## Sheet1
| Table S3. Significant associations between untargeted features and HOMA-CP, with combined dataset of boys and girls and sex-stratified. Regression models identified features from the untargeted platform (p=3272) linearly associated with the entire cohort (n=206), as well as for boys (n=98) and girls (n=108). Unannotated features are listed as "UNKNOWN." All models were adjusted for sex, age, and puberty onset (Model 1). Unadjusted p-value<0.05 highlighted in red. FDR<0.10 highlighted in green. AC, acylcarnitine; Cer, ceramide; DG, diglyceride; DiC, dicarboxylic group; FA, fatty acid; FDR, false discovery rate; HOMA-CP, homeostatic model assessment of insulin resistance using C-peptide; keto, ketone; N, negative ionization mode; OH, hydroxyl group; P, Positive ionization mode; PC, phosphatidylcholine; PE, phosphatidylethanolamine; StdErr, standard error. | 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 |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 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 |
| Metabolite | Neutral Mass | Retention time | Ionization Mode | Super Pathway | Sub Pathway | Model 1: Including sex, age, puberty onset | NaN | 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 | 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 |
| N-acetylglycine | 117.043 | 0.884938 | N | Amino Acid | Acetyl Amino Acid | -0.584082 | 0.136312 | 0.000018 | 0.008529 | -0.298207 | 0.135133 | 0.02733 | 0.273526 | -0.88479 | 0.233571 | 0.000152 | 0.041766 |
| N-acetyl-L-leucine | 173.1045 | 7.169957 | N | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.21686 | 0.136352 | 0.111736 | 0.689349 | 0.415288 | 0.120496 | 0.000568 | 0.050223 | -0.042526 | 0.253834 | 0.866949 | 0.995774 |
| lysine | 146.1055 | 0.511165 | P | Amino Acid | Lysine Metabolism | 0.436199 | 0.131679 | 0.000924 | 0.070785 | 0.275262 | 0.155293 | 0.076306 | 0.404767 | 0.517095 | 0.197787 | 0.008939 | 0.311356 |
| 3,4-hydroxyphenyl-lactate | 182.0573 | 3.796673 | N | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.16821 | 0.142796 | 0.238806 | 0.81478 | 0.491755 | 0.130194 | 0.000159 | 0.034122 | -0.182599 | 0.250771 | 0.466522 | 0.967952 |
| tyrosine | 181.0741 | 1.297716 | P | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.476021 | 0.135208 | 0.00043 | 0.045437 | 0.738259 | 0.147451 | 0.000001 | 0.001811 | 0.336269 | 0.204704 | 0.100443 | 0.75034 |
| proline | 115.0634 | 0.68809 | P | Amino Acid | Urea cycle; Arginine and Proline Metabolism | 0.487731 | 0.135784 | 0.000328 | 0.042953 | 0.384092 | 0.134456 | 0.004281 | 0.133164 | 0.606114 | 0.2297 | 0.008322 | 0.311356 |
| raffinose | 504.1699 | 0.718023 | N | Exogenous | Food Component/Plant | 0.269929 | 0.136909 | 0.048655 | 0.487836 | 0.485469 | 0.143957 | 0.000745 | 0.058264 | 0.101606 | 0.215976 | 0.638033 | 0.983456 |
| DG 32:0 | 568.5067 | 26.219461 | P | Lipid | Diacylglycerol | 0.532562 | 0.125145 | 0.000021 | 0.008529 | 0.342407 | 0.138785 | 0.013618 | 0.205733 | 0.692274 | 0.194655 | 0.000376 | 0.068338 |
