.153422 | 0.6269 | 0.1093 | 0.1429 | 0.444309 | 0.7458 | 0.2089 | 0.1897 | 0.270802 | 0.8424 |
| FA 10:1 (DiC, OH) | 216.1 | 4.325327 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.1763 | 0.1337 | 0.187223 | 0.5527 | 0.2109 | 0.1752 | 0.228629 | 0.5237 | 0.1437 | 0.1911 | 0.452043 | 0.8098 | NaN | 0.1104 | 0.1245 | 0.374972 | 0.8465 | 0.0174 | 0.1593 | 0.913124 | 0.9729 | 0.1378 | 0.1792 | 0.442086 | 0.9478 | NaN | 0.0652 | 0.1254 | 0.602902 | 0.9125 | 0.0917 | 0.1532 | 0.549536 | 0.9053 | 0.0433 | 0.1831 | 0.812875 | 0.9935 | NaN | 0.1528 | 0.1266 | 0.227464 | 0.7062 | 0.0372 | 0.1667 | 0.823229 | 0.9271 | 0.1927 | 0.1818 | 0.289043 | 0.8767 | NaN | 0.128 | 0.1258 | 0.308968 | 0.758 | 0.0632 | 0.1577 | 0.688357 | 0.8735 | 0.1376 | 0.1825 | 0.450933 | 0.9359 | NaN | 0.157 | 0.1268 | 0.215592 | 0.676 | -0.0037 | 0.1659 | 0.981973 | 0.9946 | 0.2084 | 0.1839 | 0.25713 | 0.8424 |
| FA 11:1 (DiC, OH) | 230.1147 | 5.828099 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.152 | 0.1354 | 0.261543 | 0.6341 | 0.221 | 0.1655 | 0.181639 | 0.4964 | 0.1171 | 0.1985 | 0.555184 | 0.8707 | NaN | 0.115 | 0.1255 | 0.359674 | 0.8459 | 0.0783 | 0.1489 | 0.598822 | 0.9043 | 0.1385 | 0.1861 | 0.45673 | 0.9478 | NaN | 0.0715 | 0.1261 | 0.57037 | 0.9125 | 0.1473 | 0.1436 | 0.305043 | 0.8336 | 0.0262 | 0.1894 | 0.889849 | 0.9935 | NaN | 0.1239 | 0.1282 | 0.33413 | 0.741 | 0.0489 | 0.1583 | 0.757631 | 0.8955 | 0.1751 | 0.189 | 0.354103 | 0.9134 | NaN | 0.1306 | 0.127 | 0.303996 | 0.7529 | 0.0967 | 0.1485 | 0.515147 | 0.8496 | 0.1443 | 0.1895 | 0.446386 | 0.9359 | NaN | 0.1316 | 0.1284 | 0.305564 | 0.7481 | 0.0252 | 0.1566 | 0.87198 | 0.961 | 0.1873 | 0.1913 | 0.327339 | 0.8727 |
| FA 11:1 (DiC,OH) | 244.1289 | 6.840248 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | 0.0992 | 0.1296 | 0.444032 | 0.7722 | -0.0837 | 0.149 | 0.57409 | 0.8007 | 0.1926 | 0.1969 | 0.328061 | 0.7534 | NaN | 0.0483 | 0.1203 | 0.687995 | 0.9297 | -0.1274 | 0.1305 | 0.329111 | 0.8095 | 0.1364 | 0.1856 | 0.462564 | 0.9478 | NaN | 0.0199 | 0.1206 | 0.868712 | 0.9714 | -0.044 | 0.1286 | 0.732207 | 0.9241 | 0.0467 | 0.1914 | 0.80714 | 0.9935 | NaN | 0.0402 | 0.1233 | 0.744272 | 0.913 | -0.2184 | 0.1378 | 0.113038 | 0.4439 | 0.1758 | 0.1873 | 0.348051 | 0.9127 | NaN | 0.0507 | 0.1219 | 0.677311 | 0.9097 | -0.1379 | 0.1308 | 0.291911 | 0.7544 | 0.1493 | 0.1888 | 0.429113 | 0.9359 | NaN | 0.047 | 0.1234 | 0.703309 | 0.9035 | -0.2528 | 0.1361 | 0.06327 | 0.3458 | 0.2021 | 0.1888 | 0.284453 | 0.8424 |
| FA 14:1 (DiC, OH) | 272.1624 | 12.077606 | Lipid | Fatty Acid, Dicarboxylate, hydroxy | -0.0291 | 0.1319 | 0.825657 | 0.9718 | -0.0049 | 0.1587 | 0.975473 | 0.9898 | -0.0729 | 0.1987 | 0.713699 | 0.9594 | NaN | 0.0095 | 0.1222 | 0.937938 | 0.9881 | 0.0061 | 0.1393 | 0.96494 | 0.9882 | -0.0211 | 0.187 | 0.910292 | 0.9793 | NaN | 0.009 | 0.122 | 0.941432 | 0.9728 | 0.0674 | 0.1371 | 0.62281 | 0.9053 | -0.046 | 0.1878 | 0.806428 | 0.9935 | NaN | 0.0331 | 0.1253 | 0.791434 | 0.936 | -0.0133 | 0.1451 | 0.927078 | 0.9755 | 0.0267 | 0.1913 | 0.888947 | 0.99 | NaN | 0.0183 | 0.1239 | 0.882323 | 0.9672 | 0.017 | 0.1396 | 0.903048 | 0.9744 | -0.0142 | 0.1907 | 0.940625 | 0.9834 | NaN | 0.0174 | 0.1254 | 0.889568 | 0.9591 | -0.0574 | 0.1432 | 0.68849 | 0.8757 | 0.022 | 0.1933 | 0.909604 | 0.9783 |
| 3-methyladipic acid | 160.0736 | 5.688393 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.2902 | 0.1368 | 0.033896 | 0.2621 | 0.3852 | 0.148 | 0.009251 | 0.1685 | 0.2346 | 0.2143 | 0.273623 | 0.744 | NaN | 0.1806 | 0.1288 | 0.1608 | 0.7211 | 0.2259 | 0.1365 | 0.097939 | 0.5941 | 0.1751 | 0.202 | 0.385924 | 0.9389 | NaN | 0.0874 | 0.1327 | 0.510079 | 0.9053 | 0.1922 | 0.1356 | 0.156498 | 0.7183 | 0.0243 | 0.2124 | 0.909099 | 0.9935 | NaN | 0.2425 | 0.13 | 0.062221 | 0.4641 | 0.3119 | 0.1376 | 0.023421 | 0.1989 | 0.2184 | 0.2038 | 0.283812 | 0.8705 | NaN | 0.1949 | 0.1302 | 0.134511 | 0.6708 | 0.2409 | 0.1358 | 0.07593 | 0.4631 | 0.1794 | 0.2057 | 0.383351 | 0.9106 | NaN | 0.2452 | 0.1303 | 0.059777 | 0.4541 | 0.2886 | 0.1366 | 0.034623 | 0.2595 | 0.2367 | 0.2055 | 0.249316 | 0.8424 |
| LL-2,6-diaminoheptanedioate | 190.0948 | 0.684274 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.1142 | 0.1435 | 0.426044 | 0.7581 | 0.2863 | 0.1476 | 0.05237 | 0.3003 | -0.0433 | 0.2334 | 0.852851 | 0.9732 | NaN | 0.0861 | 0.1328 | 0.516824 | 0.8832 | 0.2362 | 0.1302 | 0.069583 | 0.4801 | -0.0395 | 0.2189 | 0.856703 | 0.9765 | NaN | 0.1103 | 0.1324 | 0.405065 | 0.8502 | 0.2746 | 0.1265 | 0.030008 | 0.3503 | -0.0243 | 0.2204 | 0.912254 | 0.9935 | NaN | 0.1304 | 0.1356 | 0.336006 | 0.741 | 0.2748 | 0.1347 | 0.041421 | 0.269 | 0.0078 | 0.2224 | 0.972066 | 0.99 | NaN | 0.0813 | 0.1347 | 0.54615 | 0.867 | 0.1884 | 0.1323 | 0.154436 | 0.631 | -0.0112 | 0.2231 | 0.960027 | 0.9872 | NaN | 0.1068 | 0.1359 | 0.432203 | 0.795 | 0.2508 | 0.1333 | 0.059914 | 0.3307 | -0.0198 | 0.2241 | 0.929561 | 0.9869 |
| 2-methylmaleate | 130.0277 | 1.828859 | Lipid | Fatty Acid, Dicarboxylate-other\* | 0.0646 | 0.1344 | 0.630742 | 0.8678 | 0.0145 | 0.1369 | 0.915458 | 0.9625 | 0.1129 | 0.2235 | 0.613517 | 0.8995 | NaN | 0.0223 | 0.1246 | 0.858104 | 0.9705 | -0.0284 | 0.1204 | 0.813751 | 0.965 | 0.0643 | 0.2102 | 0.759651 | 0.954 | NaN | 0.0047 | 0.1246 | 0.969791 | 0.9794 | -0.0267 | 0.1181 | 0.821261 | 0.9425 | 0.0253 | 0.2127 | 0.905322 | 0.9935 | NaN | 0.0729 | 0.127 | 0.566244 | 0.846 | 0.0038 | 0.1252 | 0.975797 | 0.9926 | 0.136 | 0.2125 | 0.521985 | 0.9375 | NaN | 0.0426 | 0.126 | 0.735449 | 0.9269 | -0.0069 | 0.1205 | 0.954106 | 0.9923 | 0.0845 | 0.2137 | 0.692715 | 0.9621 | NaN | 0.0787 | 0.1273 | 0.536612 | 0.8487 | 0.0005 | 0.1234 | 0.996661 | 0.9978 | 0.1488 | 0.2146 | 0.487961 | 0.8887 |
| Keto 18:0 | 298.2504 | 21.835537 | Lipid | Fatty Acid, Keto | -0.2499 | 0.1331 | 0.060521 | 0.3473 | -0.0888 | 0.1441 | 0.537879 | 0.7813 | -0.3639 | 0.2104 | 0.083664 | 0.4769 | NaN | -0.3086 | 0.1227 | 0.011884 | 0.1726 | -0.1475 | 0.1263 | 0.24299 | 0.7677 | -0.4215 | 0.1964 | 0.031872 | 0.5144 | NaN | -0.3106 | 0.1225 | 0.011214 | 0.144 | -0.0334 | 0.1247 | 0.788687 | 0.9362 | -0.545 | 0.1994 | 0.006269 | 0.1494 | NaN | -0.3618 | 0.1262 | 0.004141 | 0.0737 | -0.2404 | 0.1338 | 0.07244 | 0.3762 | -0.4352 | 0.1993 | 0.029043 | 0.4788 | NaN | -0.3158 | 0.1244 | 0.011168 | 0.1927 | -0.1647 | 0.1266 | 0.193379 | 0.6684 | -0.4213 | 0.2003 | 0.035397 | 0.4772 | NaN | -0.3432 | 0.1262 | 0.006557 | 0.1065 | -0.249 | 0.1315 | 0.058211 | 0.3246 | -0.403 | 0.2013 | 0.045307 | 0.4743 |
| 5-oxo-7-octenoic acid | 156.0766 | 3.918678 | Lipid | Fatty Acid, Keto | -0.1349 | 0.1347 | 0.316495 | 0.6805 | -0.0382 | 0.1422 | 0.788114 | 0.9319 | -0.2537 | 0.2188 | 0.246193 | 0.7391 | NaN | -0.1034 | 0.1248 | 0.407323 | 0.8498 | -0.0531 | 0.1248 | 0.670529 | 0.923 | -0.1666 | 0.2072 | 0.421239 | 0.9419 | NaN | -0.1134 | 0.1245 | 0.362086 | 0.8259 | -0.008 | 0.1227 | 0.94827 | 0.9765 | -0.2118 | 0.2072 | 0.306771 | 0.9479 | NaN | -0.0806 | 0.128 | 0.528857 | 0.8293 | -0.0274 | 0.1301 | 0.833217 | 0.931 | -0.1534 | 0.211 | 0.46709 | 0.9375 | NaN | -0.1119 | 0.1263 | 0.37559 | 0.7993 | -0.0544 | 0.125 | 0.663314 | 0.8623 | -0.1896 | 0.2104 | 0.367636 | 0.9106 | NaN | -0.0845 | 0.1282 | 0.510042 | 0.8285 | -0.0374 | 0.1281 | 0.770569 | 0.9167 | -0.1568 | 0.2133 | 0.46249 | 0.8887 |
| traumatin | 212.1393 | 14.682874 | Lipid | Fatty Acid, Keto | 0.0906 | 0.1413 | 0.521151 | 0.8173 | 0.1905 | 0.1505 | 0.205665 | 0.5046 | 0.017 | 0.2247 | 0.939729 | 0.9887 | NaN | 0.0965 | 0.1306 | 0.459908 | 0.8498 | 0.109 | 0.1337 | 0.414966 | 0.847 | 0.1055 | 0.2117 | 0.618336 | 0.954 | NaN | 0.0548 | 0.1307 | 0.674908 | 0.9406 | 0.1072 | 0.1311 | 0.413735 | 0.8818 | 0.0178 | 0.2121 | 0.93317 | 0.9935 | NaN | 0.1226 | 0.1336 | 0.358753 | 0.7539 | 0.1407 | 0.1386 | 0.310022 | 0.6362 | 0.1333 | 0.2158 | 0.536852 | 0.9375 | NaN | 0.1308 | 0.1324 | 0.323193 | 0.7669 | 0.1653 | 0.1325 | 0.212092 | 0.6963 | 0.1073 | 0.216 | 0.619489 | 0.9621 | NaN | 0.13 | 0.1339 | 0.331758 | 0.7485 | 0.1378 | 0.1365 | 0.312843 | 0.6715 | 0.1367 | 0.2186 | 0.531628 | 0.8971 |
| 7-oxo-11E-tetradecenoic acid | 240.1727 | 19.634645 | Lipid | Fatty Acid, Keto | -0.3263 | 0.1361 | 0.016543 | 0.166 | -0.1547 | 0.1441 | 0.283079 | 0.5724 | -0.4505 | 0.2198 | 0.040421 | 0.3491 | NaN | -0.2814 | 0.1264 | 0.025961 | 0.3185 | -0.1569 | 0.1262 | 0.213947 | 0.7304 | -0.3629 | 0.2086 | 0.08199 | 0.7543 | NaN | -0.3399 | 0.1252 | 0.006652 | 0.0992 | -0.1126 | 0.1246 | 0.36604 | 0.8778 | -0.533 | 0.2064 | 0.009798 | 0.2003 | NaN | -0.3211 | 0.1286 | 0.012515 | 0.1645 | -0.2352 | 0.1316 | 0.073937 | 0.3762 | -0.3593 | 0.2122 | 0.090313 | 0.7393 | NaN | -0.2935 | 0.1279 | 0.021701 | 0.2786 | -0.1685 | 0.1264 | 0.182293 | 0.6534 | -0.3842 | 0.2118 | 0.069719 | 0.6053 | NaN | -0.3183 | 0.1289 | 0.013536 | 0.1779 | -0.2574 | 0.1296 | 0.047032 | 0.2877 | -0.355 | 0.2151 | 0.09885 | 0.6914 |
| 7-oxo-11-hexadecenoic acid | 268.2032 | 21.295565 | Lipid | Fatty Acid, Keto | -0.3234 | 0.1326 | 0.01474 | 0.1566 | -0.1982 | 0.1425 | 0.164334 | 0.479 | -0.4072 | 0.2113 | 0.053949 | 0.4024 | NaN | -0.3123 | 0.1225 | 0.010782 | 0.1674 | -0.1911 | 0.1248 | 0.125768 | 0.6118 | -0.3912 | 0.198 | 0.048222 | 0.5871 | NaN | -0.3558 | 0.1218 | 0.003489 | 0.0642 | -0.133 | 0.1238 | 0.282678 | 0.8127 | -0.5423 | 0.199 | 0.006415 | 0.1494 | NaN | -0.3756 | 0.1248 | 0.002621 | 0.0554 | -0.2976 | 0.1299 | 0.021938 | 0.192 | -0.4105 | 0.2004 | 0.04055 | 0.5138 | NaN | -0.324 | 0.124 | 0.008967 | 0.165 | -0.2049 | 0.1248 | 0.100664 | 0.5242 | -0.4031 | 0.2015 | 0.045429 | 0.5011 | NaN | -0.3639 | 0.1251 | 0.003634 | 0.0692 | -0.3097 | 0.1277 | 0.015258 | 0.1579 | -0.3901 | 0.2028 | 0.054429 | 0.5263 |
| 7-oxo-11-octadecenoic acid | 296.2354 | 22.077984 | Lipid | Fatty Acid, Keto | -0.1103 | 0.1333 | 0.408208 | 0.734 | -0.1936 | 0.1456 | 0.183441 | 0.4964 | -0.037 | 0.2094 | 0.859909 | 0.9732 | NaN | -0.1193 | 0.1232 | 0.333112 | 0.81 | -0.1878 | 0.1275 | 0.140866 | 0.6221 | -0.0695 | 0.1965 | 0.723385 | 0.954 | NaN | -0.1304 | 0.123 | 0.289015 | 0.7865 | -0.1224 | 0.1265 | 0.333348 | 0.8587 | -0.1505 | 0.1996 | 0.450973 | 0.9816 | NaN | -0.1704 | 0.1263 | 0.17726 | 0.6547 | -0.2679 | 0.1326 | 0.043281 | 0.2719 | -0.0951 | 0.1996 | 0.633817 | 0.9375 | NaN | -0.1236 | 0.1249 | 0.322464 | 0.7669 | -0.1949 | 0.1276 | 0.126764 | 0.5933 | -0.0679 | 0.2001 | 0.734201 | 0.9621 | NaN | -0.1489 | 0.1264 | 0.238755 | 0.7024 | -0.2609 | 0.1303 | 0.04537 | 0.2846 | -0.0635 | 0.2011 | 0.752193 | 0.9523 |
| C8 H12 N6 O2 | 224.1031 | 13.587468 | Lipid | Fatty Acid, Keto | -0.0284 | 0.135 | 0.833372 | 0.9746 | -0.0016 | 0.161 | 0.992227 | 0.9963 | -0.0593 | 0.2011 | 0.768141 | 0.9647 | NaN | -0.061 | 0.1249 | 0.625513 | 0.9079 | -0.0488 | 0.1415 | 0.730071 | 0.9386 | -0.0824 | 0.1886 | 0.662366 | 0.954 | NaN | -0.0687 | 0.1248 | 0.581858 | 0.9125 | 0.0271 | 0.1388 | 0.845392 | 0.95 | -0.1327 | 0.1906 | 0.486418 | 0.9848 | NaN | -0.0693 | 0.1279 | 0.587919 | 0.8473 | -0.1317 | 0.1496 | 0.378613 | 0.6808 | -0.0484 | 0.1912 | 0.800059 | 0.9662 | NaN | -0.0555 | 0.1266 | 0.661145 | 0.9055 | -0.0645 | 0.142 | 0.649368 | 0.8623 | -0.0654 | 0.192 | 0.733471 | 0.9621 | NaN | -0.0637 | 0.1281 | 0.619259 | 0.8808 | -0.1481 | 0.1474 | 0.315164 | 0.6717 | -0.0367 | 0.1932 | 0.849184 | 0.9641 |
| 7-oxo-13-tetradecadienoic acid | 238.1186 | 15.035772 | Lipid | Fatty Acid, Keto | -0.2278 | 0.1291 | 0.077718 | 0.3936 | -0.2469 | 0.1255 | 0.049131 | 0.2996 | -0.1943 | 0.2247 | 0.387176 | 0.7552 | NaN | -0.1219 | 0.1215 | 0.31552 | 0.7898 | -0.1661 | 0.1122 | 0.13871 | 0.6175 | -0.0725 | 0.2138 | 0.734687 | 0.954 | NaN | -0.1151 | 0.1215 | 0.343297 | 0.8224 | -0.2247 | 0.1079 | 0.037303 | 0.3993 | 0.0061 | 0.2204 | 0.978089 | 0.9976 | NaN | -0.1443 | 0.1239 | 0.244149 | 0.7131 | -0.1845 | 0.1165 | 0.11338 | 0.4439 | -0.0914 | 0.2164 | 0.672615 | 0.9472 | NaN | -0.1549 | 0.1223 | 0.20526 | 0.6855 | -0.2027 | 0.111 | 0.067679 | 0.4198 | -0.1008 | 0.2171 | 0.642554 | 0.9621 | NaN | -0.167 | 0.1234 | 0.175948 | 0.6413 | -0.1774 | 0.1149 | 0.122691 | 0.4838 | -0.1531 | 0.2163 | 0.479091 | 0.8887 |
| FA 5:0 (OH) | 118.0634 | 3.490162 | Lipid | Fatty acid,hydroxy | 0.0977 | 0.1372 | 0.476312 | 0.7972 | 0.2048 | 0.1251 | 0.10161 | 0.3816 | -0.0717 | 0.2638 | 0.785762 | 0.9647 | NaN | 0.0485 | 0.1272 | 0.702814 | 0.9314 | 0.1162 | 0.112 | 0.29935 | 0.8095 | -0.0744 | 0.2474 | 0.763557 | 0.954 | NaN | 0.0329 | 0.1272 | 0.795837 | 0.9641 | 0.0726 | 0.1116 | 0.515143 | 0.9053 | -0.0526 | 0.2492 | 0.832689 | 0.9935 | NaN | 0.0558 | 0.13 | 0.667911 | 0.8697 | 0.1432 | 0.116 | 0.216952 | 0.5546 | -0.1136 | 0.2509 | 0.650829 | 0.9375 | NaN | 0.0587 | 0.1288 | 0.648412 | 0.9016 | 0.1148 | 0.1123 | 0.306534 | 0.7544 | -0.0552 | 0.252 | 0.826539 | 0.9621 | NaN | 0.0602 | 0.1303 | 0.643802 | 0.8907 | 0.1425 | 0.1141 | 0.211951 | 0.5763 | -0.1037 | 0.2532 | 0.682281 | 0.9459 |
| FA 9:0 (OH) | 174.1256 | 11.971786 | Lipid | Fatty acid,hydroxy | 0.078 | 0.1365 | 0.567919 | 0.8382 | 0.1799 | 0.1459 | 0.217629 | 0.5107 | -0.0106 | 0.217 | 0.96092 | 0.9887 | NaN | 0.0719 | 0.1262 | 0.568894 | 0.9079 | 0.137 | 0.1285 | 0.286565 | 0.7996 | 0.0161 | 0.2037 | 0.937177 | 0.9911 | NaN | 0.0105 | 0.1267 | 0.934143 | 0.9728 | 0.1214 | 0.1265 | 0.336908 | 0.8587 | -0.0827 | 0.2057 | 0.687801 | 0.9894 | NaN | 0.0729 | 0.1291 | 0.572251 | 0.8469 | 0.1465 | 0.1339 | 0.273677 | 0.6067 | 0.0059 | 0.2064 | 0.97737 | 0.9923 | NaN | 0.085 | 0.1279 | 0.506202 | 0.8625 | 0.1396 | 0.1287 | 0.278241 | 0.7544 | 0.0323 | 0.2076 | 0.876217 | 0.9621 | NaN | 0.0776 | 0.1293 | 0.548516 | 0.8553 | 0.1159 | 0.1326 | 0.382189 | 0.6983 | 0.038 | 0.2088 | 0.855741 | 0.9641 |
| FA 10:0 (OH) | 188.1411 | 16.303364 | Lipid | Fatty acid,hydroxy | -0.3054 | 0.136 | 0.024755 | 0.2102 | -0.12 | 0.1437 | 0.403891 | 0.6737 | -0.4481 | 0.2192 | 0.040912 | 0.3491 | NaN | -0.2644 | 0.1262 | 0.036127 | 0.3763 | -0.1468 | 0.1258 | 0.243364 | 0.7677 | -0.3473 | 0.2087 | 0.096182 | 0.7567 | NaN | -0.3192 | 0.1252 | 0.010779 | 0.1417 | -0.1086 | 0.1238 | 0.380109 | 0.8818 | -0.4978 | 0.2059 | 0.015596 | 0.2532 | NaN | -0.3026 | 0.1284 | 0.018457 | 0.2168 | -0.2145 | 0.1318 | 0.103453 | 0.4326 | -0.3534 | 0.2118 | 0.095169 | 0.7399 | NaN | -0.2742 | 0.1277 | 0.031824 | 0.332 | -0.154 | 0.126 | 0.221693 | 0.7033 | -0.3706 | 0.2119 | 0.080318 | 0.6055 | NaN | -0.3054 | 0.1287 | 0.017636 | 0.2163 | -0.2387 | 0.1298 | 0.065974 | 0.3536 | -0.3575 | 0.2141 | 0.094954 | 0.6807 |
| FA 12:0 (OH) | 216.1724 | 19.386652 | Lipid | Fatty acid,hydroxy | -0.3436 | 0.1325 | 0.009512 | 0.1221 | -0.1763 | 0.141 | 0.211032 | 0.5065 | -0.4701 | 0.2124 | 0.026909 | 0.3016 | NaN | -0.2991 | 0.123 | 0.01502 | 0.2126 | -0.1871 | 0.1233 | 0.128927 | 0.6118 | -0.3804 | 0.2019 | 0.059573 | 0.6324 | NaN | -0.3617 | 0.1218 | 0.002972 | 0.0615 | -0.1513 | 0.1215 | 0.213016 | 0.7942 | -0.5427 | 0.1992 | 0.006445 | 0.1494 | NaN | -0.3447 | 0.125 | 0.005817 | 0.0973 | -0.2597 | 0.1285 | 0.043349 | 0.2719 | -0.3983 | 0.2041 | 0.051 | 0.5592 | NaN | -0.3096 | 0.1245 | 0.012867 | 0.2029 | -0.1989 | 0.1234 | 0.1069 | 0.5464 | -0.3989 | 0.2052 | 0.051852 | 0.5267 | NaN | -0.3413 | 0.1253 | 0.006467 | 0.1065 | -0.2753 | 0.1264 | 0.02949 | 0.2359 | -0.3947 | 0.2067 | 0.056203 | 0.5263 |
| FA 14:0 (OH) | 244.2039 | 20.779514 | Lipid | Fatty acid,hydroxy | -0.0357 | 0.1298 | 0.783198 | 0.9514 | 0.1537 | 0.14 | 0.272317 | 0.5651 | -0.183 | 0.2057 | 0.373595 | 0.7534 | NaN | -0.0412 | 0.12 | 0.731076 | 0.9367 | 0.098 | 0.1237 | 0.428088 | 0.847 | -0.1556 | 0.1932 | 0.420513 | 0.9419 | NaN | -0.0981 | 0.1201 | 0.414106 | 0.8561 | 0.1048 | 0.1212 | 0.387382 | 0.8818 | -0.2719 | 0.1946 | 0.162426 | 0.7677 | NaN | -0.0536 | 0.1227 | 0.662357 | 0.8697 | 0.1041 | 0.129 | 0.419655 | 0.7106 | -0.1873 | 0.1954 | 0.33783 | 0.9044 | NaN | -0.0461 | 0.1216 | 0.704864 | 0.9116 | 0.1012 | 0.1239 | 0.414117 | 0.8188 | -0.1712 | 0.1965 | 0.383601 | 0.9106 | NaN | -0.0443 | 0.123 | 0.718412 | 0.9116 | 0.0868 | 0.1274 | 0.495798 | 0.7792 | -0.1585 | 0.1977 | 0.422746 | 0.8887 |
| FA 16:0 (OH) | 272.2351 | 22.279013 | Lipid | Fatty acid,hydroxy | 0.0036 | 0.1322 | 0.978214 | 0.9936 | -0.344 | 0.1354 | 0.01105 | 0.1697 | 0.2948 | 0.2123 | 0.165012 | 0.6553 | NaN | 0.0468 | 0.1224 | 0.702478 | 0.9314 | -0.1945 | 0.125 | 0.119871 | 0.6118 | 0.208 | 0.2013 | 0.301472 | 0.9223 | NaN | 0.0652 | 0.1224 | 0.594113 | 0.9125 | -0.1543 | 0.1249 | 0.216704 | 0.7942 | 0.2158 | 0.2025 | 0.286484 | 0.9294 | NaN | -0.0058 | 0.125 | 0.963066 | 0.9828 | -0.2688 | 0.1264 | 0.033373 | 0.2362 | 0.1807 | 0.206 | 0.380453 | 0.926 | NaN | 0.031 | 0.124 | 0.802695 | 0.952 | -0.2267 | 0.1232 | 0.065772 | 0.4198 | 0.2315 | 0.2043 | 0.2573 | 0.9039 | NaN | 0.0188 | 0.1253 | 0.881017 | 0.9588 | -0.2471 | 0.1255 | 0.048844 | 0.289 | 0.2217 | 0.206 | 0.281734 | 0.8424 |
| FA 18:0 (OH) | 300.2659 | 22.115673 | Lipid | Fatty acid,hydroxy | -0.0808 | 0.1338 | 0.54581 | 0.8252 | -0.0169 | 0.1507 | 0.910688 | 0.9594 | -0.1103 | 0.2069 | 0.594082 | 0.8909 | NaN | -0.0899 | 0.1237 | 0.467353 | 0.8498 | -0.0603 | 0.1324 | 0.648582 | 0.9079 | -0.1056 | 0.1941 | 0.58624 | 0.954 | NaN | -0.149 | 0.1237 | 0.228472 | 0.7361 | -0.0082 | 0.1298 | 0.949926 | 0.9765 | -0.265 | 0.1982 | 0.181092 | 0.8127 | NaN | -0.1256 | 0.1266 | 0.321168 | 0.741 | -0.1211 | 0.1393 | 0.384785 | 0.6816 | -0.1199 | 0.1966 | 0.542001 | 0.9375 | NaN | -0.0775 | 0.1253 | 0.536206 | 0.8632 | -0.0376 | 0.1325 | 0.776419 | 0.9247 | -0.1023 | 0.1976 | 0.604811 | 0.9621 | NaN | -0.1098 | 0.1268 | 0.386316 | 0.7698 | -0.1193 | 0.1369 | 0.383279 | 0.6983 | -0.1005 | 0.1986 | 0.612965 | 0.9445 |
| FA 24:0 (OH) | 384.3594 | 22.877468 | Lipid | Fatty acid,hydroxy | -0.0665 | 0.1448 | 0.646002 | 0.8739 | -0.1639 | 0.1448 | 0.257584 | 0.5494 | 0.0447 | 0.2438 | 0.854602 | 0.9732 | NaN | -0.0416 | 0.134 | 0.756454 | 0.9509 | -0.0166 | 0.131 | 0.899265 | 0.9729 | -0.0854 | 0.231 | 0.71152 | 0.954 | NaN | -0.0228 | 0.1339 | 0.864953 | 0.9714 | -0.0593 | 0.1268 | 0.639657 | 0.9053 | 0.0087 | 0.2304 | 0.970013 | 0.9976 | NaN | -0.0699 | 0.1368 | 0.609742 | 0.8573 | -0.0555 | 0.1357 | 0.682487 | 0.853 | -0.1064 | 0.2357 | 0.651699 | 0.9375 | NaN | -0.0479 | 0.1357 | 0.724274 | 0.9233 | -0.0371 | 0.1305 | 0.776225 | 0.9247 | -0.0509 | 0.2346 | 0.828302 | 0.9621 | NaN | -0.0713 | 0.1371 | 0.602942 | 0.8765 | -0.06 | 0.1331 | 0.65202 | 0.8652 | -0.0815 | 0.2374 | 0.731252 | 0.9459 |
| FA 25:0 (OH) | 398.3769 | 23.011435 | Lipid | Fatty acid,hydroxy | 0.0259 | 0.1438 | 0.856947 | 0.9787 | -0.1794 | 0.1387 | 0.195951 | 0.4993 | 0.2908 | 0.2536 | 0.251606 | 0.7397 | NaN | 0.0833 | 0.1332 | 0.531767 | 0.8926 | -0.0541 | 0.1251 | 0.665138 | 0.9202 | 0.2212 | 0.2391 | 0.354898 | 0.9223 | NaN | 0.1129 | 0.1334 | 0.397144 | 0.8469 | 0.0415 | 0.1268 | 0.743639 | 0.9241 | 0.1758 | 0.2426 | 0.468645 | 0.9816 | NaN | 0.0153 | 0.136 | 0.910686 | 0.9828 | -0.1398 | 0.1275 | 0.272944 | 0.6067 | 0.1844 | 0.2441 | 0.450051 | 0.9375 | NaN | 0.067 | 0.1349 | 0.619315 | 0.8971 | -0.0773 | 0.1244 | 0.534576 | 0.8528 | 0.2372 | 0.2432 | 0.329302 | 0.9106 | NaN | 0.0324 | 0.1363 | 0.811838 | 0.9477 | -0.1217 | 0.1261 | 0.334293 | 0.6758 | 0.2127 | 0.2455 | 0.386218 | 0.8887 |
| FA 26:0 (OH) | 412.3936 | 23.14789 | Lipid | Fatty acid,hydroxy | 0.0016 | 0.1368 | 0.990789 | 0.9936 | -0.2546 | 0.1554 | 0.10138 | 0.3816 | 0.1871 | 0.2121 | 0.377913 | 0.7534 | NaN | 0.0505 | 0.1267 | 0.690525 | 0.9297 | -0.0872 | 0.1419 | 0.538796 | 0.8967 | 0.1171 | 0.2002 | 0.558801 | 0.954 | NaN | 0.0706 | 0.1267 | 0.577538 | 0.9125 | -0.0149 | 0.1426 | 0.916928 | 0.973 | 0.1024 | 0.2022 | 0.612615 | 0.9894 | NaN | -0.0092 | 0.1293 | 0.943127 | 0.9828 | -0.1919 | 0.1436 | 0.181419 | 0.5327 | 0.0915 | 0.2043 | 0.654262 | 0.9375 | NaN | 0.0415 | 0.1284 | 0.746568 | 0.9324 | -0.1014 | 0.1415 | 0.473446 | 0.8272 | 0.1316 | 0.2036 | 0.518224 | 0.9524 | NaN | 0.0103 | 0.1296 | 0.936468 | 0.9794 | -0.1673 | 0.1422 | 0.23944 | 0.613 | 0.1197 | 0.2052 | 0.559629 | 0.914 |
| FA 27:0 (OH) | 426.4057 | 23.29134 | Lipid | Fatty acid,hydroxy | 0.1399 | 0.1353 | 0.301025 | 0.6742 | -0.1726 | 0.1408 | 0.220178 | 0.5107 | 0.4306 | 0.2227 | 0.053127 | 0.4017 | NaN | 0.1919 | 0.125 | 0.124708 | 0.6749 | -0.0103 | 0.1284 | 0.935988 | 0.973 | 0.3389 | 0.2114 | 0.109001 | 0.7818 | NaN | 0.2027 | 0.1249 | 0.104548 | 0.5628 | 0.0382 | 0.1278 | 0.764843 | 0.9284 | 0.3292 | 0.2136 | 0.12336 | 0.6991 | NaN | 0.1424 | 0.1278 | 0.265342 | 0.7279 | -0.0909 | 0.1309 | 0.487675 | 0.7494 | 0.3179 | 0.2162 | 0.141474 | 0.8157 | NaN | 0.1764 | 0.1267 | 0.163828 | 0.6753 | -0.0361 | 0.1275 | 0.777267 | 0.9247 | 0.3587 | 0.2148 | 0.09497 | 0.6636 | NaN | 0.1687 | 0.1281 | 0.187721 | 0.6463 | -0.0596 | 0.1301 | 0.646724 | 0.8623 | 0.3562 | 0.2162 | 0.099502 | 0.6914 |