| DG 34:0 | 618.5204 | 27.634111 | P | Lipid | Diacylglycerol | 0.470698 | 0.128342 | 0.000245 | 0.039163 | 0.336521 | 0.160405 | 0.03591 | 0.30323 | 0.548049 | 0.187612 | 0.003487 | 0.202256 |
| DG 30:1 | 560.4423 | 24.64577 | P | Lipid | Diacylglycerol | 0.424917 | 0.129851 | 0.001067 | 0.074253 | 0.233257 | 0.146329 | 0.110923 | 0.456334 | 0.551936 | 0.199455 | 0.005654 | 0.264269 |
| DG 32:1 | 588.4736 | 25.42276 | P | Lipid | Diacylglycerol | 0.447053 | 0.128931 | 0.000526 | 0.053739 | 0.185415 | 0.137974 | 0.179 | 0.544569 | 0.67838 | 0.204787 | 0.000924 | 0.116318 |
| DG 34:1 | 616.5049 | 26.494192 | P | Lipid | Diacylglycerol | 0.418648 | 0.128929 | 0.001166 | 0.076287 | 0.179312 | 0.144565 | 0.214844 | 0.562376 | 0.616428 | 0.198704 | 0.001921 | 0.194379 |
| DG 36:1 | 644.5369 | 28.001514 | P | Lipid | Diacylglycerol | 0.430119 | 0.130312 | 0.000964 | 0.070785 | 0.245832 | 0.156761 | 0.116835 | 0.46791 | 0.54628 | 0.192729 | 0.004591 | 0.234693 |
| FA 12:2 | 196.1463 | 20.184414 | N | Lipid | Fatty Acid | -0.419716 | 0.133413 | 0.001655 | 0.091796 | -0.144506 | 0.134446 | 0.28245 | 0.619006 | -0.692943 | 0.22555 | 0.002125 | 0.194379 |
| FA 14:2 | 224.1775 | 21.617804 | N | Lipid | Fatty Acid | -0.442623 | 0.135525 | 0.001091 | 0.074359 | -0.280741 | 0.143534 | 0.050474 | 0.34396 | -0.582059 | 0.219736 | 0.008076 | 0.311078 |
| Decanoyl-L-carnitine | 315.2413 | 15.299243 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.460998 | 0.138412 | 0.000867 | 0.070785 | -0.464768 | 0.152803 | 0.002353 | 0.104047 | -0.447814 | 0.214403 | 0.036739 | 0.53105 |
| AC 12:1 | 341.2561 | 16.741268 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.482715 | 0.135658 | 0.000373 | 0.045231 | -0.420955 | 0.143181 | 0.003282 | 0.121779 | -0.517723 | 0.217609 | 0.017353 | 0.38836 |
| AC 14:1 | 369.2874 | 18.959509 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.471444 | 0.133614 | 0.000418 | 0.045437 | -0.457487 | 0.142682 | 0.001344 | 0.081426 | -0.465033 | 0.212287 | 0.028482 | 0.477908 |
| AC 12:2 | 339.2397 | 15.794398 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.586434 | 0.126722 | 0.000004 | 0.003024 | -0.295736 | 0.141806 | 0.037024 | 0.306375 | -0.79072 | 0.195262 | 0.000051 | 0.027985 |
| AC 14:2 | 367.2715 | 17.837961 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.458928 | 0.126722 | 0.000293 | 0.040897 | -0.337832 | 0.130857 | 0.009832 | 0.185948 | -0.5483 | 0.208265 | 0.008471 | 0.311356 |
| AC 11:3 | 323.2119 | 20.819927 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine) | -0.234048 | 0.124669 | 0.060469 | 0.533085 | -0.527895 | 0.122768 | 0.000017 | 0.010666 | 0.002886 | 0.201331 | 0.988563 | 0.997187 |
| AC 8:0 (OH) | 303.2045 | 7.959024 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.543455 | 0.13457 | 0.000054 | 0.016004 | -0.521567 | 0.154704 | 0.000748 | 0.058264 | -0.541714 | 0.204198 | 0.007981 | 0.311078 |
| AC 10:0 (OH) | 331.2357 | 12.493725 | P | Lipid | Fatty Acid Metabolism(Acyl Carnitine), hydroxy | -0.545119 | 0.137317 | 0.000072 | 0.019505 | -0.505196 | 0.155291 | 0.001141 | 0.079436 | -0.564644 | 0.209841 | 0.007128 | 0.304593 |
| Keto 14:0 | 242.1884 | 20.796713 | N | Lipid | Fatty Acid, Keto | -0.432825 | 0.133805 | 0.001217 | 0.07721 | -0.284456 | 0.139951 | 0.042099 | 0.319201 | -0.548831 | 0.218035 | 0.01183 | 0.34255 |
| myo-inositol | 180.0635 | 0.624334 | P | Lipid | Inositol Metabolism | 0.466587 | 0.145822 | 0.001376 | 0.081838 | 0.101592 | 0.146029 | 0.486618 | 0.780824 | 0.864055 | 0.244295 | 0.000405 | 0.06971 |
| PC 33:3/PE 36:3 | 741.568 | 25.137949 | P | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.465731 | 0.122905 | 0.000151 | 0.029069 | -0.192363 | 0.142101 | 0.175832 | 0.540812 | -0.62545 | 0.188513 | 0.000907 | 0.116318 |
| PC 38:6/PE 41:6 | 805.5625 | 24.26375 | P | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.229169 | 0.140176 | 0.102078 | 0.664161 | -0.454239 | 0.140418 | 0.001217 | 0.079629 | -0.024376 | 0.229813 | 0.915527 | 0.995774 |
| glycochenodeoxycholate | 449.315 | 20.243961 | N | Lipid | Primary Bile Acid Metabolism | 0.676991 | 0.124144 | 0.0 | 0.000162 | 0.299852 | 0.128868 | 0.019975 | 0.242658 | 1.056754 | 0.201323 | 0.0 | 0.0005 |
| glycocholate | 465.309 | 18.850445 | N | Lipid | Primary Bile Acid Metabolism | 0.630707 | 0.126082 | 0.000001 | 0.000927 | 0.365003 | 0.13344 | 0.006232 | 0.150635 | 0.873226 | 0.202838 | 0.000017 | 0.014573 |
| taurocholate | 515.2836 | 24.507624 | N | Lipid | Primary Bile Acid Metabolism | -0.243156 | 0.132718 | 0.066932 | 0.561394 | 0.188123 | 0.12453 | 0.130876 | 0.487555 | -0.8494 | 0.231899 | 0.000249 | 0.054419 |
| norhyodeoxycholic acid | 378.2799 | 22.721872 | N | Lipid | Secondary Bile Acid Metabolism | 0.193944 | 0.131316 | 0.139696 | 0.733683 | 0.459414 | 0.132195 | 0.00051 | 0.047709 | -0.018548 | 0.21269 | 0.930507 | 0.995774 |
| dipeptide (tyrosine proline) | 279.132 | 1.012568 | P | Peptide | Dipeptide | 0.192967 | 0.128385 | 0.132832 | 0.713674 | 0.411703 | 0.127703 | 0.001264 | 0.081126 | 0.037419 | 0.212649 | 0.860322 | 0.995774 |
| UNKNOWN [M+H] | 133.0191 | 0.717814 | P | NaN | NaN | -0.368883 | 0.140017 | 0.008424 | 0.21245 | 0.068319 | 0.138672 | 0.622248 | 0.846014 | -0.833677 | 0.237218 | 0.000441 | 0.07211 |
| UNKNOWN [M-H] | 133.9307 | 24.502043 | N | NaN | NaN | -0.265193 | 0.133187 | 0.046465 | 0.487836 | 0.141223 | 0.129829 | 0.276699 | 0.615054 | -0.761812 | 0.224996 | 0.000709 | 0.096725 |
| UNKNOWN [M+H] | 153.1152 | 1.71102 | P | NaN | NaN | -0.399598 | 0.120714 | 0.000932 | 0.070785 | -0.33658 | 0.124182 | 0.006721 | 0.152793 | -0.462205 | 0.197186 | 0.019078 | 0.407989 |
| UNKNOWN [M+H] | 199.1213 | 1.35627 | P | NaN | NaN | 0.468552 | 0.129602 | 0.0003 | 0.040897 | 0.483694 | 0.144169 | 0.000793 | 0.060379 | 0.465364 | 0.200389 | 0.020217 | 0.410866 |