| PA 17:3 | 418.2211 | 16.179428 | Lipid | Phosphatidic Acid | 0.0672 | 0.1307 | 0.607073 | 0.8575 | 0.206 | 0.1248 | 0.098666 | 0.3816 | -0.1423 | 0.2399 | 0.552909 | 0.8707 | NaN | 0.0922 | 0.1209 | 0.445632 | 0.8498 | 0.1489 | 0.1106 | 0.178022 | 0.692 | -0.0122 | 0.2279 | 0.957192 | 0.9911 | NaN | 0.0856 | 0.1207 | 0.477999 | 0.8967 | 0.173 | 0.1077 | 0.108192 | 0.6422 | -0.0574 | 0.228 | 0.801325 | 0.9935 | NaN | 0.1043 | 0.1237 | 0.399048 | 0.7795 | 0.1666 | 0.1149 | 0.14702 | 0.4863 | -0.0203 | 0.2313 | 0.930068 | 0.99 | NaN | 0.0954 | 0.1225 | 0.435853 | 0.8472 | 0.1551 | 0.1106 | 0.160773 | 0.631 | -0.0266 | 0.2323 | 0.908841 | 0.9693 | NaN | 0.0907 | 0.1239 | 0.464068 | 0.8132 | 0.1312 | 0.1144 | 0.251262 | 0.627 | -0.0123 | 0.2346 | 0.95827 | 0.9892 |
| PA 18:3 | 432.237 | 16.17762 | Lipid | Phosphatidic Acid | 0.0423 | 0.1361 | 0.756072 | 0.9343 | 0.1968 | 0.1377 | 0.153011 | 0.4692 | -0.1245 | 0.2285 | 0.58575 | 0.887 | NaN | -0.0042 | 0.1261 | 0.973674 | 0.9952 | 0.0715 | 0.1243 | 0.565129 | 0.9016 | -0.0902 | 0.2146 | 0.674157 | 0.954 | NaN | -0.014 | 0.126 | 0.911421 | 0.9717 | 0.1059 | 0.1205 | 0.379452 | 0.8818 | -0.1477 | 0.2156 | 0.493453 | 0.9848 | NaN | 0.0318 | 0.1287 | 0.804889 | 0.9433 | 0.1262 | 0.1278 | 0.323362 | 0.6497 | -0.0825 | 0.2177 | 0.704675 | 0.9477 | NaN | 0.0072 | 0.1277 | 0.955266 | 0.9796 | 0.0642 | 0.125 | 0.607265 | 0.8623 | -0.0741 | 0.2189 | 0.734881 | 0.9621 | NaN | 0.0309 | 0.129 | 0.810836 | 0.9477 | 0.0988 | 0.1268 | 0.435861 | 0.7458 | -0.0634 | 0.2204 | 0.77341 | 0.9525 |
| PA 19.3 | 446.2526 | 18.066814 | Lipid | Phosphatidic Acid | -0.19 | 0.1292 | 0.141494 | 0.5159 | -0.1002 | 0.1514 | 0.508318 | 0.7648 | -0.2952 | 0.1986 | 0.137277 | 0.6043 | NaN | -0.1653 | 0.1197 | 0.167213 | 0.7251 | -0.1369 | 0.1327 | 0.301896 | 0.8095 | -0.2309 | 0.1877 | 0.218637 | 0.9223 | NaN | -0.1349 | 0.12 | 0.260864 | 0.7619 | -0.0975 | 0.1304 | 0.454713 | 0.8952 | -0.1919 | 0.191 | 0.314914 | 0.9479 | NaN | -0.1594 | 0.1225 | 0.193031 | 0.6616 | -0.1476 | 0.1384 | 0.286456 | 0.6122 | -0.2239 | 0.1908 | 0.240576 | 0.8705 | NaN | -0.1472 | 0.1216 | 0.225926 | 0.7052 | -0.1377 | 0.1329 | 0.300096 | 0.7544 | -0.2071 | 0.1927 | 0.282521 | 0.9039 | NaN | -0.1734 | 0.1225 | 0.157122 | 0.6278 | -0.1864 | 0.1366 | 0.172176 | 0.5537 | -0.2291 | 0.1926 | 0.23425 | 0.8424 |
| PA 20:3 | 460.2681 | 17.864069 | Lipid | Phosphatidic Acid | 0.0836 | 0.1383 | 0.545311 | 0.8252 | 0.1814 | 0.1393 | 0.192859 | 0.4993 | -0.0408 | 0.2379 | 0.863833 | 0.9735 | NaN | 0.0812 | 0.1279 | 0.525415 | 0.8924 | 0.099 | 0.1239 | 0.424514 | 0.847 | 0.037 | 0.2241 | 0.868705 | 0.977 | NaN | 0.0477 | 0.1279 | 0.709236 | 0.9481 | 0.1254 | 0.1208 | 0.299279 | 0.8336 | -0.0617 | 0.2247 | 0.783702 | 0.9935 | NaN | 0.1217 | 0.1308 | 0.352085 | 0.7467 | 0.1504 | 0.1278 | 0.239249 | 0.5767 | 0.0557 | 0.2279 | 0.806897 | 0.9662 | NaN | 0.0803 | 0.1296 | 0.535738 | 0.8632 | 0.1043 | 0.124 | 0.40044 | 0.8162 | 0.0182 | 0.2279 | 0.936233 | 0.9806 | NaN | 0.1177 | 0.1311 | 0.369134 | 0.7603 | 0.1146 | 0.1269 | 0.366295 | 0.6901 | 0.0823 | 0.2317 | 0.722311 | 0.9459 |
| PA 21:3 | 474.2836 | 19.388664 | Lipid | Phosphatidic Acid | -0.1859 | 0.1278 | 0.145831 | 0.516 | -0.1102 | 0.1429 | 0.440522 | 0.711 | -0.2993 | 0.204 | 0.14231 | 0.6043 | NaN | -0.1413 | 0.1186 | 0.233561 | 0.7495 | -0.0917 | 0.1255 | 0.464823 | 0.8665 | -0.238 | 0.1925 | 0.21637 | 0.9223 | NaN | -0.156 | 0.1182 | 0.187079 | 0.7122 | -0.0929 | 0.1231 | 0.450584 | 0.8947 | -0.2457 | 0.1937 | 0.20462 | 0.8462 | NaN | -0.149 | 0.1212 | 0.218986 | 0.7062 | -0.1349 | 0.1305 | 0.301226 | 0.6322 | -0.2293 | 0.1958 | 0.241555 | 0.8705 | NaN | -0.1417 | 0.1203 | 0.238782 | 0.7125 | -0.0944 | 0.1257 | 0.452587 | 0.8246 | -0.2373 | 0.1964 | 0.226847 | 0.8892 | NaN | -0.1581 | 0.1213 | 0.192609 | 0.6472 | -0.1585 | 0.1285 | 0.217383 | 0.5853 | -0.2317 | 0.1978 | 0.241512 | 0.8424 |
| PA 23:3 | 502.3153 | 20.654627 | Lipid | Phosphatidic Acid | -0.2163 | 0.1299 | 0.095864 | 0.4484 | -0.0967 | 0.1467 | 0.509884 | 0.7648 | -0.3541 | 0.2048 | 0.083795 | 0.4769 | NaN | -0.1568 | 0.1209 | 0.194605 | 0.7307 | -0.0846 | 0.1288 | 0.511371 | 0.8967 | -0.2619 | 0.1947 | 0.178695 | 0.879 | NaN | -0.1385 | 0.1211 | 0.252646 | 0.7458 | -0.0454 | 0.1269 | 0.720415 | 0.9241 | -0.2446 | 0.1973 | 0.215114 | 0.8605 | NaN | -0.168 | 0.1235 | 0.173467 | 0.6514 | -0.1155 | 0.134 | 0.388886 | 0.6838 | -0.2688 | 0.1975 | 0.173509 | 0.8705 | NaN | -0.1555 | 0.1226 | 0.204684 | 0.6855 | -0.0946 | 0.1289 | 0.463259 | 0.8272 | -0.258 | 0.1993 | 0.195408 | 0.8608 | NaN | -0.1782 | 0.1235 | 0.148985 | 0.6183 | -0.1464 | 0.132 | 0.267229 | 0.6386 | -0.2702 | 0.1997 | 0.176109 | 0.8194 |
| PA 24:3 | 516.3306 | 21.119514 | Lipid | Phosphatidic Acid | -0.1645 | 0.1304 | 0.207193 | 0.5776 | -0.0608 | 0.1487 | 0.682847 | 0.8645 | -0.2908 | 0.2064 | 0.158857 | 0.6354 | NaN | -0.1133 | 0.1211 | 0.349434 | 0.8386 | -0.0813 | 0.1304 | 0.533025 | 0.8967 | -0.1918 | 0.1963 | 0.328658 | 0.9223 | NaN | -0.1033 | 0.1211 | 0.393762 | 0.8457 | -0.0434 | 0.1282 | 0.734979 | 0.9241 | -0.1892 | 0.198 | 0.33938 | 0.957 | NaN | -0.113 | 0.1239 | 0.361912 | 0.7539 | -0.092 | 0.136 | 0.498545 | 0.756 | -0.1937 | 0.1994 | 0.33146 | 0.9044 | NaN | -0.1012 | 0.123 | 0.410974 | 0.8283 | -0.0788 | 0.1307 | 0.546346 | 0.8618 | -0.1795 | 0.2015 | 0.373045 | 0.9106 | NaN | -0.121 | 0.1241 | 0.329472 | 0.7485 | -0.1254 | 0.1341 | 0.349859 | 0.6824 | -0.1912 | 0.2021 | 0.344153 | 0.8785 |
| PA 25:3 | 530.3468 | 21.493023 | Lipid | Phosphatidic Acid | -0.0611 | 0.131 | 0.64059 | 0.8731 | 0.0257 | 0.1405 | 0.854907 | 0.932 | -0.194 | 0.2205 | 0.37895 | 0.7534 | NaN | -0.0097 | 0.1215 | 0.93633 | 0.9881 | 0.007 | 0.1234 | 0.954825 | 0.9836 | -0.0845 | 0.2094 | 0.686592 | 0.954 | NaN | -0.0063 | 0.1213 | 0.958384 | 0.9747 | 0.0467 | 0.121 | 0.699511 | 0.9195 | -0.0992 | 0.2104 | 0.637207 | 0.9894 | NaN | -0.0061 | 0.1244 | 0.961029 | 0.9828 | 0.0044 | 0.1286 | 0.972675 | 0.9926 | -0.0884 | 0.2126 | 0.67737 | 0.9476 | NaN | -0.0005 | 0.1233 | 0.99649 | 0.9991 | 0.0062 | 0.1236 | 0.959681 | 0.9923 | -0.0719 | 0.2147 | 0.737808 | 0.9621 | NaN | -0.0122 | 0.1246 | 0.922275 | 0.9775 | -0.0233 | 0.127 | 0.854504 | 0.951 | -0.0798 | 0.2157 | 0.71161 | 0.9459 |
| PA 26:3 | 544.3617 | 21.772911 | Lipid | Phosphatidic Acid | 0.0138 | 0.1312 | 0.916169 | 0.9809 | -0.0092 | 0.1296 | 0.943089 | 0.9731 | -0.0178 | 0.2413 | 0.941129 | 0.9887 | NaN | 0.0854 | 0.1218 | 0.483162 | 0.8576 | 0.031 | 0.1139 | 0.785634 | 0.9616 | 0.083 | 0.2276 | 0.715502 | 0.954 | NaN | 0.0701 | 0.1214 | 0.563576 | 0.9125 | 0.0519 | 0.112 | 0.642856 | 0.9053 | 0.0455 | 0.2284 | 0.842152 | 0.9935 | NaN | 0.0736 | 0.1245 | 0.554283 | 0.8434 | 0.0091 | 0.1186 | 0.939089 | 0.9799 | 0.0646 | 0.2305 | 0.779159 | 0.961 | NaN | 0.0885 | 0.1236 | 0.473664 | 0.8625 | 0.0293 | 0.1141 | 0.797279 | 0.9324 | 0.0964 | 0.2328 | 0.678794 | 0.9621 | NaN | 0.0778 | 0.1249 | 0.533366 | 0.8482 | 0.0003 | 0.1167 | 0.99782 | 0.9978 | 0.0914 | 0.2341 | 0.696273 | 0.9459 |
| PC 20:0 | 565.3707 | 22.624731 | Lipid | Phosphatidylcholine | -0.1961 | 0.128 | 0.125617 | 0.4924 | -0.2426 | 0.1214 | 0.045634 | 0.2929 | -0.1363 | 0.2266 | 0.547455 | 0.8684 | NaN | -0.2284 | 0.1181 | 0.053127 | 0.4443 | -0.2724 | 0.1052 | 0.009643 | 0.1622 | -0.1755 | 0.2125 | 0.408812 | 0.9419 | NaN | -0.2057 | 0.118 | 0.081309 | 0.5159 | -0.2104 | 0.1047 | 0.044434 | 0.446 | -0.2088 | 0.2143 | 0.329964 | 0.957 | NaN | -0.235 | 0.1209 | 0.051842 | 0.4336 | -0.2862 | 0.1099 | 0.009198 | 0.12 | -0.1717 | 0.2154 | 0.425464 | 0.9375 | NaN | -0.2436 | 0.1198 | 0.041949 | 0.3925 | -0.2861 | 0.1052 | 0.006563 | 0.1424 | -0.1925 | 0.2166 | 0.374239 | 0.9106 | NaN | -0.2264 | 0.1211 | 0.061552 | 0.4591 | -0.2945 | 0.108 | 0.006385 | 0.1007 | -0.1454 | 0.2174 | 0.503662 | 0.8946 |
| PC 34:0 | 761.5932 | 25.417608 | Lipid | Phosphatidylcholine | -0.0421 | 0.1302 | 0.746385 | 0.9321 | -0.1908 | 0.1332 | 0.151938 | 0.4685 | 0.1383 | 0.2175 | 0.524928 | 0.8655 | NaN | -0.0217 | 0.1204 | 0.857168 | 0.9705 | -0.1018 | 0.1189 | 0.392012 | 0.8387 | 0.0663 | 0.2052 | 0.746494 | 0.954 | NaN | -0.0128 | 0.1203 | 0.915398 | 0.9717 | -0.0558 | 0.1183 | 0.637021 | 0.9053 | 0.024 | 0.2082 | 0.908164 | 0.9935 | NaN | -0.0751 | 0.1232 | 0.541769 | 0.84 | -0.1763 | 0.1219 | 0.148014 | 0.4863 | 0.0481 | 0.2088 | 0.818029 | 0.969 | NaN | -0.0401 | 0.122 | 0.742133 | 0.9289 | -0.128 | 0.1183 | 0.2794 | 0.7544 | 0.0697 | 0.2091 | 0.738748 | 0.9621 | NaN | -0.0531 | 0.1233 | 0.666978 | 0.9035 | -0.1637 | 0.1203 | 0.173547 | 0.5537 | 0.0847 | 0.2097 | 0.686152 | 0.9459 |
| SN-glycero-3-phosphocholine | 257.1031 | 0.614226 | Lipid | Phosphatidylcholine | 0.0119 | 0.1339 | 0.929335 | 0.982 | -0.108 | 0.1485 | 0.467311 | 0.737 | 0.0934 | 0.2104 | 0.657286 | 0.9185 | NaN | -0.1119 | 0.1253 | 0.37153 | 0.8459 | -0.1208 | 0.1302 | 0.353188 | 0.8148 | -0.1125 | 0.2044 | 0.58204 | 0.954 | NaN | -0.1149 | 0.1251 | 0.358367 | 0.8251 | -0.1898 | 0.1276 | 0.136764 | 0.6741 | -0.0474 | 0.2026 | 0.814941 | 0.9935 | NaN | -0.0754 | 0.1277 | 0.554596 | 0.8434 | -0.0879 | 0.136 | 0.517905 | 0.7667 | -0.0777 | 0.2064 | 0.706606 | 0.9477 | NaN | -0.0883 | 0.1267 | 0.485647 | 0.8625 | -0.1054 | 0.1305 | 0.419251 | 0.8188 | -0.0674 | 0.2071 | 0.744979 | 0.9621 | NaN | -0.0516 | 0.1274 | 0.685287 | 0.9035 | -0.0474 | 0.1347 | 0.724681 | 0.8975 | -0.0509 | 0.2076 | 0.806182 | 0.9623 |
| PC 32:0/PE 35:0 | 733.5648 | 24.662941 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0578 | 0.1416 | 0.683146 | 0.9021 | -0.078 | 0.1578 | 0.620946 | 0.8279 | -0.0077 | 0.222 | 0.972327 | 0.9935 | NaN | 0.0261 | 0.1318 | 0.842988 | 0.9694 | 0.0452 | 0.1405 | 0.747912 | 0.949 | 0.0361 | 0.2085 | 0.862698 | 0.977 | NaN | 0.0448 | 0.1319 | 0.733927 | 0.957 | 0.0772 | 0.1385 | 0.577108 | 0.9053 | 0.0296 | 0.2098 | 0.887742 | 0.9935 | NaN | 0.0079 | 0.1346 | 0.953182 | 0.9828 | 0.0242 | 0.1464 | 0.868907 | 0.9545 | 0.0322 | 0.2113 | 0.878965 | 0.99 | NaN | 0.0044 | 0.1333 | 0.973688 | 0.9861 | 0.0296 | 0.1404 | 0.832909 | 0.9444 | 0.0143 | 0.212 | 0.946108 | 0.9854 | NaN | 0.0015 | 0.1348 | 0.990879 | 0.9956 | 0.0286 | 0.1441 | 0.842847 | 0.9453 | 0.0182 | 0.2132 | 0.93208 | 0.9869 |
| PC 34:0/PE 37:0 | 761.5923 | 25.413399 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1725 | 0.132 | 0.191198 | 0.5541 | -0.2291 | 0.1159 | 0.048077 | 0.2996 | -0.0696 | 0.2598 | 0.788917 | 0.9647 | NaN | -0.0529 | 0.1243 | 0.670574 | 0.9208 | -0.0508 | 0.1098 | 0.643528 | 0.9079 | -0.0864 | 0.2437 | 0.723067 | 0.954 | NaN | -0.0814 | 0.1232 | 0.509145 | 0.9053 | -0.082 | 0.1051 | 0.435403 | 0.8947 | -0.0871 | 0.2453 | 0.722606 | 0.99 | NaN | -0.1076 | 0.1258 | 0.392162 | 0.7731 | -0.1063 | 0.1121 | 0.343105 | 0.67 | -0.1433 | 0.2476 | 0.562673 | 0.9375 | NaN | -0.0913 | 0.125 | 0.465038 | 0.8625 | -0.106 | 0.1064 | 0.319075 | 0.7579 | -0.0629 | 0.2481 | 0.800005 | 0.9621 | NaN | -0.0949 | 0.1265 | 0.452947 | 0.8014 | -0.1007 | 0.1101 | 0.360636 | 0.6888 | -0.086 | 0.2494 | 0.730295 | 0.9459 |
| PC 32:1/PE 35:1 | 731.5476 | 24.215395 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2995 | 0.1327 | 0.023994 | 0.2069 | 0.062 | 0.1306 | 0.635055 | 0.8406 | 0.5682 | 0.2271 | 0.012334 | 0.1929 | NaN | 0.1828 | 0.1253 | 0.144731 | 0.6828 | -0.0371 | 0.1162 | 0.749591 | 0.949 | 0.4323 | 0.2187 | 0.048027 | 0.5871 | NaN | 0.2715 | 0.1227 | 0.026865 | 0.27 | 0.1028 | 0.1124 | 0.360477 | 0.873 | 0.4639 | 0.2183 | 0.033586 | 0.3815 | NaN | 0.2018 | 0.128 | 0.1148 | 0.5709 | -0.0437 | 0.122 | 0.720483 | 0.876 | 0.4766 | 0.2193 | 0.029739 | 0.4788 | NaN | 0.1811 | 0.1275 | 0.155514 | 0.6753 | -0.0749 | 0.1176 | 0.524253 | 0.8496 | 0.4646 | 0.2214 | 0.035886 | 0.4772 | NaN | 0.1897 | 0.129 | 0.141392 | 0.605 | -0.0677 | 0.1207 | 0.574944 | 0.8092 | 0.4721 | 0.2224 | 0.033737 | 0.4663 |
| PC 34:1/PE 37:1 | 759.5781 | 24.803432 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0379 | 0.1308 | 0.772134 | 0.9439 | -0.1154 | 0.1213 | 0.34165 | 0.6305 | 0.2685 | 0.2401 | 0.263552 | 0.7397 | NaN | 0.0456 | 0.1209 | 0.705881 | 0.9314 | -0.0982 | 0.1066 | 0.356516 | 0.8148 | 0.2666 | 0.225 | 0.236237 | 0.9223 | NaN | 0.0642 | 0.1208 | 0.594807 | 0.9125 | -0.0538 | 0.1054 | 0.609906 | 0.9053 | 0.2391 | 0.227 | 0.292349 | 0.9294 | NaN | 0.0188 | 0.1237 | 0.879439 | 0.9749 | -0.1107 | 0.1109 | 0.318175 | 0.6457 | 0.2238 | 0.2289 | 0.32839 | 0.9044 | NaN | 0.055 | 0.1225 | 0.653739 | 0.9044 | -0.0835 | 0.107 | 0.435232 | 0.8205 | 0.2688 | 0.2291 | 0.240695 | 0.9039 | NaN | 0.0214 | 0.124 | 0.86316 | 0.9576 | -0.1138 | 0.1092 | 0.297486 | 0.6559 | 0.2362 | 0.2309 | 0.306324 | 0.8671 |
| PC 36:1/PE 39:1 | 787.6113 | 25.608099 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0217 | 0.1336 | 0.870662 | 0.9809 | -0.0847 | 0.1432 | 0.554299 | 0.7957 | 0.0387 | 0.2133 | 0.856102 | 0.9732 | NaN | -0.054 | 0.1236 | 0.662198 | 0.9185 | -0.0937 | 0.1255 | 0.455203 | 0.8559 | -0.0279 | 0.2008 | 0.889348 | 0.977 | NaN | -0.046 | 0.1234 | 0.709357 | 0.9481 | -0.0066 | 0.1243 | 0.957629 | 0.9785 | -0.093 | 0.2045 | 0.649325 | 0.9894 | NaN | -0.0721 | 0.1266 | 0.568919 | 0.846 | -0.1445 | 0.1311 | 0.270094 | 0.6036 | -0.0148 | 0.2034 | 0.94186 | 0.99 | NaN | -0.0797 | 0.1255 | 0.525606 | 0.8625 | -0.1241 | 0.1257 | 0.323425 | 0.7597 | -0.0442 | 0.2053 | 0.829614 | 0.9621 | NaN | -0.0627 | 0.1268 | 0.621088 | 0.8808 | -0.1436 | 0.129 | 0.265595 | 0.6386 | 0.001 | 0.2051 | 0.995997 | 0.9991 |
| PC 32:2/PE 35:2 | 729.5338 | 23.893877 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1011 | 0.1277 | 0.428514 | 0.7581 | 0.0013 | 0.1465 | 0.992668 | 0.9963 | 0.166 | 0.197 | 0.399496 | 0.7684 | NaN | 0.0857 | 0.1182 | 0.467982 | 0.8498 | 0.0593 | 0.1289 | 0.645435 | 0.9079 | 0.0766 | 0.1867 | 0.68148 | 0.954 | NaN | 0.0886 | 0.1179 | 0.45234 | 0.8854 | 0.1041 | 0.127 | 0.412395 | 0.8818 | 0.0589 | 0.189 | 0.755456 | 0.9935 | NaN | 0.0777 | 0.1209 | 0.52017 | 0.8227 | 0.0116 | 0.134 | 0.93092 | 0.9769 | 0.0929 | 0.1889 | 0.622818 | 0.9375 | NaN | 0.0944 | 0.1197 | 0.430262 | 0.8452 | 0.0326 | 0.1289 | 0.800307 | 0.9326 | 0.1217 | 0.1889 | 0.519468 | 0.9524 | NaN | 0.0806 | 0.1211 | 0.505828 | 0.8285 | 0.0015 | 0.132 | 0.990784 | 0.9978 | 0.1126 | 0.1902 | 0.553941 | 0.9114 |
| PC 34:2/PE 37:2 | 757.5632 | 24.41449 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0174 | 0.1399 | 0.900818 | 0.9809 | 0.3416 | 0.1525 | 0.025111 | 0.2446 | -0.2419 | 0.2159 | 0.26251 | 0.7397 | NaN | -0.0414 | 0.1294 | 0.749133 | 0.9484 | 0.3472 | 0.1327 | 0.008854 | 0.1606 | -0.2861 | 0.2021 | 0.156924 | 0.879 | NaN | 0.012 | 0.1293 | 0.926171 | 0.9728 | 0.3095 | 0.1311 | 0.018268 | 0.2586 | -0.1714 | 0.2054 | 0.403998 | 0.9816 | NaN | -0.0494 | 0.1324 | 0.709141 | 0.8896 | 0.3715 | 0.1381 | 0.007156 | 0.1015 | -0.3199 | 0.2053 | 0.119164 | 0.7964 | NaN | -0.0116 | 0.1311 | 0.929781 | 0.9796 | 0.3606 | 0.1326 | 0.006543 | 0.1424 | -0.2414 | 0.206 | 0.241283 | 0.9039 | NaN | -0.0663 | 0.1328 | 0.617796 | 0.8808 | 0.3548 | 0.1362 | 0.009189 | 0.1247 | -0.3346 | 0.2079 | 0.107485 | 0.7063 |
| PC 36:2/PE 39:2 | 785.5938 | 25.064062 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1618 | 0.1405 | 0.249419 | 0.6174 | 0.0409 | 0.168 | 0.807795 | 0.932 | 0.2775 | 0.2117 | 0.189936 | 0.6943 | NaN | 0.1416 | 0.13 | 0.276193 | 0.7644 | 0.1418 | 0.148 | 0.337828 | 0.8095 | 0.1621 | 0.202 | 0.422312 | 0.9419 | NaN | 0.154 | 0.1297 | 0.235104 | 0.7361 | 0.1632 | 0.1453 | 0.261331 | 0.8057 | 0.1589 | 0.2039 | 0.435755 | 0.9816 | NaN | 0.1204 | 0.1333 | 0.366421 | 0.7543 | 0.0864 | 0.1538 | 0.574407 | 0.7987 | 0.1691 | 0.205 | 0.409422 | 0.9375 | NaN | 0.1454 | 0.1317 | 0.26966 | 0.7442 | 0.14 | 0.1483 | 0.345001 | 0.7839 | 0.1854 | 0.2052 | 0.366315 | 0.9106 | NaN | 0.1275 | 0.1335 | 0.339347 | 0.7513 | 0.0866 | 0.1515 | 0.567466 | 0.8092 | 0.1889 | 0.2063 | 0.359675 | 0.8785 |
| PC 33:3/PE 36:3 | 741.5698 | 24.691595 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0572 | 0.1303 | 0.660685 | 0.883 | -0.1629 | 0.1406 | 0.246561 | 0.538 | 0.2021 | 0.2052 | 0.324764 | 0.7534 | NaN | 0.0282 | 0.1207 | 0.815121 | 0.9614 | -0.0995 | 0.1244 | 0.424064 | 0.847 | 0.095 | 0.1952 | 0.626651 | 0.954 | NaN | 0.0536 | 0.1203 | 0.6559 | 0.9331 | -0.0912 | 0.1222 | 0.4554 | 0.8952 | 0.1529 | 0.1946 | 0.431984 | 0.9816 | NaN | 0.0244 | 0.1234 | 0.843474 | 0.962 | -0.1201 | 0.1293 | 0.352831 | 0.6762 | 0.0962 | 0.1984 | 0.627837 | 0.9375 | NaN | 0.0571 | 0.1221 | 0.640165 | 0.8992 | -0.0713 | 0.1255 | 0.569869 | 0.8623 | 0.1384 | 0.1974 | 0.483199 | 0.9403 | NaN | 0.0427 | 0.1235 | 0.729758 | 0.9166 | -0.0955 | 0.128 | 0.455731 | 0.7516 | 0.1232 | 0.1993 | 0.53633 | 0.8971 |
| PC 34:3/PE 37:3 | 755.5473 | 24.082075 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1017 | 0.1357 | 0.453641 | 0.7825 | -0.0655 | 0.1337 | 0.624342 | 0.8305 | 0.306 | 0.2329 | 0.188957 | 0.6943 | NaN | 0.0366 | 0.1262 | 0.771585 | 0.9527 | -0.0762 | 0.1172 | 0.515591 | 0.8967 | 0.1769 | 0.2223 | 0.426146 | 0.9419 | NaN | 0.1167 | 0.1253 | 0.351586 | 0.8224 | 0.0316 | 0.1165 | 0.785972 | 0.935 | 0.2197 | 0.222 | 0.32245 | 0.9479 | NaN | 0.0001 | 0.1302 | 0.999346 | 0.9993 | -0.1449 | 0.1228 | 0.238039 | 0.5767 | 0.1848 | 0.2256 | 0.412684 | 0.9375 | NaN | 0.0437 | 0.1278 | 0.732291 | 0.9262 | -0.0903 | 0.1174 | 0.442168 | 0.8205 | 0.2145 | 0.2252 | 0.340715 | 0.9106 | NaN | 0.0019 | 0.1305 | 0.988284 | 0.9956 | -0.1437 | 0.1208 | 0.234113 | 0.6096 | 0.1877 | 0.2283 | 0.411184 | 0.8887 |
| PC 35:3/PE 38:3 | 769.5958 | 24.92041 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1975 | 0.135 | 0.143365 | 0.516 | 0.0063 | 0.1453 | 0.965592 | 0.987 | -0.3287 | 0.2173 | 0.130372 | 0.6043 | NaN | -0.1145 | 0.126 | 0.363558 | 0.8459 | 0.044 | 0.1276 | 0.730466 | 0.9386 | -0.2177 | 0.2071 | 0.293211 | 0.9223 | NaN | -0.1278 | 0.1255 | 0.308517 | 0.7952 | 0.0249 | 0.1252 | 0.84217 | 0.95 | -0.2513 | 0.2071 | 0.225069 | 0.8771 | NaN | -0.1553 | 0.1281 | 0.225383 | 0.7062 | 0.0299 | 0.133 | 0.822147 | 0.9271 | -0.2711 | 0.2079 | 0.192067 | 0.8705 | NaN | -0.1135 | 0.1279 | 0.375077 | 0.7993 | 0.0713 | 0.1281 | 0.578015 | 0.8623 | -0.2426 | 0.2103 | 0.248578 | 0.9039 | NaN | -0.149 | 0.1285 | 0.246374 | 0.7047 | 0.0329 | 0.131 | 0.801348 | 0.9273 | -0.2678 | 0.2102 | 0.202711 | 0.8424 |
| PC 35:3/PE 38:3 | 769.5964 | 26.10005 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2677 | 0.1339 | 0.045684 | 0.3113 | -0.1657 | 0.1533 | 0.279866 | 0.5701 | -0.3074 | 0.2078 | 0.139087 | 0.6043 | NaN | -0.1884 | 0.1252 | 0.132245 | 0.6772 | -0.0643 | 0.1366 | 0.637804 | 0.9073 | -0.2371 | 0.1965 | 0.227541 | 0.9223 | NaN | -0.2371 | 0.1239 | 0.055601 | 0.3885 | -0.0645 | 0.1339 | 0.630081 | 0.9053 | -0.3402 | 0.1957 | 0.082182 | 0.5886 | NaN | -0.2019 | 0.1278 | 0.114172 | 0.5709 | -0.0448 | 0.1439 | 0.755846 | 0.8953 | -0.2632 | 0.1984 | 0.18466 | 0.8705 | NaN | -0.2002 | 0.1266 | 0.113986 | 0.6708 | -0.0443 | 0.1376 | 0.747218 | 0.9085 | -0.2704 | 0.1991 | 0.174451 | 0.8447 | NaN | -0.1796 | 0.129 | 0.163777 | 0.6278 | -0.0149 | 0.1428 | 0.917078 | 0.979 | -0.2422 | 0.2013 | 0.229106 | 0.8424 |
| PC 36:3/PE 39:3 | 783.5786 | 24.554457 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1265 | 0.1335 | 0.343154 | 0.7042 | -0.1063 | 0.1426 | 0.456007 | 0.7254 | 0.351 | 0.2133 | 0.099828 | 0.5278 | NaN | 0.0852 | 0.1238 | 0.491357 | 0.8632 | -0.0783 | 0.1254 | 0.532523 | 0.8967 | 0.2396 | 0.2035 | 0.239164 | 0.9223 | NaN | 0.115 | 0.1233 | 0.350777 | 0.8224 | 0.028 | 0.1254 | 0.823244 | 0.9428 | 0.1996 | 0.208 | 0.337353 | 0.957 | NaN | 0.0445 | 0.1276 | 0.727141 | 0.902 | -0.1498 | 0.1303 | 0.250343 | 0.5831 | 0.235 | 0.2073 | 0.25692 | 0.8705 | NaN | 0.0803 | 0.1255 | 0.522582 | 0.8625 | -0.1078 | 0.1253 | 0.389766 | 0.815 | 0.2649 | 0.2065 | 0.199597 | 0.8608 | NaN | 0.0658 | 0.1273 | 0.605483 | 0.8772 | -0.1544 | 0.1283 | 0.228545 | 0.6007 | 0.2793 | 0.207 | 0.177139 | 0.8194 |
| PC 32:4/PE 35:4 | 725.5072 | 23.725977 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1831 | 0.1373 | 0.18254 | 0.5518 | 0.0619 | 0.1341 | 0.64423 | 0.8471 | 0.3225 | 0.24 | 0.179002 | 0.6772 | NaN | 0.1608 | 0.1271 | 0.206017 | 0.7401 | 0.0056 | 0.1183 | 0.96243 | 0.9875 | 0.3315 | 0.2247 | 0.140122 | 0.8611 | NaN | 0.2688 | 0.1267 | 0.03394 | 0.2852 | 0.1402 | 0.1155 | 0.224761 | 0.8003 | 0.3993 | 0.2261 | 0.077408 | 0.5774 | NaN | 0.1236 | 0.1307 | 0.34414 | 0.7421 | -0.0303 | 0.1246 | 0.808037 | 0.9197 | 0.2885 | 0.2285 | 0.20679 | 0.8705 | NaN | 0.1498 | 0.129 | 0.245522 | 0.7211 | -0.0337 | 0.1194 | 0.77784 | 0.9247 | 0.3462 | 0.2287 | 0.130073 | 0.772 | NaN | 0.1214 | 0.1311 | 0.354482 | 0.7573 | -0.0499 | 0.1231 | 0.685534 | 0.8747 | 0.2987 | 0.2305 | 0.195005 | 0.8424 |