| UNKNOWN [M+H] | 204.0221 | 0.96207 | P | NaN | NaN | -0.561287 | 0.122955 | 0.000005 | 0.003269 | -0.291181 | 0.12295 | 0.017871 | 0.234295 | -0.875646 | 0.20715 | 0.000024 | 0.01549 |
| UNKNOWN [M+H] | 218.0908 | 0.849892 | P | NaN | NaN | -0.011016 | 0.136478 | 0.935667 | 0.997984 | 0.397353 | 0.125074 | 0.001488 | 0.083962 | -0.475452 | 0.235984 | 0.043929 | 0.54997 |
| UNKNOWN [M-H] | 234.0852 | 0.689233 | N | NaN | NaN | 0.410436 | 0.142854 | 0.004064 | 0.149739 | 0.609316 | 0.134214 | 0.000006 | 0.00608 | 0.191585 | 0.244555 | 0.43339 | 0.961381 |
| UNKNOWN [M+H] | 236.1031 | 13.22092 | P | NaN | NaN | -0.333336 | 0.127092 | 0.008721 | 0.217836 | -0.458187 | 0.145137 | 0.001594 | 0.088425 | -0.279109 | 0.191991 | 0.146013 | 0.832003 |
| UNKNOWN [M-H] | 241.9439 | 0.858534 | N | NaN | NaN | 0.080518 | 0.136513 | 0.555312 | 0.97219 | 0.474811 | 0.124324 | 0.000134 | 0.033706 | -0.321897 | 0.237283 | 0.174909 | 0.877222 |
| UNKNOWN [M+H] | 248.1485 | 0.664849 | P | NaN | NaN | 0.527999 | 0.127821 | 0.000036 | 0.01183 | 0.247061 | 0.140083 | 0.077787 | 0.406578 | 0.738763 | 0.200334 | 0.000226 | 0.054419 |
| UNKNOWN [M-H] | 255.9597 | 1.587606 | N | NaN | NaN | 0.056408 | 0.139764 | 0.686513 | 0.993261 | 0.470841 | 0.131009 | 0.000326 | 0.042626 | -0.330618 | 0.237081 | 0.163156 | 0.861888 |
| UNKNOWN [M-H] | 256.9434 | 5.498513 | N | NaN | NaN | -0.453352 | 0.128382 | 0.000414 | 0.045437 | -0.263024 | 0.13738 | 0.055547 | 0.352915 | -0.593012 | 0.205336 | 0.003877 | 0.215006 |
| UNKNOWN [M+H] | 268.1134 | 0.886952 | P | NaN | NaN | 0.419102 | 0.13393 | 0.001752 | 0.095567 | 0.321519 | 0.142145 | 0.023703 | 0.260254 | 0.495655 | 0.215562 | 0.021484 | 0.423475 |
| UNKNOWN [M-H] | 306.923 | 3.809026 | N | NaN | NaN | 0.371893 | 0.135015 | 0.005879 | 0.18166 | 0.451004 | 0.122415 | 0.000229 | 0.039005 | 0.314074 | 0.246102 | 0.201887 | 0.915771 |
| UNKNOWN [M+H] | 318.1586 | 6.124557 | P | NaN | NaN | 0.387109 | 0.122618 | 0.001594 | 0.090686 | 0.259584 | 0.143602 | 0.070659 | 0.391195 | 0.466058 | 0.183904 | 0.011269 | 0.338277 |
| UNKNOWN [M+H] | 318.1876 | 22.69893 | P | NaN | NaN | -0.411272 | 0.132028 | 0.001839 | 0.097063 | -0.294483 | 0.129053 | 0.022496 | 0.258619 | -0.533198 | 0.231351 | 0.021183 | 0.421634 |
| UNKNOWN [M+H] | 319.2218 | 0.670699 | P | NaN | NaN | 0.577528 | 0.127934 | 0.000006 | 0.003465 | 0.316806 | 0.139563 | 0.023209 | 0.258619 | 0.783491 | 0.200487 | 0.000093 | 0.03561 |
| UNKNOWN [M+H] | 320.2037 | 22.90022 | P | NaN | NaN | -0.419592 | 0.130728 | 0.001329 | 0.081838 | -0.306278 | 0.118456 | 0.009721 | 0.185708 | -0.588974 | 0.247767 | 0.017448 | 0.38836 |
| UNKNOWN [M+H] | 322.2183 | 23.15732 | P | NaN | NaN | -0.482968 | 0.145913 | 0.000933 | 0.070785 | -0.262479 | 0.171551 | 0.126007 | 0.482259 | -0.599973 | 0.219102 | 0.006175 | 0.276787 |
| UNKNOWN [M-H] | 326.1314 | 0.632932 | N | NaN | NaN | 0.326776 | 0.140561 | 0.020082 | 0.325999 | 0.484895 | 0.142958 | 0.000694 | 0.056784 | 0.17459 | 0.22964 | 0.44709 | 0.961381 |
| UNKNOWN [M+H] | 326.2198 | 22.89422 | P | NaN | NaN | -0.273389 | 0.129221 | 0.034372 | 0.418091 | -0.496783 | 0.128646 | 0.000113 | 0.033504 | -0.084176 | 0.211279 | 0.690327 | 0.986893 |
| UNKNOWN [M-H] | 354.1504 | 22.53625 | N | NaN | NaN | -0.407337 | 0.130437 | 0.001791 | 0.096065 | -0.438444 | 0.125832 | 0.000493 | 0.047475 | -0.358854 | 0.224479 | 0.109908 | 0.77459 |
| UNKNOWN [M+H] | 366.2092 | 22.89956 | P | NaN | NaN | -0.427344 | 0.130045 | 0.001016 | 0.07225 | -0.320591 | 0.117057 | 0.006167 | 0.150588 | -0.588952 | 0.248294 | 0.017692 | 0.391142 |
| UNKNOWN [M+H] | 372.205 | 22.68437 | P | NaN | NaN | -0.459695 | 0.132923 | 0.000543 | 0.053886 | -0.379098 | 0.135857 | 0.005264 | 0.141175 | -0.544114 | 0.220458 | 0.013583 | 0.352579 |
| UNKNOWN [M-H] | 373.1252 | 22.53523 | N | NaN | NaN | -0.453068 | 0.128687 | 0.00043 | 0.045437 | -0.386391 | 0.124444 | 0.001903 | 0.097296 | -0.510715 | 0.223189 | 0.022122 | 0.42812 |
| UNKNOWN [M-H] | 380.166 | 22.69135 | N | NaN | NaN | -0.438678 | 0.131013 | 0.000813 | 0.068585 | -0.351723 | 0.127281 | 0.005721 | 0.145938 | -0.516279 | 0.228604 | 0.023921 | 0.447249 |
| UNKNOWN [M-H] | 382.182 | 22.88448 | N | NaN | NaN | -0.367103 | 0.131667 | 0.005302 | 0.173467 | -0.412689 | 0.126723 | 0.001128 | 0.079436 | -0.30409 | 0.226541 | 0.179493 | 0.877222 |
| UNKNOWN [M+H] | 390.1761 | 22.49085 | P | NaN | NaN | -0.442946 | 0.130032 | 0.000658 | 0.059822 | -0.299043 | 0.126304 | 0.017902 | 0.234295 | -0.591185 | 0.227389 | 0.009325 | 0.311356 |
| UNKNOWN [M+H] | 392.1921 | 22.70167 | P | NaN | NaN | -0.453325 | 0.132473 | 0.000622 | 0.058107 | -0.32379 | 0.128133 | 0.011504 | 0.193597 | -0.589052 | 0.235941 | 0.012539 | 0.346851 |
| UNKNOWN [M+H] | 394.2077 | 22.90065 | P | NaN | NaN | -0.445952 | 0.131772 | 0.000714 | 0.063114 | -0.391518 | 0.112359 | 0.000493 | 0.047475 | -0.533282 | 0.268938 | 0.047377 | 0.575679 |
| UNKNOWN [M+H] | 394.2145 | 22.80924 | P | NaN | NaN | -0.499378 | 0.128313 | 0.000099 | 0.021697 | -0.402119 | 0.112472 | 0.00035 | 0.04276 | -0.656564 | 0.259673 | 0.011458 | 0.34081 |
| UNKNOWN [M+H] | 396.2253 | 23.12257 | P | NaN | NaN | -0.498616 | 0.1302 | 0.000128 | 0.026246 | -0.332831 | 0.134138 | 0.013092 | 0.204967 | -0.641514 | 0.214146 | 0.002738 | 0.202256 |
| UNKNOWN [M-H] | 399.141 | 22.6912 | N | NaN | NaN | -0.501067 | 0.126788 | 0.000077 | 0.019505 | -0.321412 | 0.126399 | 0.010996 | 0.193597 | -0.676252 | 0.21535 | 0.001688 | 0.190459 |
| UNKNOWN [M-H] | 400.1678 | 10.72078 | N | NaN | NaN | 0.317791 | 0.135787 | 0.019265 | 0.321608 | 0.481614 | 0.136929 | 0.000436 | 0.045139 | 0.1902 | 0.220456 | 0.38827 | 0.94482 |
| UNKNOWN [M-H] | 401.1561 | 22.87746 | N | NaN | NaN | -0.365493 | 0.127588 | 0.004175 | 0.150638 | -0.49218 | 0.133442 | 0.000226 | 0.039005 | -0.264895 | 0.202308 | 0.190412 | 0.891314 |
| UNKNOWN [M-H] | 402.1566 | 22.54156 | N | NaN | NaN | -0.357035 | 0.132919 | 0.007229 | 0.199352 | -0.424488 | 0.13028 | 0.001121 | 0.079436 | -0.285952 | 0.225136 | 0.204039 | 0.915771 |