| PC 33:4/PE 36:4 | 739.5503 | 24.66426 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2026 | 0.1502 | 0.177288 | 0.5449 | -0.2379 | 0.1631 | 0.144772 | 0.4547 | -0.1384 | 0.2399 | 0.563872 | 0.8721 | NaN | -0.1436 | 0.1395 | 0.303365 | 0.7864 | -0.2157 | 0.1431 | 0.131896 | 0.6118 | -0.0565 | 0.2263 | 0.802923 | 0.9617 | NaN | -0.1337 | 0.1394 | 0.337783 | 0.8142 | -0.1191 | 0.1431 | 0.405418 | 0.8818 | -0.144 | 0.2264 | 0.524931 | 0.9894 | NaN | -0.1498 | 0.1426 | 0.293489 | 0.7388 | -0.2428 | 0.1488 | 0.102817 | 0.4326 | -0.0248 | 0.2309 | 0.914348 | 0.99 | NaN | -0.1531 | 0.1412 | 0.278476 | 0.7462 | -0.2143 | 0.1435 | 0.135165 | 0.5986 | -0.0803 | 0.23 | 0.727018 | 0.9621 | NaN | -0.1504 | 0.1429 | 0.292616 | 0.7478 | -0.237 | 0.1466 | 0.105883 | 0.4566 | -0.0444 | 0.2326 | 0.848729 | 0.9641 |
| PC 35:4/PE 38:4 | 767.5821 | 24.73068 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.079 | 0.1343 | 0.556362 | 0.8309 | 0.0631 | 0.1422 | 0.656952 | 0.8482 | -0.1643 | 0.2182 | 0.451519 | 0.8098 | NaN | -0.0626 | 0.1243 | 0.614237 | 0.9079 | 0.0669 | 0.1247 | 0.591759 | 0.904 | -0.1498 | 0.2048 | 0.464435 | 0.9478 | NaN | -0.047 | 0.1242 | 0.704874 | 0.9481 | 0.0313 | 0.1227 | 0.798372 | 0.9363 | -0.1089 | 0.2069 | 0.598796 | 0.9894 | NaN | -0.0947 | 0.127 | 0.455781 | 0.7844 | 0.0801 | 0.13 | 0.537641 | 0.7845 | -0.2217 | 0.2076 | 0.285447 | 0.8705 | NaN | -0.0603 | 0.126 | 0.632172 | 0.8971 | 0.066 | 0.125 | 0.597491 | 0.8623 | -0.1454 | 0.2085 | 0.485697 | 0.9403 | NaN | -0.0948 | 0.1272 | 0.456402 | 0.8023 | 0.0671 | 0.128 | 0.600472 | 0.8225 | -0.2066 | 0.2095 | 0.323964 | 0.8727 |
| PC 36:4/PE 39:4 | 781.5616 | 24.310883 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0262 | 0.1329 | 0.843732 | 0.9778 | 0.0117 | 0.133 | 0.92997 | 0.9696 | 0.0119 | 0.2269 | 0.95834 | 0.9887 | NaN | 0.0044 | 0.123 | 0.971715 | 0.9952 | -0.0328 | 0.1169 | 0.779213 | 0.9615 | 0.0162 | 0.2128 | 0.939367 | 0.9911 | NaN | -0.0116 | 0.1229 | 0.924835 | 0.9728 | -0.1113 | 0.1159 | 0.337021 | 0.8587 | 0.0757 | 0.2148 | 0.724438 | 0.99 | NaN | 0.0008 | 0.1258 | 0.994759 | 0.9985 | -0.0039 | 0.1217 | 0.974751 | 0.9926 | -0.0398 | 0.2161 | 0.853765 | 0.9772 | NaN | 0.0127 | 0.1246 | 0.918667 | 0.9796 | -0.0239 | 0.1171 | 0.838303 | 0.946 | 0.0209 | 0.2166 | 0.923246 | 0.9774 | NaN | -0.0044 | 0.1261 | 0.972092 | 0.9893 | -0.0005 | 0.1198 | 0.996886 | 0.9978 | -0.0491 | 0.2186 | 0.822221 | 0.9641 |
| PC 37:4/PE 40:4 | 795.6124 | 25.543018 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.3444 | 0.138 | 0.012588 | 0.1478 | -0.318 | 0.1534 | 0.038197 | 0.2877 | -0.3296 | 0.2213 | 0.136431 | 0.6043 | NaN | -0.2368 | 0.13 | 0.068421 | 0.5202 | -0.2056 | 0.1378 | 0.135658 | 0.6175 | -0.2372 | 0.21 | 0.258586 | 0.9223 | NaN | -0.2541 | 0.1291 | 0.049157 | 0.3618 | -0.1986 | 0.1353 | 0.142233 | 0.6948 | -0.3049 | 0.2092 | 0.145052 | 0.7483 | NaN | -0.2871 | 0.1315 | 0.029001 | 0.3194 | -0.2422 | 0.1425 | 0.089165 | 0.4173 | -0.2868 | 0.2111 | 0.174382 | 0.8705 | NaN | -0.2462 | 0.1316 | 0.061472 | 0.4979 | -0.1921 | 0.1388 | 0.166407 | 0.631 | -0.2624 | 0.2131 | 0.218201 | 0.8892 | NaN | -0.2813 | 0.132 | 0.033108 | 0.3264 | -0.2319 | 0.1406 | 0.099088 | 0.4447 | -0.2857 | 0.2133 | 0.180415 | 0.8194 |
| PC 40:4/PE 43:4 | 837.6238 | 25.627386 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0462 | 0.1345 | 0.731406 | 0.9287 | 0.0622 | 0.1368 | 0.6494 | 0.8471 | 0.0999 | 0.2316 | 0.666284 | 0.9264 | NaN | -0.0968 | 0.1266 | 0.444133 | 0.8498 | -0.0855 | 0.123 | 0.487213 | 0.8847 | -0.062 | 0.2214 | 0.779415 | 0.954 | NaN | 0.0011 | 0.1244 | 0.993063 | 0.9939 | -0.0019 | 0.1185 | 0.987248 | 0.9908 | 0.019 | 0.22 | 0.931086 | 0.9935 | NaN | -0.0975 | 0.1303 | 0.453912 | 0.7844 | -0.0615 | 0.1284 | 0.631728 | 0.8283 | -0.0751 | 0.2262 | 0.739793 | 0.9572 | NaN | -0.1033 | 0.1289 | 0.42305 | 0.84 | -0.1019 | 0.1239 | 0.410725 | 0.8188 | -0.0621 | 0.2269 | 0.784356 | 0.9621 | NaN | -0.1094 | 0.1312 | 0.404093 | 0.7874 | -0.0782 | 0.1267 | 0.537066 | 0.8003 | -0.0883 | 0.2307 | 0.701858 | 0.9459 |
| PC 31:5/PE 34:5 | 707.509 | 25.409264 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2617 | 0.1276 | 0.040179 | 0.288 | -0.0268 | 0.1443 | 0.852772 | 0.932 | 0.478 | 0.1947 | 0.014073 | 0.1992 | NaN | 0.1074 | 0.1222 | 0.379519 | 0.8465 | -0.0967 | 0.1269 | 0.445933 | 0.8547 | 0.2713 | 0.1968 | 0.167949 | 0.879 | NaN | 0.1333 | 0.1208 | 0.269687 | 0.7794 | -0.0679 | 0.1243 | 0.585131 | 0.9053 | 0.2963 | 0.1963 | 0.13127 | 0.7174 | NaN | 0.1216 | 0.1254 | 0.332265 | 0.741 | -0.1232 | 0.1332 | 0.355025 | 0.6762 | 0.3125 | 0.197 | 0.112632 | 0.787 | NaN | 0.1488 | 0.1224 | 0.224029 | 0.7052 | -0.085 | 0.1271 | 0.503551 | 0.848 | 0.3417 | 0.1949 | 0.079537 | 0.6055 | NaN | 0.1402 | 0.1247 | 0.261059 | 0.7205 | -0.129 | 0.131 | 0.324986 | 0.6724 | 0.3521 | 0.1955 | 0.071695 | 0.6024 |
| PC 32:5/PE 35:5 | 723.5265 | 24.594513 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2349 | 0.1321 | 0.075384 | 0.3896 | 0.1877 | 0.132 | 0.15506 | 0.4721 | 0.3405 | 0.2267 | 0.133138 | 0.6043 | NaN | 0.1423 | 0.1238 | 0.250448 | 0.7495 | 0.1248 | 0.117 | 0.285905 | 0.7996 | 0.2015 | 0.2174 | 0.353957 | 0.9223 | NaN | 0.18 | 0.1227 | 0.142258 | 0.6585 | 0.111 | 0.1151 | 0.335084 | 0.8587 | 0.2735 | 0.2155 | 0.204511 | 0.8462 | NaN | 0.1909 | 0.1255 | 0.128243 | 0.5896 | 0.1875 | 0.1205 | 0.119543 | 0.4541 | 0.2437 | 0.2185 | 0.264781 | 0.8705 | NaN | 0.1698 | 0.1248 | 0.173622 | 0.6753 | 0.1201 | 0.1174 | 0.306346 | 0.7544 | 0.2662 | 0.2185 | 0.223079 | 0.8892 | NaN | 0.1888 | 0.1258 | 0.133597 | 0.605 | 0.1753 | 0.1188 | 0.140012 | 0.5193 | 0.2559 | 0.2204 | 0.245594 | 0.8424 |
| PC 34:5/PE 37:5 | 751.5536 | 25.308743 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.2271 | 0.1342 | 0.090614 | 0.4349 | 0.0778 | 0.155 | 0.615853 | 0.8251 | 0.3574 | 0.206 | 0.082706 | 0.4769 | NaN | 0.1923 | 0.1244 | 0.12214 | 0.6749 | 0.0727 | 0.136 | 0.593114 | 0.904 | 0.2792 | 0.1952 | 0.152518 | 0.879 | NaN | 0.211 | 0.1239 | 0.088677 | 0.5342 | 0.0866 | 0.1334 | 0.516411 | 0.9053 | 0.2894 | 0.1962 | 0.140241 | 0.7444 | NaN | 0.2193 | 0.1268 | 0.083798 | 0.5283 | 0.1099 | 0.1417 | 0.437974 | 0.7301 | 0.3045 | 0.197 | 0.122136 | 0.8026 | NaN | 0.1891 | 0.1262 | 0.13388 | 0.6708 | 0.0577 | 0.1364 | 0.672531 | 0.8623 | 0.2912 | 0.1986 | 0.142479 | 0.8056 | NaN | 0.2174 | 0.1272 | 0.087268 | 0.5441 | 0.0907 | 0.1396 | 0.515623 | 0.7928 | 0.3182 | 0.1985 | 0.108885 | 0.7071 |
| PC 35:5/PE 38:5 | 765.5646 | 24.605843 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.074 | 0.1399 | 0.596946 | 0.8537 | -0.1366 | 0.1405 | 0.330846 | 0.6191 | -0.0122 | 0.2366 | 0.958728 | 0.9887 | NaN | 0.0468 | 0.131 | 0.720931 | 0.9325 | -0.0149 | 0.126 | 0.905602 | 0.9729 | 0.0885 | 0.2233 | 0.691809 | 0.954 | NaN | 0.036 | 0.1305 | 0.782499 | 0.9641 | -0.0385 | 0.1227 | 0.753525 | 0.9264 | 0.0931 | 0.2251 | 0.679204 | 0.9894 | NaN | 0.0568 | 0.1349 | 0.673952 | 0.8746 | -0.0102 | 0.1325 | 0.938563 | 0.9799 | 0.1062 | 0.2273 | 0.640463 | 0.9375 | NaN | 0.0475 | 0.1331 | 0.720977 | 0.9229 | -0.0046 | 0.1267 | 0.970747 | 0.9923 | 0.0866 | 0.2278 | 0.703845 | 0.9621 | NaN | 0.0396 | 0.1347 | 0.768997 | 0.9344 | -0.0147 | 0.1299 | 0.909598 | 0.9768 | 0.0802 | 0.2289 | 0.726033 | 0.9459 |
| PC 35:5/PE 38:5 | 765.5672 | 25.150826 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1846 | 0.1343 | 0.16918 | 0.531 | -0.3904 | 0.1446 | 0.006922 | 0.147 | -0.0102 | 0.2138 | 0.961812 | 0.9887 | NaN | -0.0048 | 0.1287 | 0.970345 | 0.9952 | -0.1499 | 0.1409 | 0.287473 | 0.7996 | 0.0893 | 0.202 | 0.658528 | 0.954 | NaN | -0.0404 | 0.127 | 0.750427 | 0.96 | -0.1798 | 0.1344 | 0.180789 | 0.7308 | 0.0389 | 0.2023 | 0.84762 | 0.9935 | NaN | -0.0641 | 0.13 | 0.621821 | 0.8606 | -0.2146 | 0.144 | 0.136233 | 0.4784 | 0.0422 | 0.2038 | 0.836079 | 0.9726 | NaN | -0.0371 | 0.1296 | 0.774581 | 0.938 | -0.163 | 0.14 | 0.244346 | 0.7302 | 0.0565 | 0.2051 | 0.782852 | 0.9621 | NaN | -0.0623 | 0.1305 | 0.633191 | 0.8817 | -0.1819 | 0.1439 | 0.206059 | 0.5756 | 0.0287 | 0.2056 | 0.888911 | 0.9702 |
| PC 36:5/PE 39:5 | 779.5674 | 24.645178 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1222 | 0.1331 | 0.358612 | 0.7161 | -0.1662 | 0.1341 | 0.215184 | 0.5076 | -0.0498 | 0.2251 | 0.824942 | 0.973 | NaN | -0.0594 | 0.1238 | 0.631574 | 0.9079 | -0.0087 | 0.1225 | 0.943552 | 0.979 | -0.0988 | 0.2113 | 0.640319 | 0.954 | NaN | -0.0666 | 0.1235 | 0.589388 | 0.9125 | -0.038 | 0.1186 | 0.74863 | 0.9243 | -0.0858 | 0.2127 | 0.686754 | 0.9894 | NaN | -0.0935 | 0.1261 | 0.458336 | 0.7844 | -0.0464 | 0.1269 | 0.714789 | 0.8729 | -0.1258 | 0.2148 | 0.558185 | 0.9375 | NaN | -0.089 | 0.125 | 0.476267 | 0.8625 | -0.056 | 0.1206 | 0.642361 | 0.8623 | -0.0946 | 0.2152 | 0.660368 | 0.9621 | NaN | -0.0803 | 0.1266 | 0.525847 | 0.8438 | -0.0358 | 0.1251 | 0.774522 | 0.9173 | -0.0925 | 0.2163 | 0.668859 | 0.9459 |
| PC 36:5/PE 39:5 | 779.5741 | 27.296911 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0318 | 0.1322 | 0.810059 | 0.9637 | -0.2692 | 0.1352 | 0.046479 | 0.2949 | 0.178 | 0.2144 | 0.406369 | 0.7758 | NaN | -0.0315 | 0.1222 | 0.796376 | 0.9571 | -0.1294 | 0.1236 | 0.294907 | 0.8059 | 0.0293 | 0.2056 | 0.886677 | 0.977 | NaN | -0.0052 | 0.1222 | 0.966052 | 0.9794 | -0.1302 | 0.1208 | 0.281291 | 0.8127 | 0.0953 | 0.2043 | 0.64077 | 0.9894 | NaN | -0.0713 | 0.1251 | 0.569101 | 0.846 | -0.1954 | 0.1259 | 0.120649 | 0.4541 | 0.0156 | 0.2104 | 0.94086 | 0.99 | NaN | -0.0427 | 0.1239 | 0.730071 | 0.9262 | -0.1702 | 0.1217 | 0.161731 | 0.631 | 0.0717 | 0.2081 | 0.730486 | 0.9621 | NaN | -0.052 | 0.1253 | 0.677876 | 0.9035 | -0.1793 | 0.1246 | 0.149964 | 0.5211 | 0.0575 | 0.2104 | 0.784731 | 0.9525 |
| PC 37:5/PE 40:5 | 793.5976 | 24.882019 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2319 | 0.1305 | 0.075519 | 0.3896 | -0.0995 | 0.143 | 0.48655 | 0.7524 | -0.3187 | 0.2064 | 0.122588 | 0.598 | NaN | -0.147 | 0.1221 | 0.228367 | 0.7495 | -0.062 | 0.1259 | 0.622313 | 0.9073 | -0.2065 | 0.1971 | 0.294862 | 0.9223 | NaN | -0.1615 | 0.1215 | 0.183781 | 0.7111 | -0.0704 | 0.1234 | 0.568327 | 0.9053 | -0.2399 | 0.197 | 0.223256 | 0.8771 | NaN | -0.1917 | 0.1239 | 0.121611 | 0.579 | -0.0983 | 0.1307 | 0.45197 | 0.7319 | -0.253 | 0.1979 | 0.200952 | 0.8705 | NaN | -0.1575 | 0.1236 | 0.202501 | 0.6855 | -0.0562 | 0.1262 | 0.655972 | 0.8623 | -0.2342 | 0.1999 | 0.241326 | 0.9039 | NaN | -0.1842 | 0.1243 | 0.138517 | 0.605 | -0.0863 | 0.1289 | 0.503104 | 0.7835 | -0.2546 | 0.1999 | 0.202974 | 0.8424 |
| PC 39:5/PE 42:5 | 821.5945 | 25.4785 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1206 | 0.1325 | 0.36281 | 0.7161 | -0.0256 | 0.1413 | 0.855967 | 0.932 | 0.2681 | 0.213 | 0.208137 | 0.7107 | NaN | 0.0832 | 0.1228 | 0.498223 | 0.8703 | -0.0248 | 0.124 | 0.841323 | 0.9729 | 0.1799 | 0.2019 | 0.372792 | 0.9312 | NaN | 0.1327 | 0.1222 | 0.277788 | 0.7865 | 0.0973 | 0.1231 | 0.429347 | 0.8947 | 0.1611 | 0.2044 | 0.430546 | 0.9816 | NaN | 0.0418 | 0.1265 | 0.741055 | 0.9111 | -0.0754 | 0.1295 | 0.560666 | 0.789 | 0.1508 | 0.2067 | 0.465694 | 0.9375 | NaN | 0.0573 | 0.1249 | 0.646353 | 0.901 | -0.0799 | 0.1244 | 0.520703 | 0.8496 | 0.1853 | 0.2058 | 0.368131 | 0.9106 | NaN | 0.0601 | 0.1263 | 0.634102 | 0.8817 | -0.0805 | 0.1275 | 0.527877 | 0.8003 | 0.1925 | 0.2067 | 0.351824 | 0.8785 |
| PC 40:5/PE 43:5 | 835.6077 | 25.139347 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1378 | 0.1383 | 0.319059 | 0.6826 | -0.0317 | 0.1648 | 0.847407 | 0.932 | 0.2404 | 0.2059 | 0.242969 | 0.7391 | NaN | 0.0882 | 0.1283 | 0.492056 | 0.8632 | -0.1998 | 0.1464 | 0.172368 | 0.6796 | 0.251 | 0.1928 | 0.193093 | 0.9189 | NaN | 0.1319 | 0.1277 | 0.301454 | 0.7865 | -0.0715 | 0.142 | 0.614606 | 0.9053 | 0.2379 | 0.1943 | 0.220797 | 0.8768 | NaN | 0.0765 | 0.1316 | 0.561024 | 0.846 | -0.1742 | 0.1531 | 0.255178 | 0.5881 | 0.2156 | 0.196 | 0.27139 | 0.8705 | NaN | 0.0746 | 0.1304 | 0.567251 | 0.8722 | -0.196 | 0.1467 | 0.181501 | 0.6534 | 0.2184 | 0.1968 | 0.267271 | 0.9039 | NaN | 0.0687 | 0.1321 | 0.602921 | 0.8765 | -0.1858 | 0.1506 | 0.217334 | 0.5853 | 0.2037 | 0.1982 | 0.304157 | 0.8671 |
| PC 36:6/PE 39:6 | 777.5297 | 24.070581 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1923 | 0.134 | 0.151307 | 0.5192 | -0.0223 | 0.1395 | 0.872732 | 0.9391 | 0.3779 | 0.2173 | 0.082026 | 0.4769 | NaN | 0.1633 | 0.1242 | 0.188328 | 0.7251 | 0.038 | 0.1229 | 0.757454 | 0.9524 | 0.26 | 0.2077 | 0.210691 | 0.9223 | NaN | 0.1756 | 0.1238 | 0.156021 | 0.6683 | 0.0743 | 0.1211 | 0.539304 | 0.9053 | 0.2631 | 0.2093 | 0.208634 | 0.8462 | NaN | 0.1549 | 0.1271 | 0.223061 | 0.7062 | -0.0079 | 0.1277 | 0.950714 | 0.987 | 0.2848 | 0.2097 | 0.174398 | 0.8705 | NaN | 0.1821 | 0.1256 | 0.147048 | 0.6708 | 0.0569 | 0.1235 | 0.644756 | 0.8623 | 0.2943 | 0.2103 | 0.161532 | 0.8292 | NaN | 0.1577 | 0.1274 | 0.215766 | 0.676 | -0.0004 | 0.1258 | 0.997367 | 0.9978 | 0.293 | 0.2117 | 0.166283 | 0.8194 |
| PC 34:7/PE 37:7 | 747.5202 | 24.72982 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.1213 | 0.1335 | 0.36353 | 0.7161 | 0.0406 | 0.1567 | 0.795618 | 0.932 | 0.1812 | 0.2012 | 0.367729 | 0.7534 | NaN | 0.143 | 0.1234 | 0.246319 | 0.7495 | 0.0473 | 0.1375 | 0.731178 | 0.9386 | 0.2015 | 0.1885 | 0.284985 | 0.9223 | NaN | 0.1296 | 0.1232 | 0.293004 | 0.7865 | 0.0452 | 0.135 | 0.737786 | 0.9241 | 0.1721 | 0.19 | 0.364987 | 0.9578 | NaN | 0.1246 | 0.1262 | 0.323443 | 0.741 | 0.0525 | 0.1433 | 0.713948 | 0.8729 | 0.1679 | 0.1913 | 0.380238 | 0.926 | NaN | 0.1483 | 0.125 | 0.235631 | 0.7108 | 0.058 | 0.1378 | 0.673945 | 0.8623 | 0.2034 | 0.1919 | 0.289167 | 0.9039 | NaN | 0.1323 | 0.1265 | 0.295619 | 0.7481 | 0.0371 | 0.1412 | 0.792606 | 0.9226 | 0.1915 | 0.1929 | 0.320806 | 0.8727 |
| PC 37:7/PE 40:7 | 789.5631 | 24.907656 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0775 | 0.1259 | 0.538224 | 0.825 | -0.0209 | 0.1345 | 0.876453 | 0.9409 | -0.0973 | 0.2029 | 0.63156 | 0.9104 | NaN | -0.0609 | 0.1165 | 0.601281 | 0.9079 | -0.0411 | 0.118 | 0.72785 | 0.9386 | -0.0577 | 0.1907 | 0.762169 | 0.954 | NaN | -0.0673 | 0.1162 | 0.562367 | 0.9125 | -0.028 | 0.1158 | 0.808963 | 0.9363 | -0.0999 | 0.1916 | 0.602062 | 0.9894 | NaN | -0.0881 | 0.119 | 0.458777 | 0.7844 | -0.046 | 0.1231 | 0.708485 | 0.8729 | -0.099 | 0.1928 | 0.607627 | 0.9375 | NaN | -0.0601 | 0.118 | 0.610356 | 0.8964 | -0.0266 | 0.1182 | 0.822171 | 0.9396 | -0.0727 | 0.194 | 0.707818 | 0.9621 | NaN | -0.0763 | 0.1192 | 0.522028 | 0.8401 | -0.0419 | 0.1212 | 0.72964 | 0.8984 | -0.0842 | 0.1948 | 0.665711 | 0.9459 |
| PC 41:7/PE 44:7 | 845.6306 | 26.31067 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.0698 | 0.137 | 0.61074 | 0.86 | 0.1129 | 0.133 | 0.395841 | 0.6662 | 0.0249 | 0.2384 | 0.916681 | 0.9838 | NaN | 0.0169 | 0.1271 | 0.894295 | 0.9705 | 0.098 | 0.1168 | 0.401573 | 0.847 | -0.0743 | 0.225 | 0.741297 | 0.954 | NaN | 0.1127 | 0.1266 | 0.373348 | 0.8283 | 0.1749 | 0.1141 | 0.125384 | 0.6704 | 0.0486 | 0.2252 | 0.829146 | 0.9935 | NaN | -0.0197 | 0.1309 | 0.880276 | 0.9749 | 0.0601 | 0.1226 | 0.624015 | 0.8241 | -0.1117 | 0.2299 | 0.626895 | 0.9375 | NaN | -0.0122 | 0.1294 | 0.924973 | 0.9796 | 0.0632 | 0.1176 | 0.590841 | 0.8623 | -0.0914 | 0.2303 | 0.691556 | 0.9621 | NaN | -0.0012 | 0.1308 | 0.992415 | 0.9956 | 0.0757 | 0.1203 | 0.529245 | 0.8003 | -0.0853 | 0.2314 | 0.712347 | 0.9459 |
| PC 43:7/PE 46:7 | 873.657 | 28.227638 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2249 | 0.1255 | 0.073163 | 0.3859 | -0.2314 | 0.1407 | 0.10009 | 0.3816 | -0.1983 | 0.1977 | 0.315868 | 0.7534 | NaN | -0.1185 | 0.1182 | 0.315853 | 0.7898 | -0.1055 | 0.1272 | 0.406807 | 0.847 | -0.1222 | 0.187 | 0.513612 | 0.954 | NaN | -0.1615 | 0.1168 | 0.166476 | 0.6736 | -0.0833 | 0.1255 | 0.50724 | 0.9053 | -0.2339 | 0.1864 | 0.209617 | 0.8462 | NaN | -0.14 | 0.1205 | 0.245501 | 0.7132 | -0.1454 | 0.1314 | 0.26847 | 0.6024 | -0.1178 | 0.19 | 0.535385 | 0.9375 | NaN | -0.1247 | 0.1198 | 0.298213 | 0.7529 | -0.0918 | 0.1282 | 0.474075 | 0.8272 | -0.1375 | 0.1902 | 0.469542 | 0.9359 | NaN | -0.1406 | 0.1208 | 0.244648 | 0.7034 | -0.1255 | 0.1301 | 0.334765 | 0.6758 | -0.1358 | 0.1913 | 0.477825 | 0.8887 |
| PC 40:7/PE 43:7 | 831.5581 | 22.282125 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1625 | 0.1302 | 0.211959 | 0.5792 | -0.0805 | 0.1294 | 0.53384 | 0.7813 | -0.2899 | 0.2249 | 0.197461 | 0.7107 | NaN | -0.1308 | 0.1206 | 0.278357 | 0.7644 | -0.0523 | 0.1138 | 0.645547 | 0.9079 | -0.2605 | 0.2112 | 0.217529 | 0.9223 | NaN | -0.1713 | 0.1201 | 0.153572 | 0.6683 | -0.0389 | 0.1118 | 0.728064 | 0.9241 | -0.3491 | 0.212 | 0.099568 | 0.6246 | NaN | -0.1286 | 0.1234 | 0.297474 | 0.7401 | -0.0797 | 0.1183 | 0.500322 | 0.7567 | -0.2303 | 0.2151 | 0.284242 | 0.8705 | NaN | -0.1342 | 0.1222 | 0.272054 | 0.7442 | -0.0486 | 0.114 | 0.669887 | 0.8623 | -0.2681 | 0.215 | 0.212293 | 0.8887 | NaN | -0.1441 | 0.1235 | 0.242992 | 0.7034 | -0.1023 | 0.1164 | 0.379341 | 0.6983 | -0.24 | 0.2169 | 0.268627 | 0.8424 |
| PC 42:7/PE 45:7 | 859.5929 | 22.454245 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1045 | 0.1351 | 0.438885 | 0.7691 | -0.0339 | 0.1384 | 0.806375 | 0.932 | -0.1618 | 0.2231 | 0.468397 | 0.8207 | NaN | -0.1551 | 0.1249 | 0.214214 | 0.7484 | -0.0546 | 0.1215 | 0.652937 | 0.9079 | -0.2444 | 0.2095 | 0.243402 | 0.9223 | NaN | -0.1546 | 0.1247 | 0.214978 | 0.7361 | 0.0056 | 0.1195 | 0.962528 | 0.9785 | -0.3104 | 0.2126 | 0.144375 | 0.7483 | NaN | -0.1979 | 0.1284 | 0.123387 | 0.579 | -0.1175 | 0.1275 | 0.356612 | 0.6762 | -0.2629 | 0.213 | 0.217079 | 0.8705 | NaN | -0.1299 | 0.1265 | 0.304414 | 0.7529 | -0.0304 | 0.1217 | 0.802537 | 0.9326 | -0.2138 | 0.2131 | 0.315806 | 0.9106 | NaN | -0.1863 | 0.1285 | 0.147188 | 0.6155 | -0.1234 | 0.1255 | 0.325229 | 0.6724 | -0.2348 | 0.2147 | 0.27411 | 0.8424 |
| PC 38:8/PE 41:8 | 801.5294 | 24.024508 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.0142 | 0.1289 | 0.912558 | 0.9809 | -0.0307 | 0.1292 | 0.812516 | 0.932 | 0.0339 | 0.2197 | 0.877307 | 0.9774 | NaN | -0.029 | 0.1193 | 0.808151 | 0.9614 | -0.0545 | 0.1134 | 0.630696 | 0.9073 | 0.0292 | 0.206 | 0.887396 | 0.977 | NaN | -0.0333 | 0.1191 | 0.779559 | 0.9641 | 0.0034 | 0.1115 | 0.975754 | 0.9847 | -0.0615 | 0.209 | 0.768751 | 0.9935 | NaN | -0.0553 | 0.1221 | 0.650522 | 0.8653 | -0.0913 | 0.1187 | 0.44187 | 0.7319 | 0.026 | 0.2088 | 0.900948 | 0.99 | NaN | -0.0412 | 0.1209 | 0.733248 | 0.9262 | -0.0506 | 0.1136 | 0.656036 | 0.8623 | -0.0033 | 0.2101 | 0.987325 | 0.9969 | NaN | -0.0326 | 0.1222 | 0.789356 | 0.9452 | -0.0702 | 0.1165 | 0.54697 | 0.8009 | 0.0429 | 0.2108 | 0.838615 | 0.9641 |
| PC 39:8/PE 42:8 | 815.5796 | 25.336128 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1403 | 0.1413 | 0.320717 | 0.6835 | -0.191 | 0.1501 | 0.203031 | 0.5003 | -0.0621 | 0.23 | 0.78722 | 0.9647 | NaN | -0.0325 | 0.1323 | 0.80564 | 0.9605 | -0.0632 | 0.1349 | 0.639361 | 0.9073 | 0.0112 | 0.2166 | 0.958789 | 0.9911 | NaN | -0.0395 | 0.1319 | 0.764304 | 0.96 | -0.0255 | 0.1337 | 0.848688 | 0.95 | -0.0539 | 0.2172 | 0.803921 | 0.9935 | NaN | -0.048 | 0.1352 | 0.722503 | 0.9 | -0.0739 | 0.1411 | 0.60059 | 0.8188 | 0.0048 | 0.2196 | 0.982553 | 0.9923 | NaN | -0.0515 | 0.1337 | 0.699972 | 0.9116 | -0.0857 | 0.1344 | 0.523769 | 0.8496 | 0 | 0.2205 | 0.999937 | 0.9999 | NaN | -0.0515 | 0.1354 | 0.703633 | 0.9035 | -0.077 | 0.1384 | 0.57772 | 0.8092 | 0.0024 | 0.2218 | 0.991522 | 0.9991 |
| PC 40:8/PE 43:8 | 829.5607 | 24.46232 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.1369 | 0.1415 | 0.333248 | 0.6942 | -0.2707 | 0.1444 | 0.06089 | 0.3144 | -0.0058 | 0.2328 | 0.980219 | 0.9935 | NaN | -0.1759 | 0.1307 | 0.178254 | 0.7251 | -0.3565 | 0.1248 | 0.004273 | 0.1179 | -0.012 | 0.2184 | 0.956347 | 0.9911 | NaN | -0.1274 | 0.1306 | 0.329317 | 0.8017 | -0.2722 | 0.1236 | 0.027662 | 0.3319 | -0.0079 | 0.2198 | 0.971416 | 0.9976 | NaN | -0.212 | 0.134 | 0.113793 | 0.5709 | -0.3722 | 0.1308 | 0.004446 | 0.0792 | -0.0679 | 0.222 | 0.759595 | 0.9586 | NaN | -0.1671 | 0.1325 | 0.207187 | 0.6855 | -0.3353 | 0.1253 | 0.007443 | 0.1424 | -0.0185 | 0.2223 | 0.93364 | 0.9803 | NaN | -0.2125 | 0.1344 | 0.113747 | 0.5578 | -0.3672 | 0.1285 | 0.00427 | 0.0793 | -0.0765 | 0.2245 | 0.733424 | 0.9459 |
| PC 41:8/PE 44:8 | 843.6115 | 25.703169 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.2173 | 0.1322 | 0.100301 | 0.4611 | -0.2871 | 0.1489 | 0.053926 | 0.3037 | -0.1313 | 0.2098 | 0.531304 | 0.8655 | NaN | -0.1463 | 0.1233 | 0.23542 | 0.7495 | -0.1648 | 0.1343 | 0.219831 | 0.7408 | -0.0989 | 0.1971 | 0.615645 | 0.954 | NaN | -0.1441 | 0.1232 | 0.242022 | 0.7381 | -0.1773 | 0.131 | 0.176045 | 0.7308 | -0.1084 | 0.1983 | 0.584722 | 0.9894 | NaN | -0.167 | 0.1257 | 0.184055 | 0.6616 | -0.1948 | 0.1393 | 0.161921 | 0.5021 | -0.095 | 0.1999 | 0.634399 | 0.9375 | NaN | -0.1563 | 0.1248 | 0.210577 | 0.6855 | -0.1454 | 0.1357 | 0.283852 | 0.7544 | -0.1265 | 0.2003 | 0.527784 | 0.9583 | NaN | -0.1655 | 0.1261 | 0.189359 | 0.6463 | -0.1694 | 0.1382 | 0.220554 | 0.5853 | -0.1131 | 0.2015 | 0.574565 | 0.9205 |