| UNKNOWN [M+H] | 406.164 | 22.90442 | P | NaN | NaN | -0.378943 | 0.125842 | 0.002602 | 0.115036 | -0.375259 | 0.104206 | 0.000317 | 0.042626 | -0.394881 | 0.265416 | 0.136809 | 0.819907 |
| UNKNOWN [M-H] | 408.1982 | 22.85601 | N | NaN | NaN | -0.300315 | 0.12782 | 0.018798 | 0.320353 | -0.412434 | 0.127403 | 0.001207 | 0.079629 | -0.196344 | 0.211445 | 0.353106 | 0.943963 |
| UNKNOWN [M-H] | 413.1327 | 22.80894 | N | NaN | NaN | -0.301449 | 0.133085 | 0.023508 | 0.355836 | -0.537691 | 0.119996 | 0.000007 | 0.00608 | -0.02121 | 0.235575 | 0.92826 | 0.995774 |
| UNKNOWN [M+H] | 416.251 | 22.21291 | P | NaN | NaN | -0.370773 | 0.130746 | 0.004571 | 0.155782 | 0.160141 | 0.1643 | 0.329716 | 0.660098 | -0.637505 | 0.18452 | 0.00055 | 0.081865 |
| UNKNOWN [M-H] | 418.3092 | 22.52272 | N | NaN | NaN | 0.402659 | 0.127644 | 0.001608 | 0.090686 | 0.18001 | 0.134214 | 0.179852 | 0.544569 | 0.639366 | 0.21383 | 0.002789 | 0.202256 |
| UNKNOWN [M+H] | 434.2493 | 12.13154 | P | NaN | NaN | -0.221736 | 0.135822 | 0.102562 | 0.664522 | -0.484415 | 0.147548 | 0.001027 | 0.076353 | -0.036231 | 0.209843 | 0.862919 | 0.995774 |
| UNKNOWN [M+H] | 434.2632 | 22.22459 | P | NaN | NaN | 0.046913 | 0.124123 | 0.705463 | 0.995015 | 0.445011 | 0.117318 | 0.000149 | 0.034122 | -0.338568 | 0.204767 | 0.098243 | 0.745829 |
| UNKNOWN [M-H] | 441.1604 | 22.54507 | N | NaN | NaN | -0.277224 | 0.129537 | 0.032345 | 0.407051 | -0.427421 | 0.1204 | 0.000385 | 0.043463 | -0.109552 | 0.226392 | 0.628455 | 0.983456 |
| UNKNOWN [M+H] | 444.2554 | 21.44807 | P | NaN | NaN | -0.216179 | 0.129521 | 0.095104 | 0.64796 | -0.435785 | 0.102671 | 0.000022 | 0.010666 | 0.24516 | 0.273545 | 0.370129 | 0.94482 |
| UNKNOWN [M-H] | 446.1944 | 21.46943 | N | NaN | NaN | 0.359032 | 0.130293 | 0.005859 | 0.18166 | -0.04462 | 0.14011 | 0.750131 | 0.90754 | 0.73157 | 0.204563 | 0.000349 | 0.067083 |
| UNKNOWN [M-H] | 458.1879 | 22.54917 | N | NaN | NaN | -0.368734 | 0.129347 | 0.004362 | 0.151824 | -0.429178 | 0.132615 | 0.001211 | 0.079629 | -0.319463 | 0.210028 | 0.128247 | 0.812591 |
| UNKNOWN [M-H] | 458.2257 | 23.17696 | N | NaN | NaN | -0.436768 | 0.13407 | 0.001123 | 0.074986 | -0.392098 | 0.142117 | 0.005798 | 0.145938 | -0.457342 | 0.214453 | 0.032958 | 0.508671 |
| UNKNOWN [M-H] | 459.2001 | 22.94147 | N | NaN | NaN | -0.244638 | 0.126653 | 0.053413 | 0.506573 | -0.482276 | 0.12375 | 0.000097 | 0.031845 | -0.018059 | 0.209343 | 0.931255 | 0.995774 |
| UNKNOWN [M+H] | 471.2968 | 20.25837 | P | NaN | NaN | 0.655202 | 0.135243 | 0.000001 | 0.001384 | 0.289834 | 0.14881 | 0.051454 | 0.345462 | 0.936548 | 0.210937 | 0.000009 | 0.014573 |
| UNKNOWN [M-H] | 478.1879 | 22.68843 | N | NaN | NaN | -0.414649 | 0.130605 | 0.001499 | 0.087599 | -0.292984 | 0.134047 | 0.028839 | 0.27789 | -0.513095 | 0.215252 | 0.01714 | 0.38677 |