| PC 43:8/PE 46:8 | 871.6412 | 26.845314 | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.229 | 0.1216 | 0.059732 | 0.3473 | -0.2437 | 0.1286 | 0.058044 | 0.3054 | -0.1997 | 0.1965 | 0.309644 | 0.7534 | NaN | -0.1378 | 0.1142 | 0.227396 | 0.7495 | -0.1712 | 0.1145 | 0.134674 | 0.6175 | -0.101 | 0.1868 | 0.588831 | 0.954 | NaN | -0.1436 | 0.1138 | 0.2068 | 0.7361 | -0.1822 | 0.1118 | 0.10315 | 0.6422 | -0.116 | 0.1876 | 0.536455 | 0.9894 | NaN | -0.1589 | 0.1164 | 0.172123 | 0.6514 | -0.1733 | 0.1197 | 0.147716 | 0.4863 | -0.1331 | 0.1883 | 0.479727 | 0.9375 | NaN | -0.1472 | 0.1156 | 0.202938 | 0.6855 | -0.1487 | 0.1157 | 0.198721 | 0.6758 | -0.1379 | 0.1891 | 0.465866 | 0.9359 | NaN | -0.1646 | 0.1165 | 0.157562 | 0.6278 | -0.1644 | 0.1181 | 0.163905 | 0.5418 | -0.1526 | 0.1896 | 0.42071 | 0.8887 |
| PE 36:2 | 620.5388 | 26.788805 | Lipid | Phosphatidylethanolamine | 0.259 | 0.1351 | 0.055227 | 0.3387 | -0.0529 | 0.1444 | 0.714241 | 0.8876 | 0.5248 | 0.2134 | 0.013901 | 0.1992 | NaN | 0.0974 | 0.1292 | 0.45115 | 0.8498 | -0.1353 | 0.127 | 0.286656 | 0.7996 | 0.3048 | 0.2148 | 0.155975 | 0.879 | NaN | 0.1445 | 0.1271 | 0.255432 | 0.75 | -0.0734 | 0.1243 | 0.55505 | 0.9053 | 0.3412 | 0.2132 | 0.109541 | 0.6502 | NaN | 0.1095 | 0.1328 | 0.409555 | 0.7796 | -0.1716 | 0.1336 | 0.199121 | 0.5448 | 0.3517 | 0.2148 | 0.101579 | 0.7577 | NaN | 0.1356 | 0.1297 | 0.296052 | 0.7529 | -0.1123 | 0.127 | 0.376785 | 0.7999 | 0.3667 | 0.2148 | 0.087764 | 0.6316 | NaN | 0.1243 | 0.1323 | 0.347653 | 0.7531 | -0.1673 | 0.1311 | 0.202127 | 0.5756 | 0.3813 | 0.2152 | 0.076386 | 0.6024 |
| PS 39.0 | 833.6163 | 25.583288 | Lipid | Phosphatidylserines | 0.1871 | 0.134 | 0.162592 | 0.531 | -0.1198 | 0.1485 | 0.419867 | 0.6877 | 0.3964 | 0.2072 | 0.055751 | 0.4103 | NaN | 0.1877 | 0.1238 | 0.12932 | 0.6772 | -0.0433 | 0.1315 | 0.741751 | 0.9456 | 0.3241 | 0.1961 | 0.098488 | 0.7567 | NaN | 0.2043 | 0.1235 | 0.098029 | 0.55 | 0.0062 | 0.1303 | 0.962067 | 0.9785 | 0.3274 | 0.1975 | 0.097316 | 0.6246 | NaN | 0.1489 | 0.1271 | 0.241251 | 0.7084 | -0.1071 | 0.1359 | 0.430665 | 0.723 | 0.3004 | 0.2005 | 0.134109 | 0.8047 | NaN | 0.1667 | 0.1256 | 0.184496 | 0.6753 | -0.0764 | 0.1311 | 0.560014 | 0.8618 | 0.3264 | 0.2001 | 0.102804 | 0.6756 | NaN | 0.168 | 0.127 | 0.185979 | 0.6463 | -0.0896 | 0.1341 | 0.503896 | 0.7835 | 0.3304 | 0.201 | 0.1002 | 0.6914 |
| PS 40:3 | 841.5442 | 22.668882 | Lipid | Phosphatidylserines | -0.0275 | 0.1405 | 0.84481 | 0.9778 | -0.124 | 0.1306 | 0.342681 | 0.6305 | 0.1091 | 0.2569 | 0.671012 | 0.9306 | NaN | -0.0328 | 0.13 | 0.801017 | 0.9571 | -0.147 | 0.1143 | 0.198372 | 0.7225 | 0.1352 | 0.2409 | 0.574743 | 0.954 | NaN | -0.0402 | 0.1298 | 0.75694 | 0.96 | -0.1193 | 0.1124 | 0.288738 | 0.8258 | 0.0702 | 0.2429 | 0.772737 | 0.9935 | NaN | -0.0973 | 0.1334 | 0.465871 | 0.7864 | -0.2239 | 0.1199 | 0.061758 | 0.3443 | 0.0902 | 0.2443 | 0.711844 | 0.9477 | NaN | -0.0612 | 0.1318 | 0.642446 | 0.9001 | -0.1767 | 0.1144 | 0.122503 | 0.588 | 0.1012 | 0.2453 | 0.679935 | 0.9621 | NaN | -0.0645 | 0.1333 | 0.628507 | 0.8817 | -0.201 | 0.1175 | 0.087187 | 0.4044 | 0.1287 | 0.2465 | 0.601733 | 0.9357 |
| PS 41:3 | 855.5623 | 24.634058 | Lipid | Phosphatidylserines | -0.1501 | 0.1248 | 0.229199 | 0.6042 | -0.1307 | 0.1125 | 0.245453 | 0.538 | -0.1424 | 0.2427 | 0.557591 | 0.8707 | NaN | -0.0628 | 0.1167 | 0.590665 | 0.9079 | -0.0481 | 0.1006 | 0.632717 | 0.9073 | -0.0635 | 0.2289 | 0.781398 | 0.9543 | NaN | -0.0617 | 0.1165 | 0.596279 | 0.9125 | -0.0474 | 0.0986 | 0.630679 | 0.9053 | -0.0786 | 0.2301 | 0.732619 | 0.9927 | NaN | -0.0924 | 0.1188 | 0.436717 | 0.7844 | -0.0536 | 0.1051 | 0.610416 | 0.8188 | -0.1261 | 0.2308 | 0.58486 | 0.9375 | NaN | -0.0921 | 0.1177 | 0.433888 | 0.8472 | -0.0876 | 0.0996 | 0.37925 | 0.8021 | -0.0697 | 0.2332 | 0.764873 | 0.9621 | NaN | -0.0945 | 0.1191 | 0.427208 | 0.795 | -0.0599 | 0.1031 | 0.560751 | 0.8092 | -0.1127 | 0.2333 | 0.629051 | 0.9459 |
| PS 42:3 | 869.6301 | 25.986755 | Lipid | Phosphatidylserines | -0.0597 | 0.129 | 0.643752 | 0.8731 | -0.1055 | 0.1277 | 0.408735 | 0.6755 | 0.0375 | 0.2249 | 0.867707 | 0.9735 | NaN | -0.0364 | 0.1194 | 0.760755 | 0.9512 | -0.0803 | 0.1123 | 0.474447 | 0.8671 | 0.0461 | 0.2109 | 0.82679 | 0.9669 | NaN | -0.0515 | 0.1192 | 0.665306 | 0.935 | -0.0908 | 0.1101 | 0.409585 | 0.8818 | -0.0011 | 0.2126 | 0.995794 | 0.9976 | NaN | -0.0588 | 0.122 | 0.629526 | 0.8606 | -0.1024 | 0.1168 | 0.380619 | 0.6816 | 0.0391 | 0.2137 | 0.854712 | 0.9772 | NaN | -0.0288 | 0.1211 | 0.812297 | 0.952 | -0.0486 | 0.1131 | 0.667725 | 0.8623 | 0.0288 | 0.2147 | 0.893303 | 0.9681 | NaN | -0.0508 | 0.1223 | 0.677549 | 0.9035 | -0.0878 | 0.1152 | 0.445854 | 0.7458 | 0.0354 | 0.2158 | 0.869608 | 0.9662 |
| PS 42:3 | 869.633 | 26.532726 | Lipid | Phosphatidylserines | -0.2891 | 0.1273 | 0.023139 | 0.2027 | -0.3626 | 0.1409 | 0.010052 | 0.1685 | -0.2446 | 0.1962 | 0.212539 | 0.7154 | NaN | -0.1729 | 0.1204 | 0.151037 | 0.6956 | -0.2331 | 0.1284 | 0.069383 | 0.4801 | -0.1401 | 0.187 | 0.453705 | 0.9478 | NaN | -0.1967 | 0.1193 | 0.099304 | 0.55 | -0.2064 | 0.1272 | 0.104629 | 0.6422 | -0.1979 | 0.1861 | 0.287539 | 0.9294 | NaN | -0.1901 | 0.1231 | 0.122421 | 0.579 | -0.274 | 0.1322 | 0.0382 | 0.2571 | -0.1342 | 0.1905 | 0.481296 | 0.9375 | NaN | -0.1937 | 0.1215 | 0.111056 | 0.6708 | -0.24 | 0.1282 | 0.061289 | 0.4149 | -0.1689 | 0.1896 | 0.373042 | 0.9106 | NaN | -0.1999 | 0.1229 | 0.103885 | 0.5529 | -0.2622 | 0.1305 | 0.044599 | 0.283 | -0.1624 | 0.1911 | 0.395369 | 0.8887 |
| PS 44:3 | 897.665 | 27.227468 | Lipid | Phosphatidylserines | -0.3056 | 0.1257 | 0.015039 | 0.1566 | -0.1861 | 0.1357 | 0.170393 | 0.4873 | -0.3811 | 0.2022 | 0.059412 | 0.4259 | NaN | -0.2651 | 0.1167 | 0.023044 | 0.3029 | -0.1854 | 0.1188 | 0.118561 | 0.6118 | -0.3197 | 0.1909 | 0.094022 | 0.7567 | NaN | -0.2489 | 0.1169 | 0.03315 | 0.2852 | -0.1792 | 0.1166 | 0.124559 | 0.6704 | -0.314 | 0.1926 | 0.103057 | 0.6251 | NaN | -0.2648 | 0.1194 | 0.026627 | 0.3062 | -0.1749 | 0.1241 | 0.158794 | 0.5021 | -0.3187 | 0.1938 | 0.100158 | 0.7574 | NaN | -0.2536 | 0.1186 | 0.032482 | 0.332 | -0.1265 | 0.1204 | 0.293267 | 0.7544 | -0.3476 | 0.1936 | 0.072531 | 0.6055 | NaN | -0.2722 | 0.1195 | 0.022753 | 0.2617 | -0.1694 | 0.1223 | 0.166156 | 0.5427 | -0.343 | 0.1948 | 0.078276 | 0.6086 |
| PS 35:4 | 769.496 | 24.213146 | Lipid | Phosphatidylserines | 0.3132 | 0.1316 | 0.017305 | 0.1685 | 0.2047 | 0.1325 | 0.122412 | 0.412 | 0.4024 | 0.2219 | 0.069749 | 0.4554 | NaN | 0.175 | 0.1253 | 0.162654 | 0.7211 | 0.0018 | 0.1244 | 0.988191 | 0.9953 | 0.331 | 0.2098 | 0.114608 | 0.7908 | NaN | 0.2506 | 0.1224 | 0.040648 | 0.316 | 0.1344 | 0.1154 | 0.24415 | 0.8037 | 0.3557 | 0.2104 | 0.090861 | 0.6117 | NaN | 0.1873 | 0.1285 | 0.145012 | 0.6151 | 0.0261 | 0.1305 | 0.84131 | 0.9382 | 0.3213 | 0.2134 | 0.132197 | 0.8047 | NaN | 0.185 | 0.127 | 0.145385 | 0.6708 | 0.0046 | 0.1245 | 0.970212 | 0.9923 | 0.3338 | 0.2139 | 0.11857 | 0.7438 | NaN | 0.1822 | 0.1293 | 0.158795 | 0.6278 | 0.0082 | 0.1288 | 0.949506 | 0.9834 | 0.3176 | 0.2161 | 0.141657 | 0.7588 |
| PS 38:4 | 811.5485 | 24.525646 | Lipid | Phosphatidylserines | -0.0608 | 0.1418 | 0.668067 | 0.8886 | -0.2189 | 0.1618 | 0.176102 | 0.4964 | 0.0283 | 0.2155 | 0.89539 | 0.9826 | NaN | 0.0302 | 0.132 | 0.81891 | 0.9614 | -0.0573 | 0.1466 | 0.695884 | 0.9323 | 0.0596 | 0.2022 | 0.768351 | 0.954 | NaN | -0.0148 | 0.1312 | 0.910451 | 0.9717 | -0.1018 | 0.1419 | 0.472818 | 0.9031 | 0.023 | 0.2035 | 0.910205 | 0.9935 | NaN | 0.018 | 0.135 | 0.8937 | 0.9771 | -0.0789 | 0.153 | 0.606315 | 0.8188 | 0.0504 | 0.2049 | 0.805859 | 0.9662 | NaN | 0.0246 | 0.1339 | 0.853984 | 0.962 | -0.0698 | 0.1464 | 0.63365 | 0.8623 | 0.0678 | 0.2061 | 0.742065 | 0.9621 | NaN | 0.0103 | 0.1352 | 0.939078 | 0.9794 | -0.0857 | 0.1498 | 0.567179 | 0.8092 | 0.0509 | 0.2069 | 0.805657 | 0.9623 |
| PS 39:4 | 825.5579 | 25.606718 | Lipid | Phosphatidylserines | 0.073 | 0.1341 | 0.585966 | 0.8423 | -0.0253 | 0.139 | 0.855475 | 0.932 | 0.1614 | 0.2233 | 0.469824 | 0.8207 | NaN | 0.1015 | 0.124 | 0.412917 | 0.8498 | -0.0073 | 0.1221 | 0.952232 | 0.9836 | 0.18 | 0.2093 | 0.389886 | 0.9389 | NaN | 0.0755 | 0.1238 | 0.542045 | 0.9125 | 0.0786 | 0.1208 | 0.515353 | 0.9053 | 0.0461 | 0.2138 | 0.829165 | 0.9935 | NaN | 0.0767 | 0.1267 | 0.545028 | 0.8404 | -0.0669 | 0.1273 | 0.599141 | 0.8188 | 0.1915 | 0.2122 | 0.366716 | 0.9223 | NaN | 0.0611 | 0.1257 | 0.626775 | 0.8971 | -0.0543 | 0.1222 | 0.656776 | 0.8623 | 0.1477 | 0.2133 | 0.488724 | 0.9403 | NaN | 0.0837 | 0.127 | 0.510001 | 0.8285 | -0.0698 | 0.1254 | 0.577641 | 0.8092 | 0.2046 | 0.2144 | 0.339963 | 0.8785 |
| PS 40:4 | 839.5813 | 25.223974 | Lipid | Phosphatidylserines | -0.2084 | 0.1427 | 0.144015 | 0.516 | -0.3197 | 0.1327 | 0.015938 | 0.2 | -0.0398 | 0.2599 | 0.878204 | 0.9774 | NaN | -0.066 | 0.1349 | 0.624865 | 0.9079 | -0.1593 | 0.1234 | 0.19667 | 0.7225 | 0.0351 | 0.2445 | 0.885881 | 0.977 | NaN | -0.0721 | 0.1344 | 0.591856 | 0.9125 | -0.1077 | 0.1241 | 0.385611 | 0.8818 | -0.0579 | 0.2454 | 0.813477 | 0.9935 | NaN | -0.0836 | 0.138 | 0.544423 | 0.8404 | -0.2048 | 0.1268 | 0.106267 | 0.4378 | 0.0773 | 0.2493 | 0.756585 | 0.9586 | NaN | -0.1018 | 0.1358 | 0.453465 | 0.8543 | -0.2091 | 0.1204 | 0.082292 | 0.4705 | 0.0406 | 0.2494 | 0.870677 | 0.9621 | NaN | -0.0949 | 0.1379 | 0.491256 | 0.8278 | -0.2019 | 0.1244 | 0.104671 | 0.4566 | 0.0522 | 0.2512 | 0.835468 | 0.9641 |
| PS 35:5 | 767.4737 | 23.664724 | Lipid | Phosphatidylserines | 0.202 | 0.1309 | 0.122776 | 0.4911 | 0.0284 | 0.1286 | 0.825413 | 0.932 | 0.4237 | 0.2305 | 0.066077 | 0.4448 | NaN | 0.1918 | 0.121 | 0.112895 | 0.6749 | -0.0114 | 0.1131 | 0.919466 | 0.9729 | 0.4256 | 0.2157 | 0.048491 | 0.5871 | NaN | 0.1834 | 0.1209 | 0.129226 | 0.6333 | -0.024 | 0.1112 | 0.828814 | 0.9453 | 0.4085 | 0.2176 | 0.060419 | 0.4905 | NaN | 0.2203 | 0.1235 | 0.07452 | 0.4957 | 0.0141 | 0.1177 | 0.904408 | 0.9695 | 0.4618 | 0.2183 | 0.034406 | 0.5133 | NaN | 0.2166 | 0.1224 | 0.07691 | 0.5579 | 0.017 | 0.1131 | 0.880858 | 0.9705 | 0.4461 | 0.2195 | 0.042073 | 0.4772 | NaN | 0.2081 | 0.1239 | 0.092962 | 0.5459 | -0.0042 | 0.1161 | 0.971246 | 0.9946 | 0.4522 | 0.2206 | 0.040331 | 0.4663 |
| PS 37:5 | 795.5063 | 24.099264 | Lipid | Phosphatidylserines | 0.1586 | 0.1334 | 0.234414 | 0.6073 | 0.0838 | 0.1387 | 0.545661 | 0.7885 | 0.2395 | 0.2207 | 0.277794 | 0.748 | NaN | 0.1261 | 0.1236 | 0.307346 | 0.7898 | 0.0217 | 0.1225 | 0.85937 | 0.9729 | 0.2171 | 0.2071 | 0.294504 | 0.9223 | NaN | 0.1773 | 0.123 | 0.149511 | 0.6683 | 0.0986 | 0.1193 | 0.408591 | 0.8818 | 0.2343 | 0.2083 | 0.2607 | 0.9 | NaN | 0.1442 | 0.1262 | 0.252936 | 0.714 | 0.0288 | 0.1277 | 0.821518 | 0.9271 | 0.25 | 0.2096 | 0.232856 | 0.8705 | NaN | 0.1317 | 0.1252 | 0.292621 | 0.7524 | 0.0106 | 0.123 | 0.93163 | 0.9852 | 0.2361 | 0.2106 | 0.262301 | 0.9039 | NaN | 0.1286 | 0.1266 | 0.309996 | 0.7485 | 0.0022 | 0.1264 | 0.985976 | 0.9968 | 0.2374 | 0.2117 | 0.262026 | 0.8424 |
| PS 39:5 | 823.5315 | 24.665892 | Lipid | Phosphatidylserines | -0.2177 | 0.1328 | 0.101069 | 0.4611 | 0.0356 | 0.1517 | 0.814492 | 0.932 | -0.3638 | 0.2032 | 0.073403 | 0.4604 | NaN | -0.0979 | 0.1252 | 0.434121 | 0.8498 | 0.2159 | 0.1353 | 0.110464 | 0.6118 | -0.2713 | 0.1933 | 0.160439 | 0.879 | NaN | -0.1252 | 0.1241 | 0.313201 | 0.7952 | 0.121 | 0.131 | 0.355522 | 0.8722 | -0.2685 | 0.195 | 0.168599 | 0.7756 | NaN | -0.1236 | 0.1276 | 0.332947 | 0.741 | 0.1841 | 0.1414 | 0.192939 | 0.5441 | -0.284 | 0.1957 | 0.146796 | 0.828 | NaN | -0.1307 | 0.126 | 0.29967 | 0.7529 | 0.188 | 0.135 | 0.16355 | 0.631 | -0.3078 | 0.1955 | 0.115337 | 0.7318 | NaN | -0.1307 | 0.1277 | 0.30617 | 0.7481 | 0.2014 | 0.1393 | 0.148243 | 0.5211 | -0.3062 | 0.1967 | 0.119527 | 0.7513 |
| PS 41:5 | 851.5624 | 25.434872 | Lipid | Phosphatidylserines | -0.118 | 0.1377 | 0.391698 | 0.726 | -0.0754 | 0.1557 | 0.627896 | 0.8332 | -0.1133 | 0.2139 | 0.596332 | 0.8909 | NaN | -0.0946 | 0.1275 | 0.457941 | 0.8498 | -0.0318 | 0.137 | 0.81637 | 0.965 | -0.1144 | 0.2006 | 0.568476 | 0.954 | NaN | -0.054 | 0.1278 | 0.672686 | 0.9401 | 0.0879 | 0.1369 | 0.520921 | 0.9053 | -0.1422 | 0.202 | 0.481361 | 0.9848 | NaN | -0.1187 | 0.1302 | 0.36163 | 0.7539 | -0.1042 | 0.1423 | 0.464113 | 0.7319 | -0.0885 | 0.2036 | 0.66376 | 0.9395 | NaN | -0.0932 | 0.1292 | 0.47068 | 0.8625 | -0.0799 | 0.1368 | 0.559077 | 0.8618 | -0.0776 | 0.2047 | 0.704624 | 0.9621 | NaN | -0.0896 | 0.1307 | 0.493013 | 0.8278 | -0.0852 | 0.1401 | 0.543203 | 0.8009 | -0.0575 | 0.2063 | 0.780457 | 0.9525 |
| PS 37:6 | 793.4957 | 24.084814 | Lipid | Phosphatidylserines | 0.1616 | 0.1398 | 0.247514 | 0.6174 | -0.1888 | 0.1483 | 0.203009 | 0.5003 | 0.453 | 0.2201 | 0.039549 | 0.3491 | NaN | 0.1354 | 0.1294 | 0.29539 | 0.7802 | -0.2054 | 0.1296 | 0.113016 | 0.6118 | 0.4137 | 0.2069 | 0.045537 | 0.5871 | NaN | 0.1894 | 0.1289 | 0.14157 | 0.6585 | -0.0269 | 0.132 | 0.838499 | 0.9485 | 0.3598 | 0.2108 | 0.087893 | 0.6065 | NaN | 0.0987 | 0.133 | 0.457984 | 0.7844 | -0.2991 | 0.1354 | 0.027221 | 0.2147 | 0.4261 | 0.2094 | 0.041885 | 0.5138 | NaN | 0.1269 | 0.1312 | 0.333426 | 0.7669 | -0.2443 | 0.1295 | 0.059295 | 0.4149 | 0.4292 | 0.2103 | 0.041261 | 0.4772 | NaN | 0.1079 | 0.1331 | 0.417555 | 0.7921 | -0.3032 | 0.1331 | 0.022712 | 0.1982 | 0.4395 | 0.2111 | 0.037379 | 0.4663 |
| PS 39:6 | 821.5289 | 24.635998 | Lipid | Phosphatidylserines | -0.0692 | 0.1416 | 0.625062 | 0.8678 | 0.081 | 0.1613 | 0.615756 | 0.8251 | -0.2088 | 0.2197 | 0.34191 | 0.7534 | NaN | 0.0274 | 0.1321 | 0.835795 | 0.9673 | 0.206 | 0.142 | 0.146948 | 0.6288 | -0.1057 | 0.2085 | 0.612125 | 0.954 | NaN | 0.0285 | 0.1319 | 0.828834 | 0.9714 | 0.1691 | 0.1389 | 0.223414 | 0.8003 | -0.0572 | 0.2128 | 0.78808 | 0.9935 | NaN | 0.0105 | 0.1349 | 0.938192 | 0.9828 | 0.1964 | 0.1486 | 0.186287 | 0.5328 | -0.137 | 0.2105 | 0.514956 | 0.9375 | NaN | 0.0292 | 0.134 | 0.827743 | 0.9564 | 0.1598 | 0.1419 | 0.259941 | 0.7339 | -0.0774 | 0.2148 | 0.718645 | 0.9621 | NaN | -0.0085 | 0.1348 | 0.949472 | 0.9794 | 0.185 | 0.1459 | 0.204712 | 0.5756 | -0.1588 | 0.2119 | 0.453424 | 0.8887 |
| PS 41:6 | 849.5462 | 24.797037 | Lipid | Phosphatidylserines | -0.1876 | 0.1332 | 0.158968 | 0.5264 | 0.084 | 0.136 | 0.536944 | 0.7813 | -0.451 | 0.2193 | 0.039764 | 0.3491 | NaN | -0.1717 | 0.1232 | 0.163289 | 0.7211 | 0.0948 | 0.1192 | 0.426346 | 0.847 | -0.4164 | 0.206 | 0.043294 | 0.5871 | NaN | -0.1704 | 0.123 | 0.165869 | 0.6736 | 0.0434 | 0.1175 | 0.7121 | 0.9206 | -0.3624 | 0.2099 | 0.084234 | 0.5886 | NaN | -0.2041 | 0.1257 | 0.104556 | 0.5709 | 0.0797 | 0.1244 | 0.521385 | 0.7695 | -0.4692 | 0.2078 | 0.023908 | 0.4551 | NaN | -0.1674 | 0.1249 | 0.18003 | 0.6753 | 0.0835 | 0.1195 | 0.484684 | 0.8301 | -0.402 | 0.2106 | 0.056198 | 0.5267 | NaN | -0.2127 | 0.126 | 0.091414 | 0.5459 | 0.0808 | 0.1225 | 0.509657 | 0.786 | -0.4878 | 0.2097 | 0.020004 | 0.4132 |
| PS 42:6 | 863.5603 | 25.18495 | Lipid | Phosphatidylserines | -0.1929 | 0.1347 | 0.152044 | 0.5192 | -0.2208 | 0.1515 | 0.144962 | 0.4547 | -0.1701 | 0.2078 | 0.413021 | 0.7762 | NaN | -0.0281 | 0.1285 | 0.826571 | 0.9667 | -0.0728 | 0.1373 | 0.596122 | 0.904 | 0.0002 | 0.2007 | 0.999086 | 0.9999 | NaN | -0.0403 | 0.1277 | 0.752572 | 0.96 | -0.0432 | 0.1357 | 0.750159 | 0.9243 | -0.0481 | 0.1998 | 0.809758 | 0.9935 | NaN | -0.0719 | 0.1304 | 0.581311 | 0.8473 | -0.1078 | 0.1423 | 0.448783 | 0.7319 | -0.0456 | 0.2016 | 0.821194 | 0.97 | NaN | -0.0484 | 0.1299 | 0.709318 | 0.9131 | -0.0633 | 0.1381 | 0.646696 | 0.8623 | -0.0425 | 0.2031 | 0.834383 | 0.9621 | NaN | -0.0849 | 0.1302 | 0.514335 | 0.8326 | -0.0831 | 0.1411 | 0.55572 | 0.8092 | -0.0878 | 0.2017 | 0.66349 | 0.9459 |
| PS 46:6 | 919.6415 | 26.437166 | Lipid | Phosphatidylserines | -0.0801 | 0.1372 | 0.559417 | 0.8323 | -0.2596 | 0.1585 | 0.101381 | 0.3816 | 0.0514 | 0.2077 | 0.804721 | 0.9678 | NaN | -0.0707 | 0.1269 | 0.577651 | 0.9079 | -0.1787 | 0.1407 | 0.20417 | 0.7304 | 0.0035 | 0.1953 | 0.985595 | 0.9964 | NaN | -0.1321 | 0.1268 | 0.297453 | 0.7865 | -0.2095 | 0.137 | 0.126306 | 0.6704 | -0.089 | 0.1998 | 0.656047 | 0.9894 | NaN | -0.0706 | 0.1297 | 0.586341 | 0.8473 | -0.2157 | 0.1457 | 0.138681 | 0.4784 | 0.0391 | 0.1975 | 0.843041 | 0.9736 | NaN | -0.0818 | 0.1285 | 0.524721 | 0.8625 | -0.1808 | 0.1409 | 0.199559 | 0.6758 | -0.0046 | 0.1992 | 0.98163 | 0.9969 | NaN | -0.0561 | 0.1301 | 0.666349 | 0.9035 | -0.2039 | 0.1438 | 0.156136 | 0.5288 | 0.0569 | 0.1993 | 0.775371 | 0.9525 |
| PS 38:7 | 805.502 | 23.481342 | Lipid | Phosphatidylserines | 0.1722 | 0.1248 | 0.16775 | 0.531 | -0.0455 | 0.1526 | 0.765579 | 0.9167 | 0.2909 | 0.1826 | 0.111142 | 0.5628 | NaN | 0.1003 | 0.1164 | 0.388664 | 0.8498 | -0.0632 | 0.1339 | 0.636716 | 0.9073 | 0.1782 | 0.1752 | 0.309166 | 0.9223 | NaN | 0.1791 | 0.1151 | 0.119665 | 0.6049 | 0.0605 | 0.1326 | 0.648045 | 0.9053 | 0.2342 | 0.1737 | 0.177759 | 0.8109 | NaN | 0.0888 | 0.1197 | 0.457876 | 0.7844 | -0.1336 | 0.1404 | 0.341262 | 0.67 | 0.1976 | 0.177 | 0.264352 | 0.8705 | NaN | 0.1254 | 0.1175 | 0.285979 | 0.7504 | 0.0041 | 0.1346 | 0.975907 | 0.9923 | 0.1929 | 0.1785 | 0.279677 | 0.9039 | NaN | 0.0935 | 0.1198 | 0.434969 | 0.795 | -0.1248 | 0.1379 | 0.365681 | 0.6901 | 0.2045 | 0.1788 | 0.252816 | 0.8424 |
| PS 39:7 | 819.5096 | 24.150833 | Lipid | Phosphatidylserines | -0.0018 | 0.1365 | 0.989356 | 0.9936 | -0.1077 | 0.1537 | 0.48357 | 0.7524 | 0.1119 | 0.2134 | 0.600111 | 0.8909 | NaN | 0.0926 | 0.1271 | 0.466296 | 0.8498 | 0.1404 | 0.1421 | 0.323261 | 0.8095 | 0.0928 | 0.2003 | 0.643091 | 0.954 | NaN | 0.0086 | 0.1261 | 0.945322 | 0.9728 | 0.1183 | 0.1378 | 0.390644 | 0.8818 | -0.0522 | 0.2068 | 0.800868 | 0.9935 | NaN | 0.0495 | 0.1294 | 0.702126 | 0.8872 | 0.0535 | 0.1458 | 0.71371 | 0.8729 | 0.0885 | 0.2031 | 0.662902 | 0.9395 | NaN | 0.0657 | 0.1285 | 0.609109 | 0.8964 | 0.0786 | 0.1398 | 0.573885 | 0.8623 | 0.0999 | 0.2038 | 0.624075 | 0.9621 | NaN | 0.0766 | 0.1302 | 0.55632 | 0.8626 | 0.049 | 0.1427 | 0.731496 | 0.8984 | 0.1472 | 0.2049 | 0.472515 | 0.8887 |
| PS 40:7 | 833.5156 | 24.11669 | Lipid | Phosphatidylserines | -0.1883 | 0.1335 | 0.158418 | 0.5264 | -0.2704 | 0.1336 | 0.042975 | 0.2929 | -0.0737 | 0.2267 | 0.745069 | 0.9647 | NaN | -0.2121 | 0.1232 | 0.085255 | 0.6033 | -0.2673 | 0.1166 | 0.021852 | 0.2566 | -0.133 | 0.2129 | 0.532231 | 0.954 | NaN | -0.1423 | 0.1237 | 0.25009 | 0.7434 | -0.1968 | 0.1165 | 0.091358 | 0.6246 | -0.0812 | 0.214 | 0.704375 | 0.9894 | NaN | -0.2234 | 0.1261 | 0.076331 | 0.4957 | -0.3019 | 0.1211 | 0.012694 | 0.14 | -0.1037 | 0.2156 | 0.630542 | 0.9375 | NaN | -0.1774 | 0.1251 | 0.156177 | 0.6753 | -0.221 | 0.1182 | 0.061594 | 0.4149 | -0.1064 | 0.2166 | 0.623142 | 0.9621 | NaN | -0.2313 | 0.1264 | 0.067236 | 0.4832 | -0.3042 | 0.1191 | 0.010644 | 0.1267 | -0.1224 | 0.2179 | 0.574191 | 0.9205 |
| PS 41:7 | 847.5315 | 24.377514 | Lipid | Phosphatidylserines | -0.1138 | 0.1352 | 0.399952 | 0.7322 | 0.0419 | 0.1384 | 0.761881 | 0.9167 | -0.2636 | 0.2239 | 0.23925 | 0.735 | NaN | -0.1579 | 0.125 | 0.206468 | 0.7401 | -0.0184 | 0.122 | 0.879888 | 0.9729 | -0.2751 | 0.2097 | 0.189599 | 0.9101 | NaN | -0.1475 | 0.1247 | 0.236949 | 0.7361 | -0.039 | 0.12 | 0.745392 | 0.9241 | -0.2349 | 0.2118 | 0.26739 | 0.9 | NaN | -0.142 | 0.1278 | 0.266384 | 0.7279 | 0.0124 | 0.1268 | 0.922292 | 0.9748 | -0.2773 | 0.2126 | 0.192122 | 0.8705 | NaN | -0.1658 | 0.1267 | 0.190829 | 0.6753 | -0.04 | 0.1226 | 0.744535 | 0.9085 | -0.2767 | 0.2136 | 0.195151 | 0.8608 | NaN | -0.1563 | 0.1281 | 0.222467 | 0.686 | 0.015 | 0.1248 | 0.904256 | 0.9732 | -0.3117 | 0.2147 | 0.146556 | 0.7588 |
| PS 42:7 | 861.5447 | 24.69211 | Lipid | Phosphatidylserine | -0.3599 | 0.1354 | 0.007863 | 0.1059 | -0.0662 | 0.1286 | 0.606614 | 0.8207 | -0.7316 | 0.2426 | 0.002561 | 0.1058 | NaN | -0.274 | 0.1269 | 0.030799 | 0.347 | 0.0257 | 0.1143 | 0.822241 | 0.9698 | -0.6586 | 0.2292 | 0.004059 | 0.16 | NaN | -0.2771 | 0.1265 | 0.028571 | 0.2816 | 0.015 | 0.1118 | 0.893003 | 0.973 | -0.6601 | 0.2309 | 0.004252 | 0.1413 | NaN | -0.2826 | 0.1298 | 0.029444 | 0.3194 | 0.0308 | 0.1199 | 0.797268 | 0.9169 | -0.6761 | 0.2318 | 0.003533 | 0.1461 | NaN | -0.2587 | 0.1294 | 0.045582 | 0.4114 | 0.0583 | 0.1155 | 0.613809 | 0.8623 | -0.6556 | 0.2342 | 0.005129 | 0.2022 | NaN | -0.2903 | 0.1298 | 0.025341 | 0.2798 | 0.0224 | 0.1175 | 0.849003 | 0.9487 | -0.6794 | 0.2341 | 0.003709 | 0.1861 |
| PS 39:8 | 817.4908 | 23.6556 | Lipid | Phosphatidylserines | 0.0919 | 0.1334 | 0.490906 | 0.8041 | -0.0439 | 0.1379 | 0.750134 | 0.9087 | 0.217 | 0.2193 | 0.322489 | 0.7534 | NaN | 0.0762 | 0.1235 | 0.536995 | 0.8926 | -0.003 | 0.1213 | 0.980238 | 0.9953 | 0.1292 | 0.2076 | 0.533683 | 0.954 | NaN | 0.1306 | 0.1232 | 0.288986 | 0.7865 | 0.0879 | 0.1206 | 0.466456 | 0.9003 | 0.1557 | 0.2082 | 0.45461 | 0.9816 | NaN | 0.0268 | 0.127 | 0.833122 | 0.9581 | -0.0945 | 0.1263 | 0.454651 | 0.7319 | 0.1211 | 0.2111 | 0.566128 | 0.9375 | NaN | 0.0666 | 0.1252 | 0.59488 | 0.8924 | -0.0049 | 0.1215 | 0.968057 | 0.9923 | 0.1261 | 0.212 | 0.551846 | 0.9621 | NaN | 0.0281 | 0.1273 | 0.825163 | 0.9491 | -0.1038 | 0.1244 | 0.404444 | 0.7211 | 0.1361 | 0.2128 | 0.522466 | 0.8957 |
| 16-bromo-9E-hexadecenoic acid | 332.1376 | 11.983191 | Lipid | Halogenated Fatty Acids | -0.2565 | 0.1306 | 0.049536 | 0.318 | -0.137 | 0.1328 | 0.302243 | 0.5924 | -0.3937 | 0.2183 | 0.071339 | 0.4554 | NaN | -0.1787 | 0.122 | 0.143164 | 0.6828 | -0.028 | 0.119 | 0.813829 | 0.965 | -0.3372 | 0.2058 | 0.101336 | 0.7663 | NaN | -0.2029 | 0.1213 | 0.094248 | 0.5363 | -0.061 | 0.1157 | 0.597937 | 0.9053 | -0.338 | 0.2073 | 0.102948 | 0.6251 | NaN | -0.2013 | 0.1244 | 0.105599 | 0.5709 | -0.0611 | 0.1233 | 0.62031 | 0.8228 | -0.3525 | 0.2082 | 0.090481 | 0.7393 | NaN | -0.1702 | 0.1241 | 0.170283 | 0.6753 | -0.0155 | 0.1198 | 0.89691 | 0.9727 | -0.3266 | 0.2104 | 0.12053 | 0.7476 | NaN | -0.2041 | 0.1246 | 0.10133 | 0.5529 | -0.0706 | 0.121 | 0.559533 | 0.8092 | -0.3439 | 0.2107 | 0.102639 | 0.6941 |
| LysoPA 20.5 | 456.2297 | 14.845019 | Lipid | Lysolipid, PA | 0.2579 | 0.1257 | 0.040159 | 0.288 | 0.3373 | 0.1262 | 0.007524 | 0.1497 | 0.1817 | 0.2079 | 0.382225 | 0.7534 | NaN | 0.1531 | 0.1184 | 0.195915 | 0.7307 | 0.1868 | 0.1176 | 0.112271 | 0.6118 | 0.1372 | 0.1956 | 0.48292 | 0.954 | NaN | 0.0885 | 0.121 | 0.464517 | 0.8953 | 0.1848 | 0.1149 | 0.107772 | 0.6422 | 0.0014 | 0.2036 | 0.994458 | 0.9976 | NaN | 0.2172 | 0.1194 | 0.068777 | 0.4931 | 0.2613 | 0.1182 | 0.027132 | 0.2147 | 0.1861 | 0.1975 | 0.346054 | 0.9127 | NaN | 0.1759 | 0.1194 | 0.14083 | 0.6708 | 0.2137 | 0.1159 | 0.065181 | 0.4198 | 0.1428 | 0.1991 | 0.473318 | 0.9365 | NaN | 0.2181 | 0.1196 | 0.068241 | 0.4832 | 0.2414 | 0.1174 | 0.039823 | 0.2717 | 0.2014 | 0.1994 | 0.312345 | 0.8727 |
| LysoPC 15:0 | 481.3168 | 21.947886 | Lipid | Lysolipid, PC | 0.1417 | 0.1327 | 0.285575 | 0.6651 | 0.0043 | 0.1149 | 0.969843 | 0.987 | 0.4148 | 0.2738 | 0.129707 | 0.6043 | NaN | 0.0362 | 0.1243 | 0.770811 | 0.9527 | -0.06 | 0.1013 | 0.553978 | 0.9009 | 0.2326 | 0.2634 | 0.377224 | 0.9322 | NaN | 0.0947 | 0.1229 | 0.440947 | 0.8792 | 0.0164 | 0.0989 | 0.868558 | 0.9581 | 0.2553 | 0.2643 | 0.334005 | 0.957 | NaN | 0.0525 | 0.1271 | 0.679735 | 0.8746 | -0.063 | 0.106 | 0.552358 | 0.7858 | 0.2842 | 0.2647 | 0.283045 | 0.8705 | NaN | 0.0628 | 0.1255 | 0.616906 | 0.8971 | -0.0457 | 0.1013 | 0.651976 | 0.8623 | 0.2852 | 0.2662 | 0.284065 | 0.9039 | NaN | 0.0692 | 0.1269 | 0.585466 | 0.8765 | -0.053 | 0.104 | 0.610392 | 0.8279 | 0.3134 | 0.2661 | 0.238966 | 0.8424 |
| LysoPC 16:0 | 495.3327 | 22.244642 | Lipid | Lysolipid, PC | 0.1175 | 0.1325 | 0.375174 | 0.7191 | -0.1879 | 0.1356 | 0.165757 | 0.479 | 0.4374 | 0.2172 | 0.044038 | 0.3491 | NaN | 0.06 | 0.1231 | 0.626093 | 0.9079 | -0.1498 | 0.1194 | 0.209798 | 0.7304 | 0.2827 | 0.2105 | 0.179283 | 0.879 | NaN | 0.0852 | 0.1225 | 0.486991 | 0.8991 | -0.1189 | 0.118 | 0.31338 | 0.8421 | 0.2951 | 0.2115 | 0.163006 | 0.7677 | NaN | 0.0269 | 0.1269 | 0.831889 | 0.9581 | -0.2092 | 0.1235 | 0.090369 | 0.4174 | 0.2874 | 0.2144 | 0.180102 | 0.8705 | NaN | 0.0862 | 0.1244 | 0.48811 | 0.8625 | -0.149 | 0.1197 | 0.213294 | 0.6963 | 0.3444 | 0.211 | 0.1026 | 0.6756 | NaN | 0.049 | 0.1265 | 0.698843 | 0.9035 | -0.1942 | 0.1218 | 0.110826 | 0.4635 | 0.3221 | 0.2144 | 0.132919 | 0.7588 |
| LysoPC 18:0 | 523.3636 | 22.659883 | Lipid | Lysolipid, PC | 0.169 | 0.1348 | 0.209863 | 0.5792 | -0.0993 | 0.1422 | 0.48501 | 0.7524 | 0.4404 | 0.2176 | 0.043026 | 0.3491 | NaN | 0.1007 | 0.1255 | 0.422244 | 0.8498 | -0.12 | 0.1245 | 0.335398 | 0.8095 | 0.3249 | 0.2081 | 0.11855 | 0.8079 | NaN | 0.1074 | 0.1252 | 0.3907 | 0.8424 | -0.064 | 0.1227 | 0.602285 | 0.9053 | 0.2796 | 0.2135 | 0.190498 | 0.8412 | NaN | 0.0545 | 0.1301 | 0.675385 | 0.8746 | -0.2078 | 0.1308 | 0.112252 | 0.4439 | 0.3229 | 0.2119 | 0.127594 | 0.8047 | NaN | 0.1413 | 0.1265 | 0.263947 | 0.7442 | -0.0717 | 0.1252 | 0.566978 | 0.8623 | 0.3654 | 0.2103 | 0.08227 | 0.6055 | NaN | 0.0979 | 0.1289 | 0.447433 | 0.801 | -0.1745 | 0.1281 | 0.173068 | 0.5537 | 0.3745 | 0.211 | 0.075908 | 0.6024 |
| LysoPC 16:1 | 493.3177 | 21.817492 | Lipid | Lysolipid, PC | 0.2182 | 0.1355 | 0.10741 | 0.4706 | -0.1674 | 0.1571 | 0.286861 | 0.5742 | 0.4973 | 0.2037 | 0.01464 | 0.202 | NaN | 0.1015 | 0.1276 | 0.426515 | 0.8498 | -0.1977 | 0.1374 | 0.150032 | 0.634 | 0.3266 | 0.2005 | 0.103326 | 0.7708 | NaN | 0.1634 | 0.1258 | 0.193732 | 0.7268 | -0.0817 | 0.1367 | 0.550358 | 0.9053 | 0.3475 | 0.2006 | 0.0832 | 0.5886 | NaN | 0.0901 | 0.1317 | 0.493631 | 0.8047 | -0.2644 | 0.1436 | 0.065594 | 0.3599 | 0.3553 | 0.2021 | 0.078683 | 0.7239 | NaN | 0.1408 | 0.1283 | 0.272349 | 0.7442 | -0.1698 | 0.1379 | 0.21815 | 0.7001 | 0.3824 | 0.2007 | 0.056734 | 0.5267 | NaN | 0.1202 | 0.1307 | 0.357698 | 0.7574 | -0.226 | 0.141 | 0.109027 | 0.4629 | 0.3856 | 0.202 | 0.056325 | 0.5263 |
| LysoPC 18:1 | 521.3471 | 22.368698 | Lipid | Lysolipid, PC | 0.0041 | 0.1349 | 0.976024 | 0.9936 | -0.1466 | 0.125 | 0.240884 | 0.534 | 0.2949 | 0.2554 | 0.248194 | 0.7397 | NaN | 0.0514 | 0.1249 | 0.680924 | 0.9237 | -0.0221 | 0.113 | 0.845103 | 0.9729 | 0.177 | 0.2425 | 0.465564 | 0.9478 | NaN | 0.0479 | 0.1247 | 0.700842 | 0.9481 | -0.007 | 0.1112 | 0.949769 | 0.9765 | 0.128 | 0.2471 | 0.604523 | 0.9894 | NaN | 0.0426 | 0.1277 | 0.738645 | 0.9111 | -0.0402 | 0.1179 | 0.733068 | 0.8813 | 0.1988 | 0.2453 | 0.417623 | 0.9375 | NaN | 0.0266 | 0.1264 | 0.833411 | 0.9564 | -0.0799 | 0.1111 | 0.47239 | 0.8272 | 0.2279 | 0.2453 | 0.352943 | 0.9106 | NaN | 0.07 | 0.1284 | 0.585687 | 0.8765 | -0.0083 | 0.1174 | 0.943526 | 0.9823 | 0.2392 | 0.2462 | 0.331374 | 0.8727 |
| LysoPC 18:3 | 517.4306 | 23.745913 | Lipid | Lysolipid, PC | 0.1348 | 0.1312 | 0.304385 | 0.6742 | -0.1622 | 0.1388 | 0.242573 | 0.5356 | 0.3856 | 0.2083 | 0.064117 | 0.4426 | NaN | 0.1405 | 0.1213 | 0.24663 | 0.7495 | -0.0588 | 0.1241 | 0.635628 | 0.9073 | 0.2899 | 0.1982 | 0.143522 | 0.8611 | NaN | 0.1603 | 0.121 | 0.185494 | 0.7111 | -0.0202 | 0.123 | 0.869569 | 0.9581 | 0.2982 | 0.1993 | 0.13464 | 0.7286 | NaN | 0.1041 | 0.1243 | 0.402428 | 0.7795 | -0.1211 | 0.1276 | 0.342375 | 0.67 | 0.2799 | 0.2021 | 0.166197 | 0.8705 | NaN | 0.1335 | 0.1229 | 0.277444 | 0.7462 | -0.0608 | 0.1243 | 0.625019 | 0.8623 | 0.2982 | 0.2021 | 0.140047 | 0.8053 | NaN | 0.1246 | 0.1244 | 0.31662 | 0.7485 | -0.1048 | 0.126 | 0.405893 | 0.7211 | 0.3136 | 0.2023 | 0.12113 | 0.7513 |
| LysoPC 20:3 | 545.3462 | 22.560707 | Lipid | Lysolipid, PC | 0.1584 | 0.1301 | 0.223244 | 0.6011 | -0.0303 | 0.1669 | 0.855881 | 0.932 | 0.276 | 0.1877 | 0.141471 | 0.6043 | NaN | 0.0639 | 0.1218 | 0.599425 | 0.9079 | -0.0799 | 0.1465 | 0.585658 | 0.904 | 0.1524 | 0.1805 | 0.398348 | 0.9398 | NaN | 0.0452 | 0.1221 | 0.711119 | 0.9481 | -0.0171 | 0.1438 | 0.905279 | 0.973 | 0.0865 | 0.1877 | 0.644812 | 0.9894 | NaN | 0.0656 | 0.1248 | 0.599205 | 0.8569 | -0.1264 | 0.1537 | 0.410689 | 0.6997 | 0.184 | 0.1816 | 0.311074 | 0.8963 | NaN | 0.0697 | 0.1234 | 0.57212 | 0.8773 | -0.0861 | 0.1469 | 0.557789 | 0.8618 | 0.1713 | 0.1836 | 0.350716 | 0.9106 | NaN | 0.0704 | 0.125 | 0.573276 | 0.8765 | -0.1346 | 0.1513 | 0.373513 | 0.6983 | 0.1956 | 0.1831 | 0.285526 | 0.8424 |
| LysoPC 20:4 | 543.3407 | 19.784397 | Lipid | Lysolipid, PC | 0.0932 | 0.1372 | 0.496994 | 0.8054 | -0.1747 | 0.147 | 0.234525 | 0.5274 | 0.3222 | 0.2195 | 0.142036 | 0.6043 | NaN | 0.1283 | 0.1268 | 0.311752 | 0.7898 | -0.0656 | 0.1315 | 0.617643 | 0.9073 | 0.2637 | 0.2069 | 0.202536 | 0.9223 | NaN | 0.1457 | 0.1267 | 0.250248 | 0.7434 | -0.0285 | 0.1301 | 0.826579 | 0.9447 | 0.2638 | 0.2084 | 0.205639 | 0.8462 | NaN | 0.0799 | 0.1298 | 0.537976 | 0.8389 | -0.1177 | 0.1356 | 0.385254 | 0.6816 | 0.2196 | 0.2121 | 0.300495 | 0.8823 | NaN | 0.1226 | 0.1285 | 0.340063 | 0.7724 | -0.0746 | 0.1314 | 0.570038 | 0.8623 | 0.2773 | 0.2104 | 0.187652 | 0.8608 | NaN | 0.1063 | 0.1299 | 0.41327 | 0.791 | -0.1021 | 0.1339 | 0.445705 | 0.7458 | 0.2669 | 0.212 | 0.207947 | 0.8424 |
| LysoPE 16:0 | 453.2871 | 22.236048 | Lipid | Lysolipid, PE | 0.2031 | 0.1288 | 0.114887 | 0.4809 | -0.1844 | 0.1435 | 0.198708 | 0.4993 | 0.4836 | 0.1958 | 0.013503 | 0.1992 | NaN | 0.1837 | 0.1192 | 0.123322 | 0.6749 | -0.0912 | 0.1279 | 0.47595 | 0.8671 | 0.3706 | 0.1882 | 0.048926 | 0.5871 | NaN | 0.1928 | 0.1189 | 0.10502 | 0.5628 | -0.0533 | 0.1267 | 0.673961 | 0.9163 | 0.3638 | 0.1905 | 0.056163 | 0.477 | NaN | 0.1522 | 0.1225 | 0.214 | 0.6949 | -0.155 | 0.1316 | 0.23875 | 0.5767 | 0.3677 | 0.192 | 0.055508 | 0.5776 | NaN | 0.1935 | 0.1207 | 0.108966 | 0.6683 | -0.0903 | 0.1282 | 0.481058 | 0.8272 | 0.402 | 0.1903 | 0.034594 | 0.4772 | NaN | 0.1833 | 0.1222 | 0.133548 | 0.605 | -0.1222 | 0.1305 | 0.348944 | 0.6824 | 0.4051 | 0.1913 | 0.034194 | 0.4663 |
| LysoPE 18:0 | 481.3184 | 22.637491 | Lipid | Lysolipid, PE | 0.2224 | 0.1291 | 0.08492 | 0.4185 | -0.1582 | 0.1408 | 0.261261 | 0.5505 | 0.5188 | 0.1991 | 0.00915 | 0.1629 | NaN | 0.189 | 0.1197 | 0.114127 | 0.6749 | -0.0638 | 0.1256 | 0.611528 | 0.9043 | 0.3764 | 0.1938 | 0.052098 | 0.5991 | NaN | 0.2012 | 0.1193 | 0.091707 | 0.5342 | -0.0307 | 0.1242 | 0.8049 | 0.9363 | 0.3795 | 0.1956 | 0.052313 | 0.477 | NaN | 0.1533 | 0.1233 | 0.213977 | 0.6949 | -0.1321 | 0.1291 | 0.30605 | 0.6359 | 0.3715 | 0.1989 | 0.061779 | 0.5957 | NaN | 0.1986 | 0.1211 | 0.101047 | 0.6358 | -0.0688 | 0.1257 | 0.584123 | 0.8623 | 0.4155 | 0.1954 | 0.033444 | 0.4772 | NaN | 0.183 | 0.1228 | 0.13614 | 0.605 | -0.1092 | 0.1277 | 0.392404 | 0.7125 | 0.4158 | 0.1969 | 0.034722 | 0.4663 |
| LysoPE 18:0 | 481.3465 | 22.425735 | Lipid | Lysolipid, PE | -0.0342 | 0.1249 | 0.7842 | 0.9514 | -0.1182 | 0.127 | 0.352153 | 0.6332 | 0.0696 | 0.2082 | 0.738266 | 0.9647 | NaN | 0.0081 | 0.1157 | 0.944289 | 0.9906 | -0.0405 | 0.1129 | 0.719648 | 0.9386 | 0.0637 | 0.1953 | 0.744248 | 0.954 | NaN | 0.0482 | 0.1161 | 0.678232 | 0.9406 | -0.0313 | 0.1109 | 0.777408 | 0.9309 | 0.1267 | 0.197 | 0.520139 | 0.9894 | NaN | -0.0307 | 0.1181 | 0.795019 | 0.9377 | -0.0507 | 0.1176 | 0.666685 | 0.8438 | -0.003 | 0.1992 | 0.987794 | 0.9923 | NaN | -0.0202 | 0.1171 | 0.862686 | 0.962 | -0.0929 | 0.1119 | 0.4063 | 0.8185 | 0.0662 | 0.1988 | 0.739334 | 0.9621 | NaN | -0.0304 | 0.1183 | 0.797485 | 0.9471 | -0.0593 | 0.1155 | 0.607753 | 0.8263 | 0.0166 | 0.2007 | 0.934089 | 0.9869 |
| LysoPE 18:2 | 477.2847 | 22.108313 | Lipid | Lysolipid, PE | 0.046 | 0.1252 | 0.713438 | 0.9246 | -0.215 | 0.1353 | 0.112037 | 0.3939 | 0.2221 | 0.1955 | 0.255916 | 0.7397 | NaN | 0.0503 | 0.1158 | 0.664004 | 0.9186 | -0.0933 | 0.1222 | 0.445386 | 0.8547 | 0.1276 | 0.1857 | 0.491961 | 0.954 | NaN | 0.077 | 0.1157 | 0.505535 | 0.9053 | 0.0389 | 0.1267 | 0.758735 | 0.9266 | 0.1 | 0.1887 | 0.59605 | 0.9894 | NaN | 0.0102 | 0.1187 | 0.931226 | 0.9828 | -0.2201 | 0.1233 | 0.074279 | 0.3762 | 0.1595 | 0.1872 | 0.394445 | 0.9375 | NaN | 0.0222 | 0.1175 | 0.849824 | 0.962 | -0.1689 | 0.1196 | 0.157798 | 0.631 | 0.1534 | 0.1884 | 0.415494 | 0.9359 | NaN | 0.018 | 0.1188 | 0.879526 | 0.9588 | -0.2311 | 0.1212 | 0.056581 | 0.3201 | 0.1867 | 0.1882 | 0.321113 | 0.8727 |
| LysoPS 21:0 | 567.3552 | 22.364582 | Lipid | Lysolipid, PS | 0.0187 | 0.135 | 0.889782 | 0.9809 | -0.3938 | 0.1395 | 0.004764 | 0.1195 | 0.3576 | 0.214 | 0.094812 | 0.5081 | NaN | 0.0704 | 0.125 | 0.573316 | 0.9079 | -0.2325 | 0.1298 | 0.073244 | 0.4865 | 0.2754 | 0.2028 | 0.17455 | 0.879 | NaN | 0.0597 | 0.1247 | 0.631995 | 0.9254 | -0.2105 | 0.1283 | 0.100924 | 0.6422 | 0.2441 | 0.2061 | 0.236171 | 0.888 | NaN | 0.0128 | 0.1276 | 0.920369 | 0.9828 | -0.3173 | 0.1303 | 0.014857 | 0.1422 | 0.2532 | 0.2073 | 0.221954 | 0.8705 | NaN | 0.0775 | 0.1268 | 0.541076 | 0.8632 | -0.2167 | 0.1315 | 0.099405 | 0.5226 | 0.2967 | 0.206 | 0.149676 | 0.8056 | NaN | 0.0503 | 0.128 | 0.694096 | 0.9035 | -0.279 | 0.1306 | 0.032643 | 0.2538 | 0.2991 | 0.207 | 0.148561 | 0.7593 |
| rac-glycerol-1-myristate | 302.2458 | 22.129429 | Lipid | Monoacylglycerol | 0.2722 | 0.1294 | 0.035411 | 0.2678 | 0.2369 | 0.1264 | 0.060948 | 0.3144 | 0.328 | 0.2232 | 0.141664 | 0.6043 | NaN | 0.2287 | 0.1201 | 0.056914 | 0.462 | 0.1478 | 0.1133 | 0.192091 | 0.7154 | 0.3382 | 0.2089 | 0.105497 | 0.7765 | NaN | 0.1883 | 0.1209 | 0.1195 | 0.6049 | 0.0543 | 0.1158 | 0.639454 | 0.9053 | 0.3377 | 0.2104 | 0.108447 | 0.6502 | NaN | 0.2594 | 0.1223 | 0.033975 | 0.3473 | 0.2037 | 0.1162 | 0.079554 | 0.3956 | 0.339 | 0.2118 | 0.109518 | 0.7851 | NaN | 0.2383 | 0.1216 | 0.050003 | 0.4313 | 0.148 | 0.1136 | 0.192361 | 0.6684 | 0.3476 | 0.2127 | 0.102273 | 0.6756 | NaN | 0.2476 | 0.1228 | 0.043716 | 0.389 | 0.1931 | 0.1147 | 0.09214 | 0.4238 | 0.3194 | 0.2141 | 0.135779 | 0.7588 |
| 1-octadecanoyl-rac-glycerol | 358.3087 | 22.912283 | Lipid | Monoacylglycerol | -0.0159 | 0.1277 | 0.900674 | 0.9809 | 0.0897 | 0.1549 | 0.562628 | 0.7994 | -0.0496 | 0.1888 | 0.792862 | 0.9647 | NaN | 0.0218 | 0.1183 | 0.853885 | 0.9705 | 0.0426 | 0.1364 | 0.754937 | 0.9514 | 0.0376 | 0.1786 | 0.833381 | 0.9705 | NaN | -0.0202 | 0.1179 | 0.86428 | 0.9714 | -0.1111 | 0.1376 | 0.419493 | 0.8906 | 0.034 | 0.1798 | 0.849881 | 0.9935 | NaN | 0.0332 | 0.1211 | 0.783908 | 0.936 | 0.122 | 0.1416 | 0.388948 | 0.6838 | 0.0152 | 0.1806 | 0.93297 | 0.99 | NaN | 0.0188 | 0.1199 | 0.875428 | 0.9672 | 0.0531 | 0.1366 | 0.697279 | 0.8748 | 0.0168 | 0.1815 | 0.926076 | 0.9774 | NaN | 0.0286 | 0.1213 | 0.813764 | 0.9477 | 0.1382 | 0.1395 | 0.32175 | 0.6724 | -0.0066 | 0.1818 | 0.971207 | 0.991 |
| 1-oleoyl-rac-glycerol | 356.2929 | 22.690039 | Lipid | Monoacylglycerol | 0.1277 | 0.1311 | 0.330061 | 0.6942 | -0.0394 | 0.1348 | 0.769913 | 0.9199 | 0.3238 | 0.2176 | 0.13669 | 0.6043 | NaN | 0.0313 | 0.1226 | 0.798813 | 0.9571 | -0.1238 | 0.1187 | 0.296978 | 0.8075 | 0.212 | 0.2074 | 0.306663 | 0.9223 | NaN | 0.0208 | 0.1227 | 0.865521 | 0.9714 | -0.1148 | 0.1163 | 0.323558 | 0.8505 | 0.167 | 0.2121 | 0.43123 | 0.9816 | NaN | 0.0483 | 0.1252 | 0.699565 | 0.8872 | -0.111 | 0.1239 | 0.37043 | 0.6762 | 0.2425 | 0.2092 | 0.246243 | 0.8705 | NaN | 0.081 | 0.1233 | 0.511312 | 0.8625 | -0.0843 | 0.1186 | 0.477113 | 0.8272 | 0.2714 | 0.2089 | 0.193899 | 0.8608 | NaN | 0.0619 | 0.1252 | 0.620786 | 0.8808 | -0.1012 | 0.1218 | 0.405753 | 0.7211 | 0.2572 | 0.2107 | 0.22223 | 0.8424 |
| 9,10,13-Trihydroxy-11-octadecenoic acid | 330.2412 | 20.380095 | Lipid | Octadecanoids | 0.1774 | 0.1342 | 0.18628 | 0.5527 | 0.2502 | 0.1305 | 0.055154 | 0.3047 | 0.0761 | 0.2336 | 0.744785 | 0.9647 | NaN | 0.1438 | 0.1244 | 0.247491 | 0.7495 | 0.154 | 0.1172 | 0.188714 | 0.7154 | 0.1233 | 0.2193 | 0.573812 | 0.954 | NaN | 0.0734 | 0.1256 | 0.558956 | 0.9125 | 0.1605 | 0.1145 | 0.160862 | 0.7193 | -0.0406 | 0.223 | 0.855484 | 0.9935 | NaN | 0.1812 | 0.1268 | 0.153021 | 0.6351 | 0.1966 | 0.1206 | 0.103069 | 0.4326 | 0.1461 | 0.2227 | 0.511888 | 0.9375 | NaN | 0.1563 | 0.1259 | 0.214469 | 0.689 | 0.1629 | 0.117 | 0.163902 | 0.631 | 0.1267 | 0.2234 | 0.570619 | 0.9621 | NaN | 0.1873 | 0.127 | 0.140439 | 0.605 | 0.1736 | 0.1197 | 0.146977 | 0.5201 | 0.1823 | 0.2262 | 0.420194 | 0.8887 |
| PG 31.4 | 700.4412 | 22.19887 | Lipid | Phosphatidylglycerol | 0.0434 | 0.1326 | 0.743394 | 0.9321 | 0.0749 | 0.1314 | 0.568573 | 0.8006 | -0.024 | 0.2287 | 0.916552 | 0.9838 | NaN | -0.012 | 0.123 | 0.922134 | 0.9846 | 0.0008 | 0.1164 | 0.994316 | 0.9953 | -0.053 | 0.2146 | 0.804904 | 0.9617 | NaN | -0.027 | 0.1231 | 0.826439 | 0.9714 | 0.0443 | 0.1134 | 0.695811 | 0.9195 | -0.122 | 0.2173 | 0.574412 | 0.9894 | NaN | 0.0092 | 0.1256 | 0.941473 | 0.9828 | 0.0272 | 0.1209 | 0.822249 | 0.9271 | -0.0509 | 0.2175 | 0.814937 | 0.9674 | NaN | 0.0227 | 0.1244 | 0.855333 | 0.962 | 0.0319 | 0.116 | 0.783248 | 0.9258 | -0.0181 | 0.2184 | 0.934101 | 0.9803 | NaN | 0.0187 | 0.1258 | 0.881577 | 0.9588 | 0.0004 | 0.1196 | 0.997498 | 0.9978 | 0.0008 | 0.2196 | 0.997142 | 0.9991 |
| PI 34:1 | 696.3705 | 21.316105 | Lipid | Phosphatidylinositol | -0.065 | 0.1261 | 0.60637 | 0.8575 | -0.0763 | 0.1466 | 0.602605 | 0.8198 | -0.0842 | 0.1933 | 0.663067 | 0.9243 | NaN | -0.0443 | 0.1167 | 0.704133 | 0.9314 | -0.1033 | 0.1285 | 0.421436 | 0.847 | -0.0371 | 0.1819 | 0.83824 | 0.9721 | NaN | -0.0368 | 0.1166 | 0.752441 | 0.96 | -0.0306 | 0.1267 | 0.809046 | 0.9363 | -0.0646 | 0.1827 | 0.723673 | 0.99 | NaN | -0.0331 | 0.1195 | 0.782055 | 0.936 | -0.1377 | 0.1343 | 0.305097 | 0.6359 | 0.0031 | 0.1858 | 0.986695 | 0.9923 | NaN | -0.0167 | 0.1186 | 0.888335 | 0.9672 | -0.0764 | 0.1289 | 0.553508 | 0.8618 | -0.0109 | 0.1862 | 0.953117 | 0.9854 | NaN | -0.0422 | 0.1196 | 0.724512 | 0.9153 | -0.1713 | 0.1325 | 0.196131 | 0.5756 | 0.0002 | 0.1878 | 0.999064 | 0.9991 |
| PI 35:1 | 710.3856 | 21.509493 | Lipid | Phosphatidylinositol | -0.0322 | 0.1315 | 0.80673 | 0.9618 | -0.0481 | 0.1442 | 0.738968 | 0.9065 | -0.0594 | 0.2129 | 0.780282 | 0.9647 | NaN | -0.0108 | 0.1216 | 0.929246 | 0.9861 | -0.0487 | 0.1266 | 0.700631 | 0.9328 | -0.0312 | 0.1998 | 0.876005 | 0.977 | NaN | -0.0313 | 0.1214 | 0.796494 | 0.9641 | 0.0117 | 0.1247 | 0.925441 | 0.973 | -0.1044 | 0.2012 | 0.603705 | 0.9894 | NaN | 0.0218 | 0.1248 | 0.861257 | 0.9702 | -0.0597 | 0.1319 | 0.650731 | 0.8432 | 0.0349 | 0.2043 | 0.864284 | 0.9837 | NaN | -0.0084 | 0.1233 | 0.945688 | 0.9796 | -0.0532 | 0.1268 | 0.674864 | 0.8623 | -0.0216 | 0.2037 | 0.915436 | 0.9736 | NaN | 0.0093 | 0.1249 | 0.940799 | 0.9794 | -0.0962 | 0.13 | 0.459172 | 0.7521 | 0.0373 | 0.2068 | 0.856919 | 0.9641 |
| PI 36:1 | 724.4045 | 21.826448 | Lipid | Phosphatidylinositol | -0.0396 | 0.1246 | 0.750665 | 0.9343 | -0.0611 | 0.1325 | 0.644746 | 0.8471 | -0.063 | 0.2039 | 0.757449 | 0.9647 | NaN | -0.0302 | 0.1152 | 0.793371 | 0.9571 | -0.0834 | 0.1161 | 0.47274 | 0.8671 | -0.0251 | 0.1915 | 0.895894 | 0.977 | NaN | -0.0514 | 0.115 | 0.655078 | 0.9331 | -0.0497 | 0.1141 | 0.663254 | 0.9107 | -0.0799 | 0.1925 | 0.67791 | 0.9894 | NaN | -0.0122 | 0.1179 | 0.917833 | 0.9828 | -0.0908 | 0.1211 | 0.453495 | 0.7319 | 0.009 | 0.195 | 0.963158 | 0.99 | NaN | -0.0113 | 0.1169 | 0.922837 | 0.9796 | -0.0602 | 0.1164 | 0.604971 | 0.8623 | -0.0114 | 0.1954 | 0.953589 | 0.9854 | NaN | -0.0079 | 0.1182 | 0.946433 | 0.9794 | -0.1123 | 0.1194 | 0.346747 | 0.6824 | 0.0329 | 0.1982 | 0.868053 | 0.9662 |
| PI 37:1 | 738.421 | 21.882294 | Lipid | Phosphatidylinositol | -0.1597 | 0.1331 | 0.230126 | 0.6042 | -0.1416 | 0.1392 | 0.309133 | 0.6009 | -0.2064 | 0.2181 | 0.343973 | 0.7534 | NaN | -0.1353 | 0.1232 | 0.272434 | 0.7625 | -0.1217 | 0.1222 | 0.319411 | 0.8095 | -0.182 | 0.2047 | 0.374128 | 0.9312 | NaN | -0.1313 | 0.1231 | 0.286272 | 0.7865 | -0.0485 | 0.1216 | 0.689827 | 0.9195 | -0.2287 | 0.2057 | 0.266257 | 0.9 | NaN | -0.1353 | 0.126 | 0.282987 | 0.7388 | -0.1776 | 0.127 | 0.161791 | 0.5021 | -0.1318 | 0.209 | 0.528102 | 0.9375 | NaN | -0.1244 | 0.1251 | 0.320023 | 0.7669 | -0.1132 | 0.1226 | 0.356042 | 0.7839 | -0.1669 | 0.2088 | 0.424131 | 0.9359 | NaN | -0.1494 | 0.1262 | 0.236294 | 0.7013 | -0.2091 | 0.125 | 0.094384 | 0.4306 | -0.1387 | 0.2109 | 0.510945 | 0.8946 |
| PI 38:1 | 752.4347 | 22.042263 | Lipid | Phosphatidylinositol | -0.1364 | 0.1327 | 0.303896 | 0.6742 | -0.0637 | 0.1438 | 0.657661 | 0.8482 | -0.2376 | 0.2145 | 0.267882 | 0.7397 | NaN | -0.1101 | 0.1229 | 0.370303 | 0.8459 | -0.0819 | 0.1261 | 0.516355 | 0.8967 | -0.1781 | 0.2022 | 0.378303 | 0.9322 | NaN | -0.11 | 0.1227 | 0.370157 | 0.8283 | -0.005 | 0.1244 | 0.968 | 0.9804 | -0.2283 | 0.2025 | 0.259463 | 0.9 | NaN | -0.1032 | 0.1258 | 0.411704 | 0.7798 | -0.123 | 0.1318 | 0.350762 | 0.6762 | -0.1365 | 0.2069 | 0.50961 | 0.9375 | NaN | -0.0988 | 0.1247 | 0.42807 | 0.8452 | -0.0661 | 0.1264 | 0.601211 | 0.8623 | -0.1733 | 0.2063 | 0.400781 | 0.9295 | NaN | -0.119 | 0.1258 | 0.344178 | 0.7531 | -0.1525 | 0.1301 | 0.240976 | 0.613 | -0.1522 | 0.2085 | 0.465379 | 0.8887 |
| PI 39:1 | 766.4491 | 22.154734 | Lipid | Phosphatidylinositol | -0.1254 | 0.1251 | 0.316337 | 0.6805 | -0.0834 | 0.1326 | 0.529457 | 0.7813 | -0.1922 | 0.2046 | 0.347373 | 0.7534 | NaN | -0.0978 | 0.1159 | 0.39853 | 0.8498 | -0.0774 | 0.1163 | 0.505773 | 0.8931 | -0.1525 | 0.1924 | 0.427811 | 0.9419 | NaN | -0.111 | 0.1156 | 0.336963 | 0.8142 | -0.011 | 0.1151 | 0.923862 | 0.973 | -0.2275 | 0.193 | 0.238444 | 0.888 | NaN | -0.1024 | 0.1185 | 0.387594 | 0.773 | -0.129 | 0.1212 | 0.287236 | 0.6122 | -0.1178 | 0.1962 | 0.548359 | 0.9375 | NaN | -0.0902 | 0.1176 | 0.443124 | 0.8528 | -0.0642 | 0.1167 | 0.582498 | 0.8623 | -0.1492 | 0.1961 | 0.446563 | 0.9359 | NaN | -0.11 | 0.1186 | 0.353726 | 0.7573 | -0.1509 | 0.1195 | 0.206734 | 0.5756 | -0.121 | 0.1982 | 0.541595 | 0.9005 |