| UNKNOWN [M+H] | 487.2902 | 18.95069 | P | NaN | NaN | 0.460682 | 0.13457 | 0.000619 | 0.058107 | 0.344239 | 0.147789 | 0.019846 | 0.242658 | 0.540964 | 0.209877 | 0.009951 | 0.314641 |
| UNKNOWN [M+H] | 528.9832 | 21.87873 | P | NaN | NaN | 0.393402 | 0.131545 | 0.002784 | 0.119479 | 0.031646 | 0.141344 | 0.822837 | 0.940197 | 0.706652 | 0.206472 | 0.00062 | 0.088267 |
| UNKNOWN [M-H] | 558.3295 | 22.23139 | N | NaN | NaN | 0.462884 | 0.12527 | 0.00022 | 0.037854 | -0.143587 | 0.164017 | 0.381334 | 0.696274 | 0.7414 | 0.172795 | 0.000018 | 0.014573 |
| UNKNOWN [M+H] | 558.3334 | 21.93091 | P | NaN | NaN | -0.142413 | 0.133809 | 0.287192 | 0.863688 | -0.389179 | 0.114199 | 0.000655 | 0.054923 | 0.367755 | 0.269405 | 0.172233 | 0.875074 |
| UNKNOWN [M+H] | 562.4572 | 25.22002 | P | NaN | NaN | 0.469682 | 0.12639 | 0.000202 | 0.036773 | 0.278035 | 0.136842 | 0.042175 | 0.319201 | 0.623066 | 0.199175 | 0.001759 | 0.191807 |
| UNKNOWN [M-H] | 577.2845 | 24.50501 | N | NaN | NaN | -0.34495 | 0.130945 | 0.008431 | 0.21245 | 0.093748 | 0.132337 | 0.478695 | 0.776353 | -0.83175 | 0.214922 | 0.000109 | 0.03561 |
| UNKNOWN [M+H] | 582.2485 | 23.22286 | P | NaN | NaN | -0.47189 | 0.129425 | 0.000266 | 0.039606 | -0.506253 | 0.111562 | 0.000006 | 0.00608 | -0.390438 | 0.252097 | 0.121439 | 0.802909 |
| UNKNOWN [M-H] | 584.3483 | 22.37844 | N | NaN | NaN | -0.117714 | 0.12837 | 0.35915 | 0.908389 | -0.531509 | 0.138523 | 0.000125 | 0.033706 | 0.149113 | 0.196355 | 0.447611 | 0.961381 |
| UNKNOWN [M+H] | 589.3173 | 22.08178 | P | NaN | NaN | -0.096988 | 0.145345 | 0.504582 | 0.961601 | -0.552733 | 0.157296 | 0.000441 | 0.045139 | 0.189433 | 0.221035 | 0.391429 | 0.94482 |
| UNKNOWN [M-H] | 592.4713 | 22.733011 | N | NaN | NaN | -0.105601 | 0.136789 | 0.440116 | 0.939778 | -0.472371 | 0.147562 | 0.001369 | 0.081426 | 0.131763 | 0.209219 | 0.528835 | 0.975394 |
| UNKNOWN [M+H] | 596.156 | 22.72373 | P | NaN | NaN | -0.339548 | 0.141349 | 0.016297 | 0.306027 | -0.580299 | 0.16013 | 0.00029 | 0.042626 | -0.185972 | 0.213682 | 0.384124 | 0.94482 |
| UNKNOWN [M+H] | 606.4627 | 26.22056 | P | NaN | NaN | 0.5169 | 0.12277 | 0.000026 | 0.009271 | 0.267439 | 0.138214 | 0.052996 | 0.347943 | 0.714709 | 0.188784 | 0.000153 | 0.041766 |
| UNKNOWN [M-H] | 610.2514 | 10.72204 | N | NaN | NaN | 0.282751 | 0.130147 | 0.029814 | 0.39641 | 0.416125 | 0.13389 | 0.001884 | 0.097296 | 0.185943 | 0.209444 | 0.374652 | 0.94482 |
| UNKNOWN [M-H] | 610.3743 | 22.55543 | N | NaN | NaN | -0.257436 | 0.121475 | 0.034069 | 0.418091 | -0.446705 | 0.123731 | 0.000306 | 0.042626 | -0.097713 | 0.195727 | 0.617618 | 0.983072 |
| UNKNOWN [M-H] | 616.4743 | 22.97604 | N | NaN | NaN | -0.069725 | 0.129088 | 0.589102 | 0.978387 | -0.418426 | 0.122099 | 0.00061 | 0.052563 | 0.317503 | 0.220144 | 0.149232 | 0.842721 |
| UNKNOWN [M-H] | 617.3655 | 22.47582 | N | NaN | NaN | -0.185308 | 0.133881 | 0.16632 | 0.76121 | -0.444096 | 0.120964 | 0.000241 | 0.039005 | 0.119307 | 0.238709 | 0.617216 | 0.983072 |