| PI 40:1 | 780.4654 | 22.279175 | Lipid | Phosphatidylinositol | -0.1147 | 0.1343 | 0.393261 | 0.726 | 0.0251 | 0.1333 | 0.850452 | 0.932 | -0.296 | 0.2307 | 0.199482 | 0.7107 | NaN | -0.0913 | 0.1243 | 0.462777 | 0.8498 | 0.0173 | 0.117 | 0.882558 | 0.9729 | -0.2384 | 0.2174 | 0.272668 | 0.9223 | NaN | -0.1066 | 0.124 | 0.390067 | 0.8424 | 0.0599 | 0.1148 | 0.601607 | 0.9053 | -0.308 | 0.2175 | 0.156788 | 0.7677 | NaN | -0.1004 | 0.1271 | 0.429273 | 0.7844 | -0.0146 | 0.1222 | 0.904715 | 0.9695 | -0.2263 | 0.2209 | 0.305628 | 0.8879 | NaN | -0.1018 | 0.1259 | 0.418646 | 0.8373 | 0.003 | 0.1173 | 0.979626 | 0.9923 | -0.2488 | 0.2212 | 0.260716 | 0.9039 | NaN | -0.1176 | 0.1272 | 0.35532 | 0.7573 | -0.0343 | 0.1207 | 0.776402 | 0.9173 | -0.2477 | 0.2224 | 0.265354 | 0.8424 |
| PI 41:1 | 794.4758 | 22.366863 | Lipid | Phosphatidylinositol | -0.0824 | 0.1339 | 0.538407 | 0.825 | 0.0517 | 0.1396 | 0.711245 | 0.8876 | -0.1947 | 0.2178 | 0.371414 | 0.7534 | NaN | -0.0674 | 0.1239 | 0.586409 | 0.9079 | 0.0893 | 0.1225 | 0.466216 | 0.8665 | -0.2128 | 0.2041 | 0.296986 | 0.9223 | NaN | -0.1276 | 0.1236 | 0.302048 | 0.7865 | 0.0999 | 0.1202 | 0.405979 | 0.8818 | -0.349 | 0.2076 | 0.092657 | 0.6162 | NaN | -0.0751 | 0.1266 | 0.552807 | 0.8434 | 0.0387 | 0.1278 | 0.761776 | 0.8985 | -0.1754 | 0.2072 | 0.397205 | 0.9375 | NaN | -0.0602 | 0.1256 | 0.631822 | 0.8971 | 0.0943 | 0.1228 | 0.442617 | 0.8205 | -0.1972 | 0.2079 | 0.3428 | 0.9106 | NaN | -0.0679 | 0.1269 | 0.592678 | 0.8765 | 0.0442 | 0.1258 | 0.725125 | 0.8975 | -0.1688 | 0.2093 | 0.42003 | 0.8887 |
| PI 42:1 | 808.4955 | 22.451042 | Lipid | Phosphatidylinositol | 0.0217 | 0.1352 | 0.872724 | 0.9809 | 0.1065 | 0.1445 | 0.460854 | 0.7289 | -0.0368 | 0.2152 | 0.864188 | 0.9735 | NaN | -0.0549 | 0.1256 | 0.662231 | 0.9185 | 0.0624 | 0.1272 | 0.623634 | 0.9073 | -0.1493 | 0.2034 | 0.463044 | 0.9478 | NaN | -0.0675 | 0.1256 | 0.590854 | 0.9125 | 0.1374 | 0.1241 | 0.26812 | 0.806 | -0.2489 | 0.2094 | 0.234573 | 0.888 | NaN | -0.0779 | 0.1293 | 0.546679 | 0.8406 | 0.0014 | 0.1348 | 0.992003 | 0.9938 | -0.135 | 0.2062 | 0.512411 | 0.9375 | NaN | -0.0312 | 0.1271 | 0.806214 | 0.952 | 0.0714 | 0.1274 | 0.575012 | 0.8623 | -0.1073 | 0.2064 | 0.602994 | 0.9621 | NaN | -0.0632 | 0.1292 | 0.624668 | 0.8808 | 0.004 | 0.1323 | 0.975675 | 0.9946 | -0.1114 | 0.2077 | 0.591672 | 0.9357 |
| PI 43:1 | 822.5134 | 22.551065 | Lipid | Phosphatidylinositol | -0.1166 | 0.1339 | 0.383851 | 0.7254 | -0.1818 | 0.1453 | 0.210821 | 0.5065 | -0.0583 | 0.2106 | 0.781748 | 0.9647 | NaN | -0.1405 | 0.1237 | 0.256051 | 0.7495 | -0.1973 | 0.127 | 0.120255 | 0.6118 | -0.0939 | 0.1976 | 0.634789 | 0.954 | NaN | -0.17 | 0.1236 | 0.168907 | 0.6756 | -0.137 | 0.1256 | 0.275426 | 0.806 | -0.2051 | 0.2018 | 0.309372 | 0.9479 | NaN | -0.1621 | 0.1266 | 0.200542 | 0.675 | -0.2606 | 0.1324 | 0.049093 | 0.2946 | -0.0777 | 0.2002 | 0.697824 | 0.9477 | NaN | -0.1328 | 0.1254 | 0.289417 | 0.7524 | -0.1663 | 0.1277 | 0.192884 | 0.6684 | -0.1018 | 0.2014 | 0.613146 | 0.9621 | NaN | -0.156 | 0.1269 | 0.218716 | 0.6783 | -0.2543 | 0.1302 | 0.050787 | 0.2951 | -0.0762 | 0.2021 | 0.706013 | 0.9459 |
| choline | 104.1083 | 0.63293 | Lipid | Phospholipid Metabolism | 0.0603 | 0.1325 | 0.648776 | 0.8739 | 0.2405 | 0.1309 | 0.066078 | 0.3257 | -0.1135 | 0.2264 | 0.615974 | 0.8995 | NaN | -0.0327 | 0.1236 | 0.791155 | 0.9571 | 0.1467 | 0.1174 | 0.211331 | 0.7304 | -0.1823 | 0.2126 | 0.391086 | 0.9389 | NaN | -0.0384 | 0.1235 | 0.755978 | 0.96 | 0.1604 | 0.1144 | 0.160981 | 0.7193 | -0.2168 | 0.2148 | 0.312804 | 0.9479 | NaN | -0.0374 | 0.1268 | 0.768285 | 0.9321 | 0.1579 | 0.1224 | 0.197117 | 0.5441 | -0.2055 | 0.2161 | 0.341622 | 0.9066 | NaN | -0.0447 | 0.1257 | 0.722283 | 0.9229 | 0.144 | 0.1177 | 0.221447 | 0.7033 | -0.2134 | 0.2175 | 0.326516 | 0.9106 | NaN | -0.034 | 0.1271 | 0.789243 | 0.9452 | 0.1553 | 0.1204 | 0.197286 | 0.5756 | -0.2001 | 0.2184 | 0.35953 | 0.8785 |
| 3,7-dihydroxy-5-cholestanoic acid | 434.3391 | 22.831043 | Lipid | Primary Bile Acid Metabolism | 0.1841 | 0.1393 | 0.186385 | 0.5527 | 0.1206 | 0.1341 | 0.368483 | 0.6407 | 0.2622 | 0.2511 | 0.296493 | 0.7534 | NaN | 0.2821 | 0.1289 | 0.028631 | 0.3293 | 0.1707 | 0.1172 | 0.145392 | 0.6288 | 0.405 | 0.2361 | 0.086313 | 0.7567 | NaN | 0.2884 | 0.1287 | 0.025034 | 0.27 | 0.2126 | 0.115 | 0.064444 | 0.5558 | 0.361 | 0.2372 | 0.128133 | 0.7073 | NaN | 0.2298 | 0.1316 | 0.080862 | 0.519 | 0.1414 | 0.1224 | 0.247771 | 0.5827 | 0.3142 | 0.2385 | 0.187721 | 0.8705 | NaN | 0.2731 | 0.1307 | 0.036675 | 0.3552 | 0.1632 | 0.1175 | 0.164767 | 0.631 | 0.3941 | 0.241 | 0.102059 | 0.6756 | NaN | 0.2406 | 0.132 | 0.06828 | 0.4832 | 0.1513 | 0.1205 | 0.209224 | 0.5756 | 0.3282 | 0.241 | 0.173351 | 0.8194 |
| dihomoursodeoxycholic acid | 420.3245 | 22.660122 | Lipid | Primary Bile Acid Metabolism | -0.1234 | 0.1284 | 0.3366 | 0.6985 | -0.0113 | 0.1532 | 0.940953 | 0.9727 | -0.1671 | 0.1922 | 0.38465 | 0.7534 | NaN | -0.0196 | 0.1204 | 0.870339 | 0.9705 | 0.1037 | 0.1357 | 0.444918 | 0.8547 | -0.0771 | 0.1823 | 0.672343 | 0.954 | NaN | -0.0945 | 0.1188 | 0.426148 | 0.8745 | 0.0901 | 0.1328 | 0.497115 | 0.9053 | -0.2029 | 0.1813 | 0.263105 | 0.9 | NaN | -0.03 | 0.1232 | 0.807528 | 0.9433 | 0.0777 | 0.1413 | 0.582641 | 0.804 | -0.0684 | 0.1857 | 0.712478 | 0.9477 | NaN | -0.0388 | 0.1216 | 0.749522 | 0.9339 | 0.1076 | 0.1361 | 0.429048 | 0.8205 | -0.1091 | 0.1848 | 0.55474 | 0.9621 | NaN | -0.0275 | 0.1236 | 0.824099 | 0.9491 | 0.074 | 0.1389 | 0.594149 | 0.8199 | -0.0672 | 0.1881 | 0.720943 | 0.9459 |
| ursodeoxycholic acid | 392.2928 | 20.447248 | Lipid | Primary Bile Acid Metabolism | 0.0227 | 0.129 | 0.860227 | 0.9787 | 0.0126 | 0.1259 | 0.92046 | 0.966 | 0.0651 | 0.2255 | 0.772721 | 0.9647 | NaN | 0.0017 | 0.1193 | 0.988599 | 0.9999 | -0.013 | 0.1106 | 0.906382 | 0.9729 | 0.05 | 0.2115 | 0.813033 | 0.9632 | NaN | 0.0428 | 0.1191 | 0.719187 | 0.952 | 0.0523 | 0.1086 | 0.629879 | 0.9053 | 0.0456 | 0.213 | 0.830493 | 0.9935 | NaN | -0.0093 | 0.1221 | 0.939544 | 0.9828 | -0.0126 | 0.1153 | 0.913133 | 0.9712 | 0.0332 | 0.2146 | 0.87703 | 0.99 | NaN | -0.04 | 0.1214 | 0.741517 | 0.9289 | -0.053 | 0.1113 | 0.634211 | 0.8623 | 0.0024 | 0.2163 | 0.991104 | 0.9983 | NaN | -0.0232 | 0.1226 | 0.849616 | 0.9532 | -0.0482 | 0.1141 | 0.672553 | 0.8694 | 0.0407 | 0.2166 | 0.851038 | 0.9641 |
| hyodeoxycholic acid | 392.2958 | 22.847624 | Lipid | Secondary Bile Acid Metabolism | 0.035 | 0.1373 | 0.799014 | 0.9609 | 0.0761 | 0.1348 | 0.572461 | 0.8007 | -0.0245 | 0.2446 | 0.920356 | 0.9838 | NaN | -0.0588 | 0.1279 | 0.64565 | 0.9179 | -0.0131 | 0.1197 | 0.913148 | 0.9729 | -0.0907 | 0.2299 | 0.693324 | 0.954 | NaN | -0.0493 | 0.1275 | 0.69927 | 0.9481 | 0.0127 | 0.1168 | 0.913656 | 0.973 | -0.0926 | 0.2316 | 0.689399 | 0.9894 | NaN | -0.021 | 0.1303 | 0.872124 | 0.9749 | 0.0357 | 0.1238 | 0.773167 | 0.9061 | -0.0709 | 0.2329 | 0.760623 | 0.9586 | NaN | -0.0512 | 0.1296 | 0.693019 | 0.9116 | -0.0208 | 0.1201 | 0.862619 | 0.9614 | -0.0747 | 0.234 | 0.749532 | 0.9621 | NaN | -0.0201 | 0.1306 | 0.877568 | 0.9588 | 0.0447 | 0.1217 | 0.71322 | 0.8887 | -0.0823 | 0.2354 | 0.726768 | 0.9459 |
| taurolithocholate | 483.298 | 21.677956 | Lipid | Secondary Bile Acid Metabolism | -0.1868 | 0.1345 | 0.164987 | 0.531 | -0.1539 | 0.1547 | 0.319756 | 0.6107 | -0.1953 | 0.2042 | 0.338968 | 0.7534 | NaN | -0.1491 | 0.1247 | 0.23179 | 0.7495 | -0.0796 | 0.137 | 0.561367 | 0.9009 | -0.1871 | 0.1915 | 0.328571 | 0.9223 | NaN | -0.1432 | 0.1246 | 0.250489 | 0.7434 | -0.0257 | 0.1358 | 0.850159 | 0.95 | -0.2155 | 0.1926 | 0.26335 | 0.9 | NaN | -0.1748 | 0.1272 | 0.169423 | 0.6495 | -0.1632 | 0.1413 | 0.248086 | 0.5827 | -0.1656 | 0.1945 | 0.394489 | 0.9375 | NaN | -0.1753 | 0.1261 | 0.164275 | 0.6753 | -0.0799 | 0.1372 | 0.560493 | 0.8618 | -0.2262 | 0.1948 | 0.24563 | 0.9039 | NaN | -0.1814 | 0.1274 | 0.154448 | 0.6269 | -0.1631 | 0.1391 | 0.240986 | 0.613 | -0.1809 | 0.1961 | 0.356271 | 0.8785 |
| sphingosine | 299.2791 | 20.533209 | Lipid | Sphingolipid Metabolism | 0.1984 | 0.1269 | 0.117947 | 0.4809 | -0.074 | 0.1881 | 0.694134 | 0.8728 | 0.3119 | 0.1733 | 0.071779 | 0.4554 | NaN | 0.0863 | 0.1196 | 0.470429 | 0.8514 | -0.1353 | 0.1651 | 0.412458 | 0.847 | 0.1731 | 0.1688 | 0.305118 | 0.9223 | NaN | 0.1053 | 0.1188 | 0.375156 | 0.8283 | -0.1416 | 0.162 | 0.382038 | 0.8818 | 0.1934 | 0.1689 | 0.252065 | 0.9 | NaN | 0.088 | 0.1228 | 0.473455 | 0.7944 | -0.1803 | 0.1729 | 0.297063 | 0.627 | 0.1939 | 0.1705 | 0.255458 | 0.8705 | NaN | 0.1215 | 0.1203 | 0.312509 | 0.7633 | -0.0614 | 0.1655 | 0.710448 | 0.8841 | 0.2074 | 0.1705 | 0.223937 | 0.8892 | NaN | 0.1175 | 0.1219 | 0.335136 | 0.749 | -0.1177 | 0.1694 | 0.487187 | 0.7772 | 0.2196 | 0.1708 | 0.198414 | 0.8424 |
| C16 Sphinganine | 273.267 | 16.9842 | Lipid | Sphingolipids | 0.1573 | 0.1409 | 0.264218 | 0.6341 | -0.0858 | 0.159 | 0.589264 | 0.8109 | 0.3462 | 0.2181 | 0.112458 | 0.5643 | NaN | 0.2005 | 0.1301 | 0.12337 | 0.6749 | -0.0327 | 0.1401 | 0.815416 | 0.965 | 0.36 | 0.2041 | 0.077713 | 0.7271 | NaN | 0.1847 | 0.1299 | 0.155135 | 0.6683 | -0.0705 | 0.137 | 0.606799 | 0.9053 | 0.3482 | 0.2057 | 0.090385 | 0.6117 | NaN | 0.1457 | 0.1332 | 0.274223 | 0.7361 | -0.1348 | 0.1454 | 0.353849 | 0.6762 | 0.347 | 0.2071 | 0.093753 | 0.7393 | NaN | 0.1754 | 0.1319 | 0.183479 | 0.6753 | -0.0549 | 0.14 | 0.694956 | 0.8748 | 0.3377 | 0.2082 | 0.104772 | 0.6804 | NaN | 0.173 | 0.1334 | 0.194642 | 0.6472 | -0.0865 | 0.1432 | 0.545854 | 0.8009 | 0.3573 | 0.209 | 0.087292 | 0.6512 |
| C17 Sphinganine | 287.2825 | 16.69317 | Lipid | Sphingolipids | -0.0895 | 0.1335 | 0.502647 | 0.8067 | -0.1389 | 0.1328 | 0.295534 | 0.5868 | -0.0133 | 0.2274 | 0.953412 | 0.9887 | NaN | -0.0886 | 0.1234 | 0.472891 | 0.8531 | -0.1749 | 0.116 | 0.13155 | 0.6118 | 0.026 | 0.2135 | 0.903052 | 0.9779 | NaN | -0.0368 | 0.1237 | 0.76576 | 0.96 | -0.1695 | 0.1138 | 0.136573 | 0.6741 | 0.1117 | 0.2172 | 0.606951 | 0.9894 | NaN | -0.1234 | 0.1262 | 0.328343 | 0.741 | -0.2097 | 0.1213 | 0.083697 | 0.4089 | -0.0009 | 0.2162 | 0.996797 | 0.9968 | NaN | -0.0807 | 0.1251 | 0.518592 | 0.8625 | -0.1442 | 0.1165 | 0.215695 | 0.6963 | 0.0033 | 0.2172 | 0.987909 | 0.9969 | NaN | -0.1162 | 0.1264 | 0.358102 | 0.7574 | -0.1746 | 0.1192 | 0.142994 | 0.5193 | -0.0321 | 0.2183 | 0.883205 | 0.9702 |
| SM d32:1 | 674.5378 | 23.6049 | Lipid | Sphingomyelin | 0.1557 | 0.1539 | 0.311838 | 0.6804 | 0.0424 | 0.1407 | 0.763044 | 0.9167 | 0.3959 | 0.2947 | 0.179111 | 0.6772 | NaN | 0.0843 | 0.1431 | 0.555715 | 0.9076 | 0.0112 | 0.1237 | 0.927908 | 0.9729 | 0.2374 | 0.2811 | 0.398386 | 0.9398 | NaN | 0.1334 | 0.1422 | 0.348237 | 0.8224 | 0.0923 | 0.1212 | 0.446297 | 0.8947 | 0.2105 | 0.285 | 0.460226 | 0.9816 | NaN | 0.0396 | 0.1478 | 0.788558 | 0.936 | -0.0424 | 0.1301 | 0.744816 | 0.888 | 0.2233 | 0.2868 | 0.436081 | 0.9375 | NaN | 0.0871 | 0.145 | 0.548137 | 0.867 | 0.005 | 0.124 | 0.967889 | 0.9923 | 0.2627 | 0.2859 | 0.358192 | 0.9106 | NaN | 0.051 | 0.1478 | 0.730065 | 0.9166 | -0.0523 | 0.1282 | 0.683642 | 0.8747 | 0.2645 | 0.2877 | 0.357755 | 0.8785 |
| SM d33:1 | 688.5525 | 23.80148 | Lipid | Sphingomyelin | 0.0179 | 0.1365 | 0.895943 | 0.9809 | -0.0945 | 0.1531 | 0.536975 | 0.7813 | 0.115 | 0.2115 | 0.586575 | 0.887 | NaN | -0.0175 | 0.1264 | 0.890162 | 0.9705 | -0.105 | 0.1342 | 0.434287 | 0.8531 | 0.0446 | 0.1995 | 0.823223 | 0.9668 | NaN | 0.0195 | 0.126 | 0.876829 | 0.9714 | 0.006 | 0.1333 | 0.964285 | 0.9785 | 0.0198 | 0.2018 | 0.921679 | 0.9935 | NaN | -0.0571 | 0.1299 | 0.66029 | 0.8697 | -0.1777 | 0.1404 | 0.205536 | 0.5478 | 0.0328 | 0.2028 | 0.871338 | 0.9856 | NaN | -0.0285 | 0.1282 | 0.823921 | 0.9564 | -0.108 | 0.1345 | 0.421812 | 0.8199 | 0.0343 | 0.2038 | 0.866444 | 0.9621 | NaN | -0.0523 | 0.1301 | 0.68754 | 0.9035 | -0.1945 | 0.1383 | 0.159569 | 0.5371 | 0.0519 | 0.2043 | 0.799479 | 0.9615 |
| SM d34:1 | 702.5686 | 24.01544 | Lipid | Sphingomyelin | -0.1117 | 0.1389 | 0.421144 | 0.7523 | -0.1966 | 0.16 | 0.218932 | 0.5107 | -0.0285 | 0.2124 | 0.893335 | 0.9826 | NaN | -0.0749 | 0.1287 | 0.560298 | 0.9079 | -0.1019 | 0.1423 | 0.473775 | 0.8671 | -0.0423 | 0.1993 | 0.83172 | 0.9705 | NaN | -0.0656 | 0.1286 | 0.60977 | 0.9125 | -0.0669 | 0.1406 | 0.634045 | 0.9053 | -0.0628 | 0.2008 | 0.754231 | 0.9935 | NaN | -0.1302 | 0.1312 | 0.321004 | 0.741 | -0.1588 | 0.1468 | 0.279504 | 0.6088 | -0.091 | 0.2026 | 0.653315 | 0.9375 | NaN | -0.082 | 0.1303 | 0.529207 | 0.8625 | -0.1106 | 0.1423 | 0.43678 | 0.8205 | -0.0417 | 0.2029 | 0.837103 | 0.9621 | NaN | -0.1072 | 0.1316 | 0.415396 | 0.791 | -0.1414 | 0.145 | 0.329488 | 0.6739 | -0.0585 | 0.204 | 0.774427 | 0.9525 |
| SM d36:1 | 730.6008 | 24.56354 | Lipid | Sphingomyelin | -0.0136 | 0.1321 | 0.918253 | 0.9809 | 0.1163 | 0.1458 | 0.425232 | 0.6945 | -0.099 | 0.21 | 0.637279 | 0.9104 | NaN | -0.0735 | 0.1225 | 0.54851 | 0.9038 | 0.088 | 0.1282 | 0.492278 | 0.888 | -0.1692 | 0.1973 | 0.391224 | 0.9389 | NaN | -0.0177 | 0.122 | 0.884729 | 0.9714 | 0.1217 | 0.1254 | 0.331762 | 0.8587 | -0.0918 | 0.1983 | 0.643531 | 0.9894 | NaN | -0.0998 | 0.1259 | 0.427932 | 0.7844 | 0.1139 | 0.1333 | 0.392768 | 0.6883 | -0.2509 | 0.2028 | 0.216139 | 0.8705 | NaN | -0.0531 | 0.1239 | 0.668568 | 0.9077 | 0.1292 | 0.128 | 0.31298 | 0.7544 | -0.1634 | 0.201 | 0.416268 | 0.9359 | NaN | -0.0847 | 0.1259 | 0.501106 | 0.8285 | 0.1367 | 0.1311 | 0.297336 | 0.6559 | -0.2312 | 0.2047 | 0.25857 | 0.8424 |
| SM d40:1 | 786.6598 | 26.323471 | Lipid | Sphingomyelin | 0.0446 | 0.1344 | 0.739738 | 0.9321 | -0.0358 | 0.1474 | 0.808071 | 0.932 | 0.1333 | 0.2125 | 0.530531 | 0.8655 | NaN | 0.0061 | 0.1245 | 0.96087 | 0.9952 | 0.0349 | 0.13 | 0.788205 | 0.9616 | 0.0007 | 0.2027 | 0.99708 | 0.9999 | NaN | 0.0282 | 0.1241 | 0.820251 | 0.9714 | 0.1069 | 0.1289 | 0.406884 | 0.8818 | -0.0161 | 0.2053 | 0.937688 | 0.9935 | NaN | -0.0505 | 0.1285 | 0.694375 | 0.8832 | -0.0601 | 0.1348 | 0.655763 | 0.8438 | -0.0187 | 0.2074 | 0.928335 | 0.99 | NaN | -0.0036 | 0.1263 | 0.977153 | 0.9861 | -0.001 | 0.1298 | 0.994122 | 0.9941 | 0.0251 | 0.2061 | 0.903142 | 0.9681 | NaN | -0.0245 | 0.1281 | 0.84854 | 0.9532 | -0.0499 | 0.1327 | 0.707139 | 0.8887 | 0.0284 | 0.2072 | 0.891107 | 0.9702 |
| SM d42:1 | 814.6936 | 27.731535 | Lipid | Sphingomyelin | 0.0234 | 0.1342 | 0.861684 | 0.9787 | -0.0661 | 0.1582 | 0.676262 | 0.8622 | 0.0979 | 0.2021 | 0.628077 | 0.9104 | NaN | 0.0282 | 0.1241 | 0.820316 | 0.9614 | 0.0526 | 0.1406 | 0.708483 | 0.934 | 0.0286 | 0.1906 | 0.88076 | 0.977 | NaN | 0.0117 | 0.1239 | 0.924706 | 0.9728 | 0.0667 | 0.1381 | 0.629015 | 0.9053 | -0.0093 | 0.1934 | 0.961449 | 0.9976 | NaN | -0.0243 | 0.1272 | 0.848698 | 0.962 | -0.0367 | 0.1449 | 0.800266 | 0.9172 | 0.0024 | 0.1944 | 0.990062 | 0.9923 | NaN | 0.0189 | 0.1257 | 0.880404 | 0.9672 | 0.0137 | 0.14 | 0.922331 | 0.981 | 0.047 | 0.1938 | 0.808551 | 0.9621 | NaN | 0.0029 | 0.1272 | 0.981676 | 0.9943 | -0.0151 | 0.143 | 0.915692 | 0.979 | 0.0414 | 0.195 | 0.831997 | 0.9641 |
| SM d34:2 | 700.5532 | 23.705383 | Lipid | Sphingomyelin | 0.1538 | 0.1404 | 0.273369 | 0.6449 | -0.0494 | 0.1575 | 0.753624 | 0.9103 | 0.3073 | 0.2159 | 0.154571 | 0.6351 | NaN | 0.0204 | 0.1323 | 0.877451 | 0.9705 | -0.159 | 0.1388 | 0.25204 | 0.7821 | 0.1495 | 0.2085 | 0.473248 | 0.9534 | NaN | 0.0918 | 0.1303 | 0.480979 | 0.8967 | -0.0177 | 0.1358 | 0.896406 | 0.973 | 0.1681 | 0.2091 | 0.421527 | 0.9816 | NaN | -0.0014 | 0.137 | 0.991796 | 0.9985 | -0.2059 | 0.1467 | 0.16041 | 0.5021 | 0.1438 | 0.2131 | 0.499766 | 0.9375 | NaN | 0.015 | 0.1346 | 0.911411 | 0.9796 | -0.1962 | 0.1397 | 0.160184 | 0.631 | 0.1704 | 0.2124 | 0.422456 | 0.9359 | NaN | 0.0128 | 0.1368 | 0.925654 | 0.9775 | -0.2096 | 0.144 | 0.145646 | 0.5201 | 0.1729 | 0.2139 | 0.418826 | 0.8887 |
| SM d36:2 | 728.5813 | 24.159441 | Lipid | Sphingomyelin | 0.0701 | 0.1348 | 0.602876 | 0.8575 | -0.1054 | 0.151 | 0.485252 | 0.7524 | 0.2097 | 0.2086 | 0.314777 | 0.7534 | NaN | -0.0691 | 0.1269 | 0.585974 | 0.9079 | -0.2357 | 0.1327 | 0.0758 | 0.4865 | 0.0661 | 0.2003 | 0.741499 | 0.954 | NaN | 0.033 | 0.1247 | 0.791376 | 0.9641 | -0.0843 | 0.1302 | 0.517007 | 0.9053 | 0.1273 | 0.1989 | 0.522159 | 0.9894 | NaN | -0.1038 | 0.132 | 0.431676 | 0.7844 | -0.2562 | 0.1398 | 0.066929 | 0.3622 | 0.0225 | 0.2075 | 0.913754 | 0.99 | NaN | -0.0439 | 0.1282 | 0.731869 | 0.9262 | -0.1905 | 0.1326 | 0.150919 | 0.631 | 0.0816 | 0.2042 | 0.689652 | 0.9621 | NaN | -0.0911 | 0.1319 | 0.489854 | 0.8278 | -0.2447 | 0.137 | 0.074038 | 0.3749 | 0.041 | 0.2095 | 0.844831 | 0.9641 |
| SM d41:2 | 798.6609 | 26.103058 | Lipid | Sphingomyelin | 0.0345 | 0.1404 | 0.805642 | 0.9618 | -0.0188 | 0.1465 | 0.898138 | 0.953 | 0.1388 | 0.2342 | 0.553524 | 0.8707 | NaN | -0.0812 | 0.1312 | 0.535741 | 0.8926 | -0.1308 | 0.1295 | 0.312426 | 0.8095 | 0.0127 | 0.2225 | 0.95449 | 0.9911 | NaN | -0.0322 | 0.1301 | 0.804447 | 0.9673 | -0.0583 | 0.1262 | 0.643974 | 0.9053 | 0.0129 | 0.2243 | 0.954062 | 0.9976 | NaN | -0.0956 | 0.1351 | 0.479398 | 0.7995 | -0.1275 | 0.1356 | 0.346942 | 0.6743 | -0.0058 | 0.2272 | 0.979588 | 0.9923 | NaN | -0.0613 | 0.1327 | 0.64416 | 0.9002 | -0.1044 | 0.1294 | 0.419784 | 0.8188 | 0.0258 | 0.2268 | 0.909593 | 0.9693 | NaN | -0.0646 | 0.1345 | 0.630955 | 0.8817 | -0.121 | 0.1331 | 0.363205 | 0.6901 | 0.0452 | 0.2272 | 0.842375 | 0.9641 |
| SM d42:2 | 812.6772 | 26.441246 | Lipid | Sphingomyelin | -0.0345 | 0.1386 | 0.803323 | 0.9618 | -0.1455 | 0.1574 | 0.355167 | 0.6361 | 0.0632 | 0.213 | 0.766712 | 0.9647 | NaN | -0.0507 | 0.1282 | 0.692737 | 0.9304 | -0.1115 | 0.1385 | 0.4205 | 0.847 | 0.0055 | 0.2004 | 0.978114 | 0.9943 | NaN | -0.0145 | 0.128 | 0.910146 | 0.9717 | -0.0023 | 0.1385 | 0.986481 | 0.9908 | -0.0166 | 0.2024 | 0.934513 | 0.9935 | NaN | -0.0832 | 0.1313 | 0.52636 | 0.8293 | -0.1869 | 0.1437 | 0.19336 | 0.5441 | 0.0128 | 0.2031 | 0.949566 | 0.99 | NaN | -0.0717 | 0.13 | 0.581441 | 0.8866 | -0.1602 | 0.1381 | 0.245946 | 0.7302 | 0.0083 | 0.2041 | 0.967615 | 0.9928 | NaN | -0.0597 | 0.1314 | 0.649571 | 0.8907 | -0.1636 | 0.1415 | 0.247561 | 0.624 | 0.036 | 0.2046 | 0.860424 | 0.9641 |
| 17-alpha-hydroxyprogesterone | 330.2045 | 18.162195 | Lipid | Steroid | 0.1954 | 0.1353 | 0.148666 | 0.5192 | 0.2815 | 0.1298 | 0.030036 | 0.2636 | 0.0851 | 0.2362 | 0.718619 | 0.9594 | NaN | 0.1442 | 0.1256 | 0.251143 | 0.7495 | 0.1819 | 0.1169 | 0.119473 | 0.6118 | 0.1017 | 0.2215 | 0.646261 | 0.954 | NaN | 0.0595 | 0.1277 | 0.641451 | 0.9293 | 0.1725 | 0.1149 | 0.133181 | 0.6741 | -0.0807 | 0.2277 | 0.72298 | 0.99 | NaN | 0.2125 | 0.1277 | 0.096224 | 0.5399 | 0.2561 | 0.1189 | 0.031218 | 0.2298 | 0.153 | 0.2251 | 0.496569 | 0.9375 | NaN | 0.159 | 0.1271 | 0.210971 | 0.6855 | 0.2001 | 0.1162 | 0.08506 | 0.4791 | 0.0995 | 0.2255 | 0.6592 | 0.9621 | NaN | 0.2154 | 0.128 | 0.09237 | 0.5459 | 0.2396 | 0.1176 | 0.041575 | 0.2765 | 0.1756 | 0.228 | 0.4414 | 0.8887 |
| cortisol | 362.2099 | 13.811827 | Lipid | Steroid | 0.0987 | 0.1363 | 0.468949 | 0.7972 | 0.1413 | 0.1512 | 0.350094 | 0.6332 | 0.0989 | 0.213 | 0.642379 | 0.9104 | NaN | 0.1278 | 0.126 | 0.310149 | 0.7898 | 0.1731 | 0.1323 | 0.190823 | 0.7154 | 0.1135 | 0.1997 | 0.570009 | 0.954 | NaN | 0.0991 | 0.1258 | 0.43085 | 0.8779 | 0.1417 | 0.1301 | 0.275968 | 0.806 | 0.071 | 0.2014 | 0.724551 | 0.99 | NaN | 0.1197 | 0.1288 | 0.35255 | 0.7467 | 0.1695 | 0.138 | 0.219386 | 0.5555 | 0.1098 | 0.2025 | 0.587703 | 0.9375 | NaN | 0.1275 | 0.1276 | 0.317737 | 0.7669 | 0.1587 | 0.1327 | 0.231705 | 0.7214 | 0.1243 | 0.2034 | 0.541055 | 0.9621 | NaN | 0.1011 | 0.1291 | 0.433649 | 0.795 | 0.1361 | 0.1362 | 0.317539 | 0.672 | 0.0999 | 0.2044 | 0.62498 | 0.9459 |
| cortisol 21-acetate | 404.2041 | 15.652845 | Lipid | Steroid | 0.0949 | 0.1357 | 0.484413 | 0.8041 | 0.2252 | 0.1405 | 0.108825 | 0.3922 | -0.0467 | 0.2232 | 0.834403 | 0.9732 | NaN | 0.0759 | 0.1255 | 0.545535 | 0.9016 | 0.1372 | 0.1253 | 0.273693 | 0.798 | 0.0045 | 0.2098 | 0.982977 | 0.9964 | NaN | 0.0333 | 0.1258 | 0.791296 | 0.9641 | 0.1565 | 0.1222 | 0.200209 | 0.7783 | -0.0912 | 0.211 | 0.665641 | 0.9894 | NaN | 0.1101 | 0.1282 | 0.3907 | 0.773 | 0.1827 | 0.1292 | 0.157363 | 0.5021 | 0.0176 | 0.213 | 0.934209 | 0.99 | NaN | 0.0675 | 0.1273 | 0.59602 | 0.8924 | 0.1166 | 0.1264 | 0.356439 | 0.7839 | -0.0034 | 0.2136 | 0.987245 | 0.9969 | NaN | 0.105 | 0.1285 | 0.413808 | 0.791 | 0.1471 | 0.1285 | 0.252157 | 0.627 | 0.0373 | 0.216 | 0.862838 | 0.9641 |
| cortisone | 360.1939 | 13.359143 | Lipid | Steroid | -0.0332 | 0.1325 | 0.801994 | 0.9618 | 0.1278 | 0.1441 | 0.375184 | 0.6456 | -0.1305 | 0.2129 | 0.539724 | 0.8661 | NaN | 0.1487 | 0.1258 | 0.237219 | 0.7495 | 0.2715 | 0.1265 | 0.031795 | 0.3133 | 0.0676 | 0.2066 | 0.743329 | 0.954 | NaN | 0.0909 | 0.1239 | 0.463183 | 0.8953 | 0.1675 | 0.1236 | 0.175386 | 0.7308 | 0.0244 | 0.206 | 0.905824 | 0.9935 | NaN | 0.1309 | 0.1291 | 0.310889 | 0.741 | 0.331 | 0.1346 | 0.013931 | 0.14 | 0.0025 | 0.2066 | 0.990455 | 0.9923 | NaN | 0.1627 | 0.1287 | 0.206237 | 0.6855 | 0.3324 | 0.1276 | 0.00918 | 0.1635 | 0.0452 | 0.2109 | 0.830349 | 0.9621 | NaN | 0.1262 | 0.1294 | 0.329413 | 0.7485 | 0.3153 | 0.1314 | 0.016393 | 0.1596 | 0.0029 | 0.2094 | 0.988957 | 0.9991 |
| testosterone | 288.1938 | 17.07625 | Lipid | Steroid | 0.0121 | 0.132 | 0.926641 | 0.9818 | 0.0312 | 0.1558 | 0.841321 | 0.932 | -0.0402 | 0.2046 | 0.844344 | 0.9732 | NaN | 0.0466 | 0.1221 | 0.702641 | 0.9314 | -0.0017 | 0.1369 | 0.990117 | 0.9953 | 0.0357 | 0.1929 | 0.853013 | 0.9765 | NaN | 0.0444 | 0.1219 | 0.715597 | 0.9495 | 0.0778 | 0.1342 | 0.562331 | 0.9053 | -0.0056 | 0.1935 | 0.976883 | 0.9976 | NaN | 0.0768 | 0.1253 | 0.539742 | 0.8393 | -0.0157 | 0.1429 | 0.912467 | 0.9712 | 0.0941 | 0.1982 | 0.635081 | 0.9375 | NaN | 0.0628 | 0.1239 | 0.612231 | 0.8964 | 0.0047 | 0.1371 | 0.97275 | 0.9923 | 0.055 | 0.1975 | 0.780789 | 0.9621 | NaN | 0.0634 | 0.1254 | 0.613188 | 0.8808 | -0.0551 | 0.1414 | 0.697001 | 0.8824 | 0.088 | 0.2006 | 0.660725 | 0.9459 |
| cholesterol | 386.3549 | 24.565115 | Lipid | Sterol | -0.0498 | 0.1453 | 0.731871 | 0.9287 | -0.1618 | 0.1646 | 0.325573 | 0.6183 | 0.0416 | 0.2228 | 0.851878 | 0.9732 | NaN | -0.0831 | 0.1344 | 0.536201 | 0.8926 | -0.213 | 0.1439 | 0.138598 | 0.6175 | 0.0118 | 0.2091 | 0.954913 | 0.9911 | NaN | -0.0519 | 0.1341 | 0.69892 | 0.9481 | -0.1029 | 0.1425 | 0.470064 | 0.901 | -0.023 | 0.2111 | 0.913405 | 0.9935 | NaN | -0.1045 | 0.1376 | 0.44782 | 0.7844 | -0.2545 | 0.1505 | 0.090746 | 0.4174 | 0.0091 | 0.212 | 0.965728 | 0.99 | NaN | -0.09 | 0.1363 | 0.509073 | 0.8625 | -0.2238 | 0.1441 | 0.120425 | 0.588 | 0.0065 | 0.213 | 0.975587 | 0.9969 | NaN | -0.1036 | 0.138 | 0.452561 | 0.8014 | -0.2662 | 0.148 | 0.07213 | 0.3687 | 0.0132 | 0.214 | 0.950961 | 0.9869 |
| cholesterol hydrogen sulfate | 466.3126 | 23.898865 | Lipid | Sterol | -0.0269 | 0.1512 | 0.858825 | 0.9787 | -0.0964 | 0.1628 | 0.553608 | 0.7957 | 0.0117 | 0.2423 | 0.961514 | 0.9887 | NaN | -0.1268 | 0.1406 | 0.367049 | 0.8459 | -0.1665 | 0.1427 | 0.243394 | 0.7677 | -0.0974 | 0.2288 | 0.670282 | 0.954 | NaN | -0.0854 | 0.1399 | 0.541287 | 0.9125 | -0.0736 | 0.1403 | 0.599829 | 0.9053 | -0.0866 | 0.2302 | 0.706655 | 0.99 | NaN | -0.1243 | 0.144 | 0.388332 | 0.773 | -0.1917 | 0.1494 | 0.19953 | 0.5448 | -0.0754 | 0.2316 | 0.744858 | 0.9572 | NaN | -0.0976 | 0.1422 | 0.492487 | 0.8625 | -0.1645 | 0.143 | 0.250115 | 0.7305 | -0.0456 | 0.232 | 0.844173 | 0.9621 | NaN | -0.1089 | 0.1441 | 0.449849 | 0.801 | -0.1865 | 0.1469 | 0.204212 | 0.5756 | -0.0511 | 0.2333 | 0.826814 | 0.9641 |
| TG 49:8 | 804.6346 | 25.35286 | Lipid | Triacylglycerol | -0.0147 | 0.1301 | 0.909981 | 0.9809 | -0.1562 | 0.138 | 0.257801 | 0.5494 | 0.1296 | 0.2096 | 0.536413 | 0.8655 | NaN | -0.0004 | 0.1203 | 0.997642 | 0.9999 | -0.0195 | 0.1247 | 0.875582 | 0.9729 | 0.0241 | 0.1989 | 0.90361 | 0.9779 | NaN | 0.0228 | 0.1203 | 0.849691 | 0.9714 | -0.0153 | 0.1223 | 0.900641 | 0.973 | 0.0624 | 0.1991 | 0.753787 | 0.9935 | NaN | -0.0565 | 0.1232 | 0.646725 | 0.8652 | -0.0932 | 0.1276 | 0.465273 | 0.7319 | -0.0129 | 0.2041 | 0.94959 | 0.99 | NaN | -0.0093 | 0.1219 | 0.938965 | 0.9796 | -0.0577 | 0.1235 | 0.640744 | 0.8623 | 0.0574 | 0.2017 | 0.776035 | 0.9621 | NaN | -0.0323 | 0.1233 | 0.793291 | 0.9471 | -0.0769 | 0.1261 | 0.542245 | 0.8009 | 0.0334 | 0.204 | 0.869937 | 0.9662 |
| TG 50:8 | 818.6476 | 25.808493 | Lipid | Triacylglycerol | 0.0032 | 0.1323 | 0.980984 | 0.9936 | -0.2164 | 0.1427 | 0.129495 | 0.423 | 0.188 | 0.2081 | 0.366198 | 0.7534 | NaN | 0.0198 | 0.1224 | 0.871501 | 0.9705 | -0.0349 | 0.1317 | 0.7909 | 0.9616 | 0.054 | 0.1991 | 0.786211 | 0.9557 | NaN | 0.0526 | 0.1224 | 0.667369 | 0.935 | -0.0336 | 0.1287 | 0.794159 | 0.9363 | 0.1165 | 0.1979 | 0.555993 | 0.9894 | NaN | -0.045 | 0.1254 | 0.7198 | 0.8989 | -0.1281 | 0.1332 | 0.336326 | 0.669 | 0.0121 | 0.2057 | 0.953 | 0.99 | NaN | 0.0044 | 0.1239 | 0.971399 | 0.9861 | -0.0846 | 0.1294 | 0.513041 | 0.8496 | 0.0888 | 0.2018 | 0.659842 | 0.9621 | NaN | -0.0256 | 0.1255 | 0.838252 | 0.9501 | -0.1166 | 0.1315 | 0.375216 | 0.6983 | 0.0587 | 0.2052 | 0.774696 | 0.9525 |
| TG 52:8 | 846.6828 | 26.959837 | Lipid | Triacylglycerol | -0.0101 | 0.1347 | 0.940078 | 0.9847 | -0.2439 | 0.1441 | 0.09041 | 0.3727 | 0.1948 | 0.2134 | 0.361201 | 0.7534 | NaN | 0.0113 | 0.1246 | 0.928048 | 0.9861 | -0.0786 | 0.1322 | 0.551923 | 0.9009 | 0.0767 | 0.2032 | 0.705941 | 0.954 | NaN | 0.0512 | 0.1247 | 0.681617 | 0.9406 | -0.0487 | 0.1308 | 0.709598 | 0.9195 | 0.1259 | 0.2028 | 0.534643 | 0.9894 | NaN | -0.0694 | 0.1278 | 0.587251 | 0.8473 | -0.183 | 0.1332 | 0.169608 | 0.5146 | 0.0208 | 0.2105 | 0.921189 | 0.99 | NaN | -0.0088 | 0.1262 | 0.944105 | 0.9796 | -0.1311 | 0.1298 | 0.312557 | 0.7544 | 0.1047 | 0.2063 | 0.611605 | 0.9621 | NaN | -0.0398 | 0.1277 | 0.755334 | 0.9321 | -0.1652 | 0.1318 | 0.210007 | 0.5756 | 0.0775 | 0.2093 | 0.711256 | 0.9459 |
| 2-deoxyinosine | 252.0976 | 6.110615 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.0153 | 0.1338 | 0.909057 | 0.9809 | 0.2883 | 0.1565 | 0.065503 | 0.3257 | -0.1204 | 0.1998 | 0.546769 | 0.8684 | NaN | -0.0782 | 0.1246 | 0.53018 | 0.8926 | 0.1442 | 0.1419 | 0.309731 | 0.8095 | -0.1724 | 0.1874 | 0.357577 | 0.9223 | NaN | -0.073 | 0.1243 | 0.557005 | 0.9125 | 0.1638 | 0.138 | 0.235234 | 0.8003 | -0.188 | 0.189 | 0.319766 | 0.9479 | NaN | -0.0614 | 0.1274 | 0.629935 | 0.8606 | 0.1605 | 0.1482 | 0.278983 | 0.6088 | -0.1484 | 0.1899 | 0.434439 | 0.9375 | NaN | -0.0611 | 0.1261 | 0.627839 | 0.8971 | 0.1356 | 0.1427 | 0.342078 | 0.7839 | -0.147 | 0.1907 | 0.440779 | 0.9359 | NaN | -0.0501 | 0.1274 | 0.694008 | 0.9035 | 0.1567 | 0.1457 | 0.281983 | 0.652 | -0.1361 | 0.1916 | 0.477703 | 0.8887 |
| hypoxanthine | 136.039 | 1.085038 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | -0.1502 | 0.1314 | 0.252871 | 0.6204 | -0.0442 | 0.1355 | 0.74454 | 0.9087 | -0.2309 | 0.217 | 0.287386 | 0.7534 | NaN | -0.2342 | 0.1216 | 0.054101 | 0.4457 | -0.1359 | 0.1194 | 0.255028 | 0.7821 | -0.2991 | 0.2033 | 0.141227 | 0.8611 | NaN | -0.1722 | 0.1212 | 0.155319 | 0.6683 | -0.1386 | 0.117 | 0.236318 | 0.8003 | -0.1884 | 0.2056 | 0.359339 | 0.9578 | NaN | -0.1883 | 0.1241 | 0.129247 | 0.5896 | -0.0961 | 0.1242 | 0.439116 | 0.7301 | -0.2413 | 0.2061 | 0.24161 | 0.8705 | NaN | -0.1802 | 0.123 | 0.142796 | 0.6708 | -0.0474 | 0.1191 | 0.690534 | 0.8743 | -0.2831 | 0.2071 | 0.171674 | 0.8386 | NaN | -0.1848 | 0.1244 | 0.137455 | 0.605 | -0.0749 | 0.1221 | 0.539366 | 0.8003 | -0.2611 | 0.2081 | 0.209546 | 0.8424 |
| inosine | 268.0812 | 1.800299 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | -0.219 | 0.1298 | 0.091653 | 0.4361 | -0.2052 | 0.1346 | 0.127316 | 0.4183 | -0.233 | 0.2119 | 0.271555 | 0.7421 | NaN | -0.2412 | 0.1198 | 0.043984 | 0.4204 | -0.2597 | 0.117 | 0.026429 | 0.2806 | -0.2291 | 0.1986 | 0.248716 | 0.9223 | NaN | -0.2126 | 0.1198 | 0.075933 | 0.5097 | -0.2874 | 0.1144 | 0.012003 | 0.2209 | -0.1569 | 0.2018 | 0.436973 | 0.9816 | NaN | -0.1946 | 0.1229 | 0.113441 | 0.5709 | -0.2006 | 0.1229 | 0.10259 | 0.4326 | -0.1939 | 0.202 | 0.33716 | 0.9044 | NaN | -0.2228 | 0.1215 | 0.066637 | 0.5109 | -0.1974 | 0.1181 | 0.094653 | 0.5173 | -0.2519 | 0.2021 | 0.212522 | 0.8887 | NaN | -0.2094 | 0.123 | 0.088713 | 0.5441 | -0.2106 | 0.1208 | 0.081314 | 0.3937 | -0.2159 | 0.2035 | 0.288775 | 0.8424 |
| urate | 168.0287 | 0.995372 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.3139 | 0.1427 | 0.027861 | 0.233 | 0.2427 | 0.1447 | 0.093519 | 0.381 | 0.4161 | 0.2468 | 0.091729 | 0.5013 | NaN | 0.1552 | 0.1362 | 0.254388 | 0.7495 | 0.0999 | 0.1315 | 0.44748 | 0.8547 | 0.262 | 0.237 | 0.269031 | 0.9223 | NaN | 0.1698 | 0.1353 | 0.209309 | 0.7361 | 0.17 | 0.1259 | 0.177047 | 0.7308 | 0.2208 | 0.2425 | 0.362595 | 0.9578 | NaN | 0.1806 | 0.1391 | 0.194167 | 0.6616 | 0.068 | 0.1411 | 0.629749 | 0.8277 | 0.3572 | 0.2358 | 0.129798 | 0.8047 | NaN | 0.1741 | 0.1377 | 0.206161 | 0.6855 | 0.0848 | 0.1326 | 0.522629 | 0.8496 | 0.3073 | 0.2396 | 0.199595 | 0.8608 | NaN | 0.1776 | 0.1397 | 0.203672 | 0.6633 | 0.0533 | 0.1391 | 0.701583 | 0.8862 | 0.3483 | 0.2387 | 0.144537 | 0.7588 |
| xanthine | 152.0335 | 1.282354 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | 0.1057 | 0.1548 | 0.494829 | 0.8054 | 0.3185 | 0.1592 | 0.045401 | 0.2929 | -0.0244 | 0.2552 | 0.923885 | 0.9845 | NaN | 0.0025 | 0.1444 | 0.986063 | 0.9999 | 0.1965 | 0.1432 | 0.16997 | 0.6773 | -0.1133 | 0.2402 | 0.637156 | 0.954 | NaN | 0.0339 | 0.1436 | 0.813123 | 0.9676 | 0.2358 | 0.1386 | 0.088928 | 0.6214 | -0.1217 | 0.2422 | 0.615276 | 0.9894 | NaN | 0.0182 | 0.1476 | 0.901622 | 0.9816 | 0.2345 | 0.1481 | 0.113344 | 0.4439 | -0.1089 | 0.2436 | 0.65499 | 0.9375 | NaN | 0.0121 | 0.1463 | 0.934345 | 0.9796 | 0.234 | 0.1418 | 0.099007 | 0.5226 | -0.1378 | 0.2457 | 0.575093 | 0.9621 | NaN | 0.0211 | 0.1479 | 0.886364 | 0.9591 | 0.2053 | 0.1471 | 0.162746 | 0.5412 | -0.08 | 0.2454 | 0.744444 | 0.9486 |
| xanthosine | 284.0758 | 2.258693 | Nucleotide | Purine Metabolism, (Hypo)Xanthine/Inosine containing | -0.267 | 0.131 | 0.041457 | 0.2934 | -0.1292 | 0.137 | 0.345771 | 0.632 | -0.364 | 0.2142 | 0.089191 | 0.4966 | NaN | -0.3134 | 0.1206 | 0.009347 | 0.1518 | -0.2056 | 0.1198 | 0.086047 | 0.5387 | -0.3819 | 0.2003 | 0.056479 | 0.6113 | NaN | -0.2738 | 0.1206 | 0.02321 | 0.2615 | -0.1569 | 0.1176 | 0.182051 | 0.7308 | -0.368 | 0.2018 | 0.06826 | 0.5233 | NaN | -0.3292 | 0.1235 | 0.007693 | 0.1118 | -0.2154 | 0.1254 | 0.085905 | 0.4123 | -0.3949 | 0.203 | 0.051663 | 0.5592 | NaN | -0.2749 | 0.1225 | 0.024772 | 0.2903 | -0.122 | 0.1204 | 0.3107 | 0.7544 | -0.3892 | 0.2039 | 0.056378 | 0.5267 | NaN | -0.3087 | 0.1237 | 0.012617 | 0.1699 | -0.1857 | 0.1231 | 0.131351 | 0.507 | -0.39 | 0.205 | 0.05716 | 0.5263 |
| 1-methyladenosine | 281.113 | 1.018368 | Nucleotide | Purine Metabolism, Adenine containing | 0.0153 | 0.1335 | 0.908506 | 0.9809 | -0.118 | 0.2058 | 0.566273 | 0.7994 | 0.0471 | 0.1799 | 0.793442 | 0.9647 | NaN | 0.0521 | 0.1235 | 0.672962 | 0.9208 | -0.0238 | 0.1818 | 0.895975 | 0.9729 | 0.0621 | 0.1688 | 0.712967 | 0.954 | NaN | 0.0498 | 0.1233 | 0.686376 | 0.9448 | 0.0058 | 0.1789 | 0.974297 | 0.9847 | 0.053 | 0.1699 | 0.755042 | 0.9935 | NaN | 0.0383 | 0.1262 | 0.761408 | 0.9258 | -0.1029 | 0.1883 | 0.584791 | 0.805 | 0.0678 | 0.1711 | 0.691822 | 0.9476 | NaN | 0.0284 | 0.1251 | 0.820191 | 0.9564 | -0.0425 | 0.1818 | 0.81524 | 0.9396 | 0.0394 | 0.1718 | 0.818506 | 0.9621 | NaN | 0.0273 | 0.1265 | 0.829136 | 0.9491 | -0.118 | 0.1853 | 0.5242 | 0.7998 | 0.0569 | 0.1727 | 0.741701 | 0.9477 |
| guanine | 151.0494 | 0.977411 | Nucleotide | Purine Metabolism, Adenine containing | 0.2204 | 0.1221 | 0.071076 | 0.3809 | 0.6569 | 0.2946 | 0.025774 | 0.2453 | 0.186 | 0.1528 | 0.22354 | 0.7251 | NaN | 0.1264 | 0.1147 | 0.2702 | 0.7625 | 0.6803 | 0.256 | 0.007875 | 0.1553 | 0.0682 | 0.1477 | 0.644342 | 0.954 | NaN | 0.1595 | 0.1136 | 0.160208 | 0.6683 | 0.609 | 0.2529 | 0.016038 | 0.2556 | 0.1168 | 0.1462 | 0.424112 | 0.9816 | NaN | 0.1605 | 0.1165 | 0.168324 | 0.6495 | 0.5983 | 0.2699 | 0.026633 | 0.2147 | 0.1165 | 0.1474 | 0.429249 | 0.9375 | NaN | 0.145 | 0.1158 | 0.21055 | 0.6855 | 0.6859 | 0.2564 | 0.00747 | 0.1424 | 0.0993 | 0.1493 | 0.505923 | 0.9467 | NaN | 0.1579 | 0.1168 | 0.176591 | 0.6413 | 0.6384 | 0.2643 | 0.01573 | 0.1579 | 0.1148 | 0.1493 | 0.441824 | 0.8887 |
| guanosine | 283.092 | 1.791455 | Nucleotide | Purine Metabolism, Adenine containing | -0.1484 | 0.1226 | 0.226395 | 0.6042 | -0.1787 | 0.133 | 0.17904 | 0.4964 | -0.1463 | 0.1935 | 0.449598 | 0.8098 | NaN | -0.1741 | 0.1132 | 0.124164 | 0.6749 | -0.2446 | 0.1158 | 0.034653 | 0.3298 | -0.1347 | 0.1815 | 0.458167 | 0.9478 | NaN | -0.1422 | 0.1132 | 0.209096 | 0.7361 | -0.2442 | 0.1135 | 0.031423 | 0.354 | -0.073 | 0.1842 | 0.691937 | 0.9894 | NaN | -0.1311 | 0.116 | 0.25846 | 0.7164 | -0.1906 | 0.1213 | 0.116084 | 0.445 | -0.1036 | 0.1846 | 0.574702 | 0.9375 | NaN | -0.168 | 0.1148 | 0.143198 | 0.6708 | -0.2033 | 0.1163 | 0.080461 | 0.4705 | -0.1585 | 0.1847 | 0.390799 | 0.9163 | NaN | -0.1508 | 0.1161 | 0.194185 | 0.6472 | -0.2047 | 0.1193 | 0.086115 | 0.4044 | -0.131 | 0.1858 | 0.480786 | 0.8887 |
| beta-alanine | 89.0478 | 0.671792 | Nucleotide | Pyrimidine Metabolism, Uracil containing | 0.2942 | 0.1199 | 0.014116 | 0.1558 | 0.1239 | 0.13 | 0.340281 | 0.6303 | 0.4063 | 0.1913 | 0.033692 | 0.3293 | NaN | 0.31 | 0.1104 | 0.004978 | 0.0949 | 0.1169 | 0.114 | 0.30524 | 0.8095 | 0.4444 | 0.1783 | 0.012697 | 0.4257 | NaN | 0.3147 | 0.1102 | 0.00428 | 0.0738 | 0.144 | 0.1116 | 0.196831 | 0.7706 | 0.4414 | 0.1796 | 0.014004 | 0.2416 | NaN | 0.31 | 0.1129 | 0.006057 | 0.0983 | 0.0783 | 0.1196 | 0.512688 | 0.7647 | 0.48 | 0.1809 | 0.007957 | 0.2928 | NaN | 0.2829 | 0.1122 | 0.011712 | 0.195 | 0.0911 | 0.1146 | 0.42665 | 0.8205 | 0.4128 | 0.1822 | 0.023445 | 0.4673 | NaN | 0.3122 | 0.1132 | 0.005806 | 0.103 | 0.0731 | 0.1179 | 0.535378 | 0.8003 | 0.4841 | 0.183 | 0.008153 | 0.2813 |
| deoxyuridine | 228.0759 | 1.666972 | Nucleotide | Pyrimidine Metabolism, Uracil containing | -0.0293 | 0.1343 | 0.827568 | 0.972 | 0.0685 | 0.1657 | 0.679428 | 0.8622 | -0.0904 | 0.1962 | 0.644868 | 0.9104 | NaN | -0.029 | 0.1242 | 0.815686 | 0.9614 | 0.0642 | 0.1454 | 0.659021 | 0.914 | -0.083 | 0.1841 | 0.652182 | 0.954 | NaN | -0.0199 | 0.124 | 0.872725 | 0.9714 | 0.1364 | 0.1426 | 0.339073 | 0.8587 | -0.0995 | 0.1852 | 0.591238 | 0.9894 | NaN | -0.0341 | 0.127 | 0.788364 | 0.936 | 0.0575 | 0.1516 | 0.70449 | 0.8719 | -0.0915 | 0.1865 | 0.623876 | 0.9375 | NaN | -0.0386 | 0.1259 | 0.758804 | 0.938 | 0.093 | 0.1456 | 0.52277 | 0.8496 | -0.1126 | 0.1873 | 0.547964 | 0.9621 | NaN | -0.0351 | 0.1273 | 0.782754 | 0.9414 | 0.04 | 0.1494 | 0.788908 | 0.9225 | -0.0831 | 0.1883 | 0.65911 | 0.9459 |
| uridine | 244.0701 | 1.340193 | Nucleotide | Pyrimidine Metabolism, Uracil containing | 0.1796 | 0.138 | 0.193285 | 0.5541 | 0.1199 | 0.133 | 0.367326 | 0.6407 | 0.2386 | 0.2427 | 0.325494 | 0.7534 | NaN | 0.1203 | 0.1283 | 0.34833 | 0.8386 | 0.0841 | 0.1171 | 0.472772 | 0.8671 | 0.1494 | 0.2294 | 0.515043 | 0.954 | NaN | 0.1508 | 0.1276 | 0.237351 | 0.7361 | 0.0731 | 0.1151 | 0.525765 | 0.9053 | 0.2379 | 0.2291 | 0.298888 | 0.9428 | NaN | 0.1687 | 0.1305 | 0.196043 | 0.6639 | 0.1078 | 0.1217 | 0.375984 | 0.6783 | 0.2264 | 0.2307 | 0.326543 | 0.9044 | NaN | 0.0919 | 0.1308 | 0.482082 | 0.8625 | 0.0552 | 0.118 | 0.640236 | 0.8623 | 0.1256 | 0.2353 | 0.59341 | 0.9621 | NaN | 0.1416 | 0.1312 | 0.28044 | 0.7337 | 0.0952 | 0.1201 | 0.428 | 0.7448 | 0.1813 | 0.2341 | 0.438674 | 0.8887 |
| indole-3-acetaldehyde | 159.0686 | 1.769727 | Organic Compound | 3-alkylindoles | 0.034 | 0.1331 | 0.79815 | 0.9609 | 0.1016 | 0.1312 | 0.438695 | 0.7101 | -0.0441 | 0.2312 | 0.848862 | 0.9732 | NaN | 0.0224 | 0.1231 | 0.855682 | 0.9705 | 0.0104 | 0.1168 | 0.928795 | 0.9729 | 0.0302 | 0.2177 | 0.889731 | 0.977 | NaN | 0.0511 | 0.1229 | 0.677316 | 0.9406 | 0.0372 | 0.1138 | 0.743951 | 0.9241 | 0.0511 | 0.2198 | 0.816028 | 0.9935 | NaN | 0.0605 | 0.1259 | 0.630779 | 0.8606 | 0.0364 | 0.1213 | 0.764306 | 0.8996 | 0.0892 | 0.223 | 0.689327 | 0.9476 | NaN | 0.0218 | 0.1247 | 0.861412 | 0.962 | -0.0078 | 0.1176 | 0.947187 | 0.9923 | 0.0344 | 0.2221 | 0.87672 | 0.9621 | NaN | 0.0323 | 0.1261 | 0.797839 | 0.9471 | 0.028 | 0.1196 | 0.814951 | 0.9294 | 0.018 | 0.2228 | 0.935772 | 0.9869 |
| porphobilinogen | 226.0821 | 6.687804 | Organic nitrogen compounds | Amines | 0.1221 | 0.1325 | 0.356915 | 0.7161 | 0.1347 | 0.1557 | 0.387082 | 0.6593 | 0.1011 | 0.1995 | 0.612161 | 0.8995 | NaN | 0.0441 | 0.1235 | 0.721331 | 0.9325 | 0.0008 | 0.1395 | 0.995291 | 0.9953 | 0.0538 | 0.1877 | 0.774544 | 0.954 | NaN | 0.0139 | 0.124 | 0.911003 | 0.9717 | 0.0655 | 0.135 | 0.627649 | 0.9053 | -0.0324 | 0.1922 | 0.866105 | 0.9935 | NaN | 0.0648 | 0.126 | 0.606998 | 0.8573 | -0.0029 | 0.1466 | 0.984036 | 0.9926 | 0.0866 | 0.1897 | 0.648158 | 0.9375 | NaN | 0.0605 | 0.1249 | 0.628204 | 0.8971 | 0.004 | 0.1397 | 0.97698 | 0.9923 | 0.0752 | 0.1907 | 0.693527 | 0.9621 | NaN | 0.0674 | 0.1263 | 0.593284 | 0.8765 | -0.0387 | 0.1456 | 0.790506 | 0.9225 | 0.1064 | 0.1914 | 0.578411 | 0.9205 |
| methyl beta-D-galactoside | 194.0788 | 0.883257 | Organic oxygen compounds | Carbohydrates and carbohydrate conjugates | -0.1296 | 0.1325 | 0.327701 | 0.6942 | -0.1091 | 0.14 | 0.435605 | 0.7072 | -0.1307 | 0.2144 | 0.542072 | 0.8663 | NaN | -0.0956 | 0.1227 | 0.435927 | 0.8498 | -0.0561 | 0.1235 | 0.649772 | 0.9079 | -0.1101 | 0.2012 | 0.584223 | 0.954 | NaN | -0.1786 | 0.1222 | 0.143968 | 0.6585 | -0.0779 | 0.1208 | 0.519009 | 0.9053 | -0.2594 | 0.2041 | 0.203682 | 0.8462 | NaN | -0.129 | 0.1252 | 0.302896 | 0.741 | -0.1171 | 0.1279 | 0.35986 | 0.6762 | -0.1088 | 0.204 | 0.593639 | 0.9375 | NaN | -0.0914 | 0.1245 | 0.462522 | 0.8625 | -0.0548 | 0.1238 | 0.657707 | 0.8623 | -0.1021 | 0.205 | 0.618348 | 0.9621 | NaN | -0.1102 | 0.1256 | 0.380522 | 0.7638 | -0.1015 | 0.1261 | 0.420667 | 0.7395 | -0.091 | 0.2063 | 0.658998 | 0.9459 |
| 3-hydroxybenzaldehyde | 122.0371 | 4.799146 | Organic oxygen compounds | Carbonyl compounds | -0.0136 | 0.1317 | 0.91756 | 0.9809 | -0.0594 | 0.1347 | 0.659247 | 0.8483 | 0.0501 | 0.219 | 0.81917 | 0.9713 | NaN | 0.014 | 0.1219 | 0.908468 | 0.9737 | 0.0306 | 0.1195 | 0.797675 | 0.965 | -0.0029 | 0.2059 | 0.988599 | 0.9976 | NaN | 0.0419 | 0.1219 | 0.731416 | 0.9567 | 0.045 | 0.1174 | 0.701755 | 0.9195 | 0.0355 | 0.2068 | 0.863654 | 0.9935 | NaN | -0.0043 | 0.1245 | 0.97243 | 0.9884 | -0.0004 | 0.1241 | 0.997481 | 0.9975 | -0.0041 | 0.2088 | 0.984477 | 0.9923 | NaN | -0.0064 | 0.1234 | 0.958879 | 0.9796 | 0.0105 | 0.1193 | 0.92999 | 0.9852 | -0.0104 | 0.21 | 0.960367 | 0.9872 | NaN | 0.0082 | 0.1249 | 0.947723 | 0.9794 | -0.0072 | 0.122 | 0.953066 | 0.9834 | 0.0363 | 0.2102 | 0.862728 | 0.9641 |
| 2,3-dihydroxybenzoate | 154.0262 | 4.700874 | Organoheterocyclic compounds | Benzoate and derivatives | 0.195 | 0.1274 | 0.125766 | 0.4924 | 0.2778 | 0.1328 | 0.036509 | 0.2877 | 0.1558 | 0.2085 | 0.454789 | 0.8098 | NaN | 0.1855 | 0.1178 | 0.115132 | 0.6749 | 0.2222 | 0.1175 | 0.058618 | 0.4622 | 0.2069 | 0.1955 | 0.289792 | 0.9223 | NaN | 0.149 | 0.1181 | 0.207075 | 0.7361 | 0.2422 | 0.1145 | 0.034484 | 0.3807 | 0.1002 | 0.1978 | 0.612531 | 0.9894 | NaN | 0.177 | 0.1205 | 0.142033 | 0.6148 | 0.2065 | 0.1237 | 0.095088 | 0.4302 | 0.2205 | 0.1984 | 0.266513 | 0.8705 | NaN | 0.1847 | 0.1194 | 0.121686 | 0.6708 | 0.2163 | 0.118 | 0.066868 | 0.4198 | 0.1984 | 0.1991 | 0.319037 | 0.9106 | NaN | 0.1859 | 0.1207 | 0.123563 | 0.5931 | 0.198 | 0.122 | 0.104676 | 0.4566 | 0.2325 | 0.2008 | 0.246807 | 0.8424 |
| 5-methoxytryptophol | 191.0925 | 10.292022 | Organoheterocyclic compounds | Indoles | 0.0871 | 0.1323 | 0.510247 | 0.8117 | 0.135 | 0.1572 | 0.390573 | 0.6593 | 0.0474 | 0.1976 | 0.810565 | 0.9713 | NaN | 0.026 | 0.1229 | 0.832147 | 0.967 | 0.003 | 0.1408 | 0.983226 | 0.9953 | 0.0275 | 0.1854 | 0.882177 | 0.977 | NaN | -0.0096 | 0.1234 | 0.938035 | 0.9728 | 0.0728 | 0.1362 | 0.592885 | 0.9053 | -0.0701 | 0.1893 | 0.711149 | 0.99 | NaN | 0.0405 | 0.1255 | 0.747067 | 0.9144 | -0.0204 | 0.1489 | 0.89131 | 0.9695 | 0.0631 | 0.1878 | 0.737068 | 0.9572 | NaN | 0.0374 | 0.1244 | 0.763489 | 0.938 | 0.0016 | 0.1411 | 0.990713 | 0.9941 | 0.0411 | 0.1887 | 0.827701 | 0.9621 | NaN | 0.0478 | 0.1257 | 0.703834 | 0.9035 | -0.0447 | 0.1473 | 0.761726 | 0.9096 | 0.0803 | 0.1898 | 0.672215 | 0.9459 |
| 3-indolepropionic acid | 189.0794 | 10.379467 | Organoheterocyclic compounds | Indolyl carboxylic acids and derivatives | -0.1141 | 0.1284 | 0.374352 | 0.7191 | -0.08 | 0.1361 | 0.556692 | 0.7957 | -0.179 | 0.2085 | 0.390483 | 0.7585 | NaN | -0.0637 | 0.1192 | 0.592892 | 0.9079 | 0.0756 | 0.1229 | 0.538425 | 0.8967 | -0.2166 | 0.1953 | 0.267447 | 0.9223 | NaN | -0.059 | 0.1191 | 0.620065 | 0.9181 | 0.0296 | 0.1189 | 0.803416 | 0.9363 | -0.1388 | 0.1974 | 0.481861 | 0.9848 | NaN | -0.0938 | 0.1215 | 0.440407 | 0.7844 | -0.027 | 0.1253 | 0.829292 | 0.9302 | -0.1904 | 0.198 | 0.336272 | 0.9044 | NaN | -0.1234 | 0.1203 | 0.304859 | 0.7529 | 0.0122 | 0.1212 | 0.919791 | 0.9808 | -0.2654 | 0.1997 | 0.183917 | 0.8608 | NaN | -0.1074 | 0.1217 | 0.377461 | 0.7638 | -0.0242 | 0.1234 | 0.844278 | 0.9453 | -0.2116 | 0.2 | 0.289962 | 0.8424 |
| 5-valerolactone | 100.0525 | 1.741256 | Organoheterocyclic compounds | Lactones | 0.0912 | 0.1322 | 0.490497 | 0.8041 | 0.2276 | 0.1326 | 0.086025 | 0.3625 | -0.0475 | 0.2206 | 0.829361 | 0.9732 | NaN | 0.0652 | 0.1224 | 0.594285 | 0.9079 | 0.1873 | 0.1168 | 0.108938 | 0.6118 | -0.0489 | 0.2069 | 0.813126 | 0.9632 | NaN | 0.0549 | 0.1223 | 0.653731 | 0.9331 | 0.2059 | 0.1141 | 0.071095 | 0.5732 | -0.0854 | 0.2084 | 0.681801 | 0.9894 | NaN | 0.0683 | 0.1252 | 0.585108 | 0.8473 | 0.1677 | 0.1228 | 0.171902 | 0.5146 | -0.0196 | 0.2099 | 0.925438 | 0.99 | NaN | 0.0938 | 0.1239 | 0.448847 | 0.8543 | 0.2183 | 0.1163 | 0.06046 | 0.4149 | -0.0275 | 0.2107 | 0.896109 | 0.9681 | NaN | 0.0778 | 0.1253 | 0.534724 | 0.8482 | 0.152 | 0.1214 | 0.210636 | 0.5756 | 0.0089 | 0.2125 | 0.96642 | 0.9896 |
| 2,4-dihydroxypteridine | 164.0331 | 1.32753 | Organoheterocyclic compounds | Pteridines and derivatives | -0.0213 | 0.1399 | 0.879062 | 0.9809 | 0.0475 | 0.1344 | 0.723575 | 0.8915 | -0.1147 | 0.2467 | 0.641932 | 0.9104 | NaN | -0.0149 | 0.1294 | 0.908021 | 0.9737 | 0.0792 | 0.1179 | 0.501562 | 0.8931 | -0.1406 | 0.2313 | 0.54344 | 0.954 | NaN | -0.036 | 0.1292 | 0.780298 | 0.9641 | 0.0617 | 0.1157 | 0.594003 | 0.9053 | -0.1549 | 0.233 | 0.50618 | 0.9894 | NaN | -0.0571 | 0.1324 | 0.66604 | 0.8697 | 0.0475 | 0.1229 | 0.699141 | 0.8672 | -0.2056 | 0.2354 | 0.382473 | 0.926 | NaN | -0.0366 | 0.1311 | 0.779955 | 0.938 | 0.0596 | 0.1181 | 0.613705 | 0.8623 | -0.1589 | 0.2357 | 0.500117 | 0.9436 | NaN | -0.0672 | 0.1328 | 0.612634 | 0.8808 | 0.0288 | 0.1211 | 0.812392 | 0.9294 | -0.1961 | 0.2377 | 0.409229 | 0.8887 |
| salsolinol | 179.0938 | 1.273321 | Organoheterocyclic compounds | Tetrahydroisoquinolines | 0.0288 | 0.1259 | 0.819307 | 0.9693 | -0.4065 | 0.2889 | 0.159371 | 0.4755 | 0.0733 | 0.1584 | 0.643331 | 0.9104 | NaN | 0.0444 | 0.1164 | 0.70302 | 0.9314 | -0.3124 | 0.2548 | 0.220105 | 0.7408 | 0.0749 | 0.1485 | 0.614167 | 0.954 | NaN | 0.0009 | 0.1164 | 0.99394 | 0.9939 | -0.3378 | 0.2493 | 0.175463 | 0.7308 | 0.0282 | 0.1502 | 0.851176 | 0.9935 | NaN | 0.0823 | 0.1194 | 0.490651 | 0.8037 | -0.3831 | 0.2641 | 0.146875 | 0.4863 | 0.1326 | 0.1511 | 0.380123 | 0.926 | NaN | 0.046 | 0.118 | 0.69651 | 0.9116 | -0.299 | 0.2557 | 0.24214 | 0.7302 | 0.0769 | 0.1512 | 0.610814 | 0.9621 | NaN | 0.0585 | 0.1194 | 0.624253 | 0.8808 | -0.4054 | 0.2596 | 0.118398 | 0.4771 | 0.1027 | 0.1521 | 0.499598 | 0.8946 |
| dipepetide (aspartate glutamate) | 262.0823 | 15.655098 | Peptide | Dipeptide | 0.0696 | 0.1323 | 0.599025 | 0.8544 | 0.0269 | 0.1367 | 0.843795 | 0.932 | 0.0805 | 0.221 | 0.715794 | 0.9594 | NaN | 0.0937 | 0.1223 | 0.443919 | 0.8498 | 0.0663 | 0.12 | 0.580425 | 0.904 | 0.1104 | 0.2073 | 0.594326 | 0.954 | NaN | 0.0535 | 0.1222 | 0.661686 | 0.935 | 0.0527 | 0.1177 | 0.654531 | 0.9055 | 0.0626 | 0.2088 | 0.764167 | 0.9935 | NaN | 0.1171 | 0.1253 | 0.349727 | 0.7467 | 0.0711 | 0.1253 | 0.57003 | 0.7946 | 0.1495 | 0.2107 | 0.477903 | 0.9375 | NaN | 0.0716 | 0.124 | 0.563297 | 0.8722 | 0.0584 | 0.1202 | 0.627449 | 0.8623 | 0.0746 | 0.2111 | 0.723657 | 0.9621 | NaN | 0.1078 | 0.1255 | 0.390209 | 0.7748 | 0.065 | 0.1232 | 0.597853 | 0.8209 | 0.1371 | 0.2126 | 0.518905 | 0.8946 |
| dipeptide (phenylalanine phenylalanine) | 312.1484 | 8.417695 | Peptide | Dipeptide | 0.058 | 0.1296 | 0.65433 | 0.8767 | 0.0438 | 0.1771 | 0.804569 | 0.932 | 0.0554 | 0.1815 | 0.760317 | 0.9647 | NaN | -0.0248 | 0.1207 | 0.837046 | 0.9673 | -0.1367 | 0.1584 | 0.388246 | 0.8339 | 0.0065 | 0.1708 | 0.969457 | 0.9911 | NaN | 0.0092 | 0.12 | 0.93885 | 0.9728 | -0.1026 | 0.1543 | 0.505905 | 0.9053 | 0.0434 | 0.1714 | 0.800331 | 0.9935 | NaN | 0.0324 | 0.1226 | 0.791562 | 0.936 | -0.1161 | 0.1657 | 0.483459 | 0.7493 | 0.0817 | 0.1726 | 0.635955 | 0.9375 | NaN | -0.0131 | 0.1222 | 0.91435 | 0.9796 | -0.1901 | 0.1605 | 0.236199 | 0.7254 | 0.0374 | 0.1734 | 0.829285 | 0.9621 | NaN | 0.0081 | 0.1233 | 0.947844 | 0.9794 | -0.1388 | 0.1635 | 0.395719 | 0.7162 | 0.0477 | 0.1742 | 0.784043 | 0.9525 |
| dipeptide (serine histidine) | 242.1028 | 17.227266 | Peptide | Dipeptide | 0.0125 | 0.1312 | 0.924189 | 0.9811 | -0.0971 | 0.1414 | 0.492207 | 0.7545 | 0.0646 | 0.2111 | 0.759587 | 0.9647 | NaN | 0.0206 | 0.1214 | 0.865063 | 0.9705 | -0.0787 | 0.1242 | 0.526048 | 0.8967 | 0.0583 | 0.198 | 0.768569 | 0.954 | NaN | -0.0235 | 0.1213 | 0.8467 | 0.9714 | -0.1223 | 0.1215 | 0.314251 | 0.8421 | 0.0296 | 0.1997 | 0.881967 | 0.9935 | NaN | 0.0207 | 0.1241 | 0.867222 | 0.9747 | -0.0178 | 0.1309 | 0.891762 | 0.9695 | -0.0155 | 0.2022 | 0.938904 | 0.99 | NaN | 0.0069 | 0.123 | 0.955459 | 0.9796 | -0.0804 | 0.1244 | 0.517804 | 0.8496 | 0.0393 | 0.2018 | 0.845485 | 0.9621 | NaN | 0.0343 | 0.1244 | 0.782746 | 0.9414 | -0.0127 | 0.1289 | 0.921424 | 0.979 | 0.0232 | 0.2031 | 0.90913 | 0.9783 |
| dipeptide (glutamate isoleucine/leucine) | 262.1323 | 6.182869 | Peptide | Dipeptide | 0.209 | 0.1342 | 0.119356 | 0.4809 | 0.2684 | 0.1314 | 0.041164 | 0.2929 | 0.1866 | 0.2323 | 0.421872 | 0.7762 | NaN | 0.1003 | 0.1261 | 0.426174 | 0.8498 | 0.1673 | 0.1183 | 0.157279 | 0.6528 | 0.0503 | 0.2215 | 0.820156 | 0.9653 | NaN | 0.1503 | 0.1246 | 0.22786 | 0.7361 | 0.2504 | 0.1128 | 0.026462 | 0.3319 | 0.0408 | 0.2238 | 0.855314 | 0.9935 | NaN | 0.1453 | 0.1279 | 0.256155 | 0.7164 | 0.1872 | 0.123 | 0.127896 | 0.4699 | 0.1366 | 0.2216 | 0.537458 | 0.9375 | NaN | 0.1159 | 0.1275 | 0.363528 | 0.7978 | 0.1678 | 0.1185 | 0.156844 | 0.631 | 0.0832 | 0.2247 | 0.711054 | 0.9621 | NaN | 0.1461 | 0.1282 | 0.254481 | 0.7204 | 0.1687 | 0.1218 | 0.166038 | 0.5427 | 0.1523 | 0.2234 | 0.495385 | 0.8907 |
| dipeptide (glutamate phenylalanine) | 294.1236 | 2.800813 | Peptide | Dipeptide | 0.1224 | 0.1362 | 0.368881 | 0.7161 | 0.1743 | 0.1336 | 0.19221 | 0.4993 | 0.1068 | 0.236 | 0.650888 | 0.9119 | NaN | -0.039 | 0.1292 | 0.763002 | 0.9512 | 0.0446 | 0.1209 | 0.712316 | 0.934 | -0.103 | 0.228 | 0.651555 | 0.954 | NaN | 0.03 | 0.127 | 0.813376 | 0.9676 | 0.0818 | 0.117 | 0.484129 | 0.9053 | -0.0168 | 0.2257 | 0.94077 | 0.9948 | NaN | 0.0043 | 0.1313 | 0.974109 | 0.9884 | 0.0837 | 0.1249 | 0.502773 | 0.7583 | -0.0485 | 0.2292 | 0.832375 | 0.9726 | NaN | -0.0794 | 0.1334 | 0.551717 | 0.8701 | -0.0117 | 0.124 | 0.925029 | 0.982 | -0.1243 | 0.2363 | 0.59891 | 0.9621 | NaN | -0.0081 | 0.1322 | 0.950992 | 0.9794 | 0.0554 | 0.1241 | 0.655164 | 0.8652 | -0.0437 | 0.2321 | 0.850702 | 0.9641 |
| dipeptide (isoleucine/leucine isoleucine/leucine) | 244.1532 | 5.463248 | Peptide | Dipeptide | 0.17 | 0.1957 | 0.385023 | 0.7254 | -0.0304 | 0.1717 | 0.859316 | 0.932 | 0.5333 | 0.3939 | 0.175775 | 0.6772 | NaN | 0.0434 | 0.1826 | 0.812115 | 0.9614 | -0.1003 | 0.1509 | 0.506423 | 0.8931 | 0.2939 | 0.3772 | 0.435884 | 0.9478 | NaN | 0.1528 | 0.1808 | 0.398007 | 0.8469 | 0.0581 | 0.1486 | 0.695606 | 0.9195 | 0.3138 | 0.3793 | 0.40807 | 0.9816 | NaN | 0.0951 | 0.1859 | 0.609105 | 0.8573 | -0.0647 | 0.1571 | 0.680268 | 0.853 | 0.3634 | 0.3796 | 0.338462 | 0.9044 | NaN | 0.0882 | 0.1843 | 0.63243 | 0.8971 | -0.073 | 0.151 | 0.628683 | 0.8623 | 0.3784 | 0.3809 | 0.320408 | 0.9106 | NaN | 0.0991 | 0.1863 | 0.594748 | 0.8765 | -0.083 | 0.1548 | 0.59187 | 0.8199 | 0.4184 | 0.3811 | 0.272186 | 0.8424 |
| dipeptide (isoleucine/leucine valine) | 230.1634 | 3.14795 | Peptide | Dipeptide | 0.0014 | 0.1351 | 0.991845 | 0.9936 | -0.0174 | 0.1401 | 0.901215 | 0.953 | 0.0221 | 0.2241 | 0.921417 | 0.9838 | NaN | -0.0451 | 0.1251 | 0.718518 | 0.9325 | -0.0235 | 0.123 | 0.848624 | 0.9729 | -0.0499 | 0.211 | 0.81308 | 0.9632 | NaN | 0.0064 | 0.1247 | 0.958815 | 0.9747 | -0.0089 | 0.1207 | 0.941523 | 0.9765 | 0.0431 | 0.2117 | 0.838713 | 0.9935 | NaN | -0.0339 | 0.1279 | 0.790936 | 0.936 | -0.033 | 0.1282 | 0.796652 | 0.9169 | -0.0139 | 0.2133 | 0.948027 | 0.99 | NaN | -0.0846 | 0.1274 | 0.506644 | 0.8625 | -0.1038 | 0.1238 | 0.401928 | 0.8162 | -0.0508 | 0.2151 | 0.813387 | 0.9621 | NaN | -0.0431 | 0.1283 | 0.73671 | 0.918 | -0.0561 | 0.1264 | 0.657386 | 0.8661 | -0.0106 | 0.2153 | 0.960797 | 0.9892 |
| dipeptide (isoleucine/leucine alanine) | 202.1322 | 2.070814 | Peptide | Dipeptide | 0.02 | 0.1321 | 0.879595 | 0.9809 | -0.0852 | 0.1514 | 0.573665 | 0.8007 | 0.0751 | 0.2005 | 0.708017 | 0.9556 | NaN | -0.0312 | 0.1224 | 0.798713 | 0.9571 | -0.1301 | 0.1327 | 0.326657 | 0.8095 | 0.0191 | 0.1887 | 0.919385 | 0.9835 | NaN | 0.0176 | 0.1219 | 0.885261 | 0.9714 | -0.0818 | 0.1303 | 0.530105 | 0.9053 | 0.0745 | 0.1893 | 0.693739 | 0.9894 | NaN | 0.0337 | 0.1249 | 0.787448 | 0.936 | -0.1054 | 0.1383 | 0.446243 | 0.7319 | 0.1143 | 0.1907 | 0.548996 | 0.9375 | NaN | -0.0478 | 0.1244 | 0.700968 | 0.9116 | -0.1807 | 0.1332 | 0.174867 | 0.6515 | 0.0247 | 0.1922 | 0.897573 | 0.9681 | NaN | 0.0031 | 0.1252 | 0.98017 | 0.9943 | -0.1383 | 0.1363 | 0.310202 | 0.6689 | 0.0798 | 0.1924 | 0.678208 | 0.9459 |
| possible peptide | 247.1106 | 4.573735 | Peptide | Dipeptide | -0.0268 | 0.1294 | 0.835651 | 0.9752 | -0.0527 | 0.1476 | 0.721345 | 0.8908 | -0.0098 | 0.1971 | 0.960406 | 0.9887 | NaN | -0.0621 | 0.1197 | 0.60414 | 0.9079 | -0.0873 | 0.1295 | 0.500067 | 0.8931 | -0.0425 | 0.185 | 0.818141 | 0.9653 | NaN | -0.0386 | 0.1194 | 0.74687 | 0.96 | -0.0336 | 0.1273 | 0.79155 | 0.9363 | -0.0389 | 0.1862 | 0.83454 | 0.9935 | NaN | -0.0483 | 0.1223 | 0.692733 | 0.8831 | -0.1004 | 0.1352 | 0.457554 | 0.7319 | -0.0075 | 0.1874 | 0.967962 | 0.99 | NaN | -0.0513 | 0.1213 | 0.67254 | 0.9077 | -0.0788 | 0.1298 | 0.543527 | 0.8618 | -0.0304 | 0.1883 | 0.871694 | 0.9621 | NaN | -0.0476 | 0.1226 | 0.69793 | 0.9035 | -0.1185 | 0.1332 | 0.373688 | 0.6983 | 0.0019 | 0.1892 | 0.991877 | 0.9991 |
| possible peptide | 278.1628 | 7.824666 | Peptide | Dipeptide | 0.1133 | 0.1236 | 0.359423 | 0.7161 | 0.0784 | 0.1465 | 0.592482 | 0.8115 | 0.1166 | 0.1851 | 0.528782 | 0.8655 | NaN | 0.0265 | 0.1155 | 0.818636 | 0.9614 | -0.0456 | 0.1308 | 0.727343 | 0.9386 | 0.052 | 0.1746 | 0.765834 | 0.954 | NaN | 0.115 | 0.1141 | 0.313676 | 0.7952 | 0.0834 | 0.1261 | 0.50829 | 0.9053 | 0.1263 | 0.1747 | 0.469452 | 0.9816 | NaN | 0.0562 | 0.1176 | 0.632842 | 0.8606 | -0.0608 | 0.1379 | 0.659359 | 0.8438 | 0.106 | 0.176 | 0.546812 | 0.9375 | NaN | 0.0303 | 0.1171 | 0.795763 | 0.9487 | -0.1089 | 0.1332 | 0.413926 | 0.8188 | 0.0886 | 0.177 | 0.616733 | 0.9621 | NaN | 0.0427 | 0.1183 | 0.718328 | 0.9116 | -0.0901 | 0.1366 | 0.509269 | 0.786 | 0.0944 | 0.1778 | 0.595559 | 0.9357 |
| possible peptide | 282.1234 | 8.5111 | Peptide | Dipeptide | 0.0172 | 0.1346 | 0.898433 | 0.9809 | -0.11 | 0.1696 | 0.516756 | 0.773 | 0.074 | 0.1955 | 0.705205 | 0.9541 | NaN | 0.0008 | 0.1245 | 0.994881 | 0.9999 | -0.0916 | 0.1489 | 0.538626 | 0.8967 | 0.0494 | 0.1835 | 0.787721 | 0.9557 | NaN | 0.0764 | 0.1245 | 0.539792 | 0.9125 | -0.1165 | 0.1459 | 0.424656 | 0.8947 | 0.1862 | 0.1863 | 0.317645 | 0.9479 | NaN | -0.0093 | 0.1273 | 0.94154 | 0.9828 | -0.1151 | 0.155 | 0.457584 | 0.7319 | 0.0457 | 0.1861 | 0.80618 | 0.9662 | NaN | -0.0097 | 0.1262 | 0.938553 | 0.9796 | -0.134 | 0.1489 | 0.368309 | 0.7973 | 0.055 | 0.1868 | 0.768475 | 0.9621 | NaN | -0.0262 | 0.1278 | 0.837745 | 0.9501 | -0.1134 | 0.1527 | 0.457497 | 0.7516 | 0.0204 | 0.1886 | 0.913858 | 0.9795 |
| possible peptide | 409.138 | 8.470251 | Peptide | Dipeptide | -0.0619 | 0.1567 | 0.692809 | 0.9084 | 0.1421 | 0.155 | 0.359094 | 0.6361 | -0.2747 | 0.2659 | 0.301668 | 0.7534 | NaN | -0.0487 | 0.1449 | 0.736873 | 0.9401 | 0.1479 | 0.1358 | 0.276119 | 0.798 | -0.2609 | 0.2494 | 0.295451 | 0.9223 | NaN | -0.0156 | 0.1449 | 0.914196 | 0.9717 | 0.1682 | 0.1331 | 0.206142 | 0.7942 | -0.2144 | 0.2521 | 0.395122 | 0.9816 | NaN | -0.0189 | 0.1484 | 0.898749 | 0.9805 | 0.1779 | 0.1414 | 0.208417 | 0.5478 | -0.2324 | 0.2534 | 0.35892 | 0.9215 | NaN | -0.0297 | 0.147 | 0.839926 | 0.9611 | 0.171 | 0.1359 | 0.208263 | 0.6925 | -0.2453 | 0.2542 | 0.334626 | 0.9106 | NaN | -0.027 | 0.1487 | 0.855765 | 0.9543 | 0.1435 | 0.1395 | 0.303462 | 0.6619 | -0.2119 | 0.2565 | 0.408691 | 0.8887 |
| possible peptide | 414.2051 | 18.41231 | Peptide | Dipeptide | 0.1161 | 0.1357 | 0.392313 | 0.726 | 0.2128 | 0.1776 | 0.230917 | 0.5267 | 0.1062 | 0.1952 | 0.586513 | 0.887 | NaN | 0.07 | 0.1259 | 0.578116 | 0.9079 | 0.1458 | 0.1568 | 0.35254 | 0.8148 | 0.0522 | 0.1838 | 0.776323 | 0.954 | NaN | 0.0809 | 0.1256 | 0.519659 | 0.9101 | 0.178 | 0.1532 | 0.245293 | 0.8037 | 0.0387 | 0.1855 | 0.834825 | 0.9935 | NaN | 0.0857 | 0.1286 | 0.504855 | 0.8172 | 0.1457 | 0.1637 | 0.373723 | 0.6783 | 0.0844 | 0.1857 | 0.649506 | 0.9375 | NaN | 0.0741 | 0.1276 | 0.561381 | 0.8722 | 0.1425 | 0.1572 | 0.364764 | 0.7947 | 0.0618 | 0.1871 | 0.741302 | 0.9621 | NaN | 0.0975 | 0.1287 | 0.448893 | 0.801 | 0.1602 | 0.1607 | 0.318942 | 0.672 | 0.0923 | 0.1874 | 0.622214 | 0.9459 |
| possible peptide | 445.2502 | 18.402573 | Peptide | Dipeptide | 0.0087 | 0.1387 | 0.949835 | 0.9855 | 0.0576 | 0.1572 | 0.713973 | 0.8876 | -0.0251 | 0.2124 | 0.905889 | 0.9838 | NaN | 0.0578 | 0.1284 | 0.652492 | 0.918 | 0.029 | 0.1381 | 0.833744 | 0.9729 | 0.0798 | 0.2009 | 0.691281 | 0.954 | NaN | 0.041 | 0.1281 | 0.749092 | 0.96 | 0.046 | 0.1354 | 0.734201 | 0.9241 | 0.0319 | 0.2012 | 0.873968 | 0.9935 | NaN | 0.0981 | 0.1321 | 0.457917 | 0.7844 | 0.1077 | 0.1439 | 0.454069 | 0.7319 | 0.0928 | 0.2047 | 0.65022 | 0.9375 | NaN | 0.1033 | 0.1309 | 0.43006 | 0.8452 | 0.0776 | 0.1381 | 0.574355 | 0.8623 | 0.1144 | 0.207 | 0.580336 | 0.9621 | NaN | 0.0876 | 0.1322 | 0.507499 | 0.8285 | 0.0879 | 0.1416 | 0.534788 | 0.8003 | 0.0835 | 0.2068 | 0.6863 | 0.9459 |
| dipeptide (serine isoleucine/leucine) | 218.1243 | 2.663722 | Peptide | Dipeptide | 0.2204 | 0.1384 | 0.111082 | 0.4781 | 0.2437 | 0.1394 | 0.080408 | 0.3594 | 0.2278 | 0.2318 | 0.325815 | 0.7534 | NaN | 0.1158 | 0.1298 | 0.372351 | 0.8459 | 0.0622 | 0.1293 | 0.630253 | 0.9073 | 0.2073 | 0.2175 | 0.340639 | 0.9223 | NaN | 0.1276 | 0.1292 | 0.323502 | 0.8008 | 0.1256 | 0.1231 | 0.307683 | 0.8367 | 0.1406 | 0.2208 | 0.524181 | 0.9894 | NaN | 0.1437 | 0.1322 | 0.277013 | 0.7387 | 0.094 | 0.1345 | 0.484614 | 0.7493 | 0.2446 | 0.2201 | 0.266439 | 0.8705 | NaN | 0.1027 | 0.1323 | 0.437461 | 0.8473 | 0.0978 | 0.1275 | 0.442947 | 0.8205 | 0.1309 | 0.2241 | 0.559048 | 0.9621 | NaN | 0.133 | 0.1329 | 0.317008 | 0.7485 | 0.0795 | 0.1327 | 0.549124 | 0.8019 | 0.2158 | 0.2225 | 0.332013 | 0.8727 |
| dipeptide (tyrosine histidine) | 341.1487 | 2.509147 | Peptide | Dipeptide | 0.2019 | 0.1387 | 0.145477 | 0.516 | 0.2109 | 0.156 | 0.176524 | 0.4964 | 0.2224 | 0.2139 | 0.298449 | 0.7534 | NaN | 0.0662 | 0.131 | 0.613565 | 0.9079 | 0.0255 | 0.1429 | 0.858156 | 0.9729 | 0.1185 | 0.2032 | 0.559578 | 0.954 | NaN | 0.0437 | 0.1316 | 0.740035 | 0.9589 | -0.0082 | 0.1413 | 0.953926 | 0.9769 | 0.0863 | 0.2065 | 0.675904 | 0.9894 | NaN | 0.1278 | 0.1324 | 0.334388 | 0.741 | 0.1006 | 0.1462 | 0.491454 | 0.7494 | 0.1787 | 0.204 | 0.381142 | 0.926 | NaN | 0.0833 | 0.1325 | 0.529522 | 0.8625 | 0.0401 | 0.1425 | 0.778225 | 0.9247 | 0.1327 | 0.2068 | 0.521072 | 0.9524 | NaN | 0.1268 | 0.1328 | 0.33946 | 0.7513 | 0.0803 | 0.1446 | 0.578519 | 0.8092 | 0.1843 | 0.2059 | 0.37081 | 0.8861 |
| dipeptide (methionine isoleucine/leucine) | 262.1418 | 8.063479 | Peptide | Dipeptide | -0.097 | 0.1317 | 0.461733 | 0.794 | -0.0179 | 0.1423 | 0.899634 | 0.953 | -0.2394 | 0.2226 | 0.282252 | 0.7534 | NaN | -0.0233 | 0.1226 | 0.849347 | 0.9705 | -0.0139 | 0.1249 | 0.911436 | 0.9729 | -0.1037 | 0.2129 | 0.626113 | 0.954 | NaN | -0.0248 | 0.1224 | 0.83933 | 0.9714 | -0.0125 | 0.1226 | 0.918892 | 0.973 | -0.0884 | 0.2156 | 0.681919 | 0.9894 | NaN | -0.0079 | 0.1261 | 0.94997 | 0.9828 | 0.0161 | 0.1304 | 0.90186 | 0.9695 | -0.1193 | 0.2157 | 0.580282 | 0.9375 | NaN | -0.0182 | 0.1245 | 0.883881 | 0.9672 | -0.0104 | 0.1252 | 0.933607 | 0.9854 | -0.1029 | 0.2181 | 0.63693 | 0.9621 | NaN | -0.0205 | 0.126 | 0.870847 | 0.9588 | -0.0175 | 0.1282 | 0.891357 | 0.9667 | -0.1143 | 0.2188 | 0.601374 | 0.9357 |
| L-gamma-glutamyl-L-isoleucine | 260.1368 | 4.586305 | Peptide | Gamma-glutamyl Amino Acid | 0.1873 | 0.1352 | 0.165741 | 0.531 | 0.3627 | 0.1499 | 0.015551 | 0.2 | 0.0745 | 0.2075 | 0.719582 | 0.9594 | NaN | 0.0168 | 0.1291 | 0.8963 | 0.9705 | 0.128 | 0.1438 | 0.373181 | 0.824 | -0.0339 | 0.1968 | 0.863047 | 0.977 | NaN | 0.0638 | 0.1271 | 0.615778 | 0.9162 | 0.2393 | 0.1327 | 0.071406 | 0.5732 | -0.0416 | 0.1986 | 0.833951 | 0.9935 | NaN | 0.0597 | 0.1311 | 0.648896 | 0.8652 | 0.1697 | 0.1497 | 0.257029 | 0.5881 | 0.0112 | 0.1982 | 0.954772 | 0.99 | NaN | 0.0503 | 0.13 | 0.698677 | 0.9116 | 0.1874 | 0.1394 | 0.178776 | 0.6534 | -0.0291 | 0.2008 | 0.884678 | 0.9633 | NaN | 0.0708 | 0.131 | 0.588803 | 0.8765 | 0.1559 | 0.1472 | 0.289522 | 0.6559 | 0.029 | 0.1998 | 0.884687 | 0.9702 |
| n-gamma-L-glutamyl-L-methionine | 278.0956 | 2.337805 | Peptide | Gamma-glutamyl Amino Acid | 0.27 | 0.1435 | 0.059837 | 0.3473 | 0.3778 | 0.1613 | 0.019197 | 0.2078 | 0.1869 | 0.2198 | 0.395091 | 0.7626 | NaN | 0.1677 | 0.1345 | 0.212587 | 0.7484 | 0.2396 | 0.1462 | 0.101254 | 0.6075 | 0.1133 | 0.2075 | 0.585035 | 0.954 | NaN | 0.1447 | 0.135 | 0.284052 | 0.7865 | 0.251 | 0.1425 | 0.078142 | 0.5751 | 0.0717 | 0.2107 | 0.733765 | 0.9927 | NaN | 0.2183 | 0.1364 | 0.109464 | 0.5709 | 0.278 | 0.1511 | 0.065849 | 0.3599 | 0.1694 | 0.209 | 0.417714 | 0.9375 | NaN | 0.1919 | 0.1358 | 0.157616 | 0.6753 | 0.2911 | 0.1438 | 0.042963 | 0.3563 | 0.1163 | 0.2114 | 0.582189 | 0.9621 | NaN | 0.2261 | 0.1365 | 0.097639 | 0.55 | 0.2869 | 0.1479 | 0.052455 | 0.3016 | 0.1724 | 0.211 | 0.413986 | 0.8887 |
| tripeptide (cysteine histidine lysine) | 386.1737 | 16.45213 | Peptide | Tripeptide | -0.0092 | 0.1351 | 0.94562 | 0.9855 | 0.2354 | 0.1502 | 0.117022 | 0.3987 | -0.1381 | 0.2101 | 0.510973 | 0.8599 | NaN | -0.0817 | 0.1254 | 0.514926 | 0.8827 | 0.1365 | 0.1341 | 0.308599 | 0.8095 | -0.2039 | 0.1972 | 0.301217 | 0.9223 | NaN | -0.0381 | 0.1248 | 0.760179 | 0.96 | 0.182 | 0.13 | 0.161574 | 0.7193 | -0.1834 | 0.1984 | 0.355329 | 0.9578 | NaN | -0.069 | 0.1282 | 0.590161 | 0.8484 | 0.1177 | 0.1415 | 0.405503 | 0.6951 | -0.1514 | 0.1996 | 0.448176 | 0.9375 | NaN | -0.0804 | 0.1271 | 0.527151 | 0.8625 | 0.0962 | 0.1362 | 0.479906 | 0.8272 | -0.1745 | 0.2006 | 0.384371 | 0.9106 | NaN | -0.0668 | 0.1284 | 0.603198 | 0.8765 | 0.1085 | 0.1395 | 0.436773 | 0.7458 | -0.1514 | 0.2015 | 0.452412 | 0.8887 |
| Tripeptide (glycine proline valine) | 271.1541 | 2.897597 | Peptide | Tripeptide | 0.1444 | 0.1396 | 0.300855 | 0.6742 | 0.1688 | 0.164 | 0.303518 | 0.5924 | 0.1239 | 0.2115 | 0.558055 | 0.8707 | NaN | 0.0669 | 0.13 | 0.606793 | 0.9079 | 0.0096 | 0.1479 | 0.948081 | 0.9819 | 0.0847 | 0.1988 | 0.670025 | 0.954 | NaN | 0.0915 | 0.1294 | 0.479293 | 0.8967 | 0.0836 | 0.1426 | 0.557795 | 0.9053 | 0.0786 | 0.2003 | 0.694733 | 0.9894 | NaN | 0.1207 | 0.1321 | 0.360974 | 0.7539 | 0.065 | 0.1527 | 0.670278 | 0.8447 | 0.1383 | 0.201 | 0.49152 | 0.9375 | NaN | 0.065 | 0.1319 | 0.622394 | 0.8971 | -0.0064 | 0.1489 | 0.965722 | 0.9923 | 0.0863 | 0.2025 | 0.670109 | 0.9621 | NaN | 0.0993 | 0.1328 | 0.454483 | 0.8015 | 0.0357 | 0.1513 | 0.813649 | 0.9294 | 0.1141 | 0.203 | 0.574094 | 0.9205 |
| tripeptide (tryptophan tyrosine isoleucine/leucine) | 457.2177 | 4.079669 | Peptide | Tripeptide | 0.0892 | 0.1398 | 0.523348 | 0.8184 | 0.1681 | 0.1634 | 0.303692 | 0.5924 | 0.0216 | 0.2125 | 0.919068 | 0.9838 | NaN | 0.0037 | 0.1302 | 0.977168 | 0.9952 | 0.0292 | 0.1466 | 0.842068 | 0.9729 | -0.0387 | 0.1999 | 0.84663 | 0.9765 | NaN | 0.0588 | 0.1292 | 0.649246 | 0.9331 | 0.1076 | 0.1415 | 0.447105 | 0.8947 | 0.0119 | 0.2007 | 0.95287 | 0.9976 | NaN | 0.0633 | 0.1323 | 0.63242 | 0.8606 | 0.0658 | 0.1521 | 0.665343 | 0.8438 | 0.0332 | 0.202 | 0.8694 | 0.9856 | NaN | -0.0115 | 0.1325 | 0.930659 | 0.9796 | 0.0066 | 0.1478 | 0.964601 | 0.9923 | -0.0515 | 0.2041 | 0.800702 | 0.9621 | NaN | 0.0258 | 0.1332 | 0.846717 | 0.9532 | 0.0148 | 0.1517 | 0.922243 | 0.979 | -0.0033 | 0.2041 | 0.987084 | 0.9991 |
| diethylstilbestrol | 268.1314 | 18.64137 | Phenylpropanoids and polyketides | Stilbenes | -0.0139 | 0.1427 | 0.922457 | 0.9811 | 0.3168 | 0.1535 | 0.038982 | 0.2877 | -0.2154 | 0.2249 | 0.338227 | 0.7534 | NaN | -0.1204 | 0.133 | 0.365095 | 0.8459 | 0.1275 | 0.1423 | 0.370362 | 0.824 | -0.2453 | 0.2106 | 0.244259 | 0.9223 | NaN | -0.0879 | 0.1322 | 0.506182 | 0.9053 | 0.2398 | 0.1336 | 0.072693 | 0.5732 | -0.3158 | 0.2128 | 0.137748 | 0.7382 | NaN | -0.1209 | 0.1364 | 0.375218 | 0.7615 | 0.1437 | 0.1496 | 0.336931 | 0.669 | -0.2431 | 0.2136 | 0.255001 | 0.8705 | NaN | -0.0915 | 0.1344 | 0.495839 | 0.8625 | 0.1509 | 0.1412 | 0.285018 | 0.7544 | -0.2283 | 0.2146 | 0.287212 | 0.9039 | NaN | -0.1043 | 0.1363 | 0.44408 | 0.801 | 0.1083 | 0.1493 | 0.468079 | 0.7618 | -0.2031 | 0.2159 | 0.346881 | 0.8785 |