| UNKNOWN [M-H] | 624.3653 | 21.67886 | N | NaN | NaN | -0.33942 | 0.125039 | 0.006637 | 0.193502 | -0.427055 | 0.119703 | 0.00036 | 0.04276 | -0.284093 | 0.216884 | 0.190234 | 0.891314 |
| UNKNOWN [M-H] | 632.235 | 10.72335 | N | NaN | NaN | 0.293189 | 0.133627 | 0.028229 | 0.39473 | 0.435631 | 0.139873 | 0.001843 | 0.097246 | 0.196949 | 0.212249 | 0.353452 | 0.943963 |
| UNKNOWN [M-H] | 634.3934 | 21.67741 | N | NaN | NaN | -0.293864 | 0.124842 | 0.018578 | 0.319553 | -0.461772 | 0.126101 | 0.00025 | 0.039005 | -0.185322 | 0.205289 | 0.366665 | 0.94482 |
| UNKNOWN [M-H] | 635.2293 | 19.90286 | N | NaN | NaN | -0.456174 | 0.124608 | 0.000251 | 0.039163 | -0.367959 | 0.140797 | 0.008965 | 0.179955 | -0.540478 | 0.191561 | 0.004781 | 0.240658 |
| UNKNOWN [M-H] | 643.4054 | 22.68533 | N | NaN | NaN | -0.333394 | 0.134877 | 0.013442 | 0.283758 | -0.403275 | 0.128509 | 0.0017 | 0.091212 | -0.234108 | 0.235629 | 0.320445 | 0.943963 |
| UNKNOWN [M-H] | 647.4372 | 22.87978 | N | NaN | NaN | -0.376899 | 0.131161 | 0.004059 | 0.149739 | -0.462451 | 0.12435 | 0.0002 | 0.038505 | -0.271079 | 0.226872 | 0.232145 | 0.925187 |
| UNKNOWN [M-H] | 663.4318 | 22.95292 | N | NaN | NaN | -0.431561 | 0.128947 | 0.000817 | 0.068585 | -0.513187 | 0.124944 | 0.00004 | 0.014552 | -0.334446 | 0.218441 | 0.125754 | 0.810727 |
| UNKNOWN [M-H] | 667.406 | 22.6741 | N | NaN | NaN | -0.212046 | 0.13485 | 0.115843 | 0.690852 | -0.423856 | 0.132878 | 0.001424 | 0.083183 | 0.004762 | 0.224773 | 0.983098 | 0.996599 |
| UNKNOWN [M-H] | 675.2957 | 21.79783 | N | NaN | NaN | -0.012714 | 0.129567 | 0.921833 | 0.997984 | -0.444879 | 0.140011 | 0.001486 | 0.083962 | 0.288565 | 0.20073 | 0.150553 | 0.842721 |
| UNKNOWN [M+H] | 684.4939 | 26.49437 | P | NaN | NaN | 0.397094 | 0.127794 | 0.001888 | 0.098056 | 0.089864 | 0.139949 | 0.520795 | 0.802657 | 0.650247 | 0.198812 | 0.001073 | 0.125383 |
| UNKNOWN [M-H] | 713.2542 | 21.68026 | N | NaN | NaN | -0.336578 | 0.12185 | 0.005741 | 0.18166 | -0.400351 | 0.124629 | 0.001317 | 0.08128 | -0.317809 | 0.201507 | 0.114757 | 0.788837 |
| UNKNOWN [M+H] | 831.5717 | 24.71593 | P | NaN | NaN | -0.241198 | 0.130393 | 0.064345 | 0.549706 | -0.423028 | 0.122636 | 0.000562 | 0.050223 | -0.015087 | 0.227821 | 0.9472 | 0.996599 |
| UNKNOWN [M+H] | 873.5479 | 24.56265 | P | NaN | NaN | -0.395331 | 0.134942 | 0.003394 | 0.133782 | -0.066697 | 0.140733 | 0.635551 | 0.851915 | -0.799938 | 0.223205 | 0.000339 | 0.067083 |
| UNKNOWN [M-H] | 877.5814 | 24.40452 | N | NaN | NaN | -0.398326 | 0.123225 | 0.001227 | 0.07721 | -0.547759 | 0.12933 | 0.000023 | 0.010666 | -0.276762 | 0.195342 | 0.156539 | 0.848008 |
| UNKNOWN [M+H] | 915.5538 | 22.68628 | P | NaN | NaN | -0.201754 | 0.129458 | 0.119126 | 0.697282 | -0.352897 | 0.112435 | 0.001697 | 0.091212 | 0.051995 | 0.249154 | 0.834692 | 0.995774 |
| UNKNOWN [M-H] | 919.5557 | 24.24036 | N | NaN | NaN | -0.322207 | 0.131796 | 0.014496 | 0.290542 | 0.084838 | 0.133206 | 0.524192 | 0.804105 | -0.74815 | 0.215885 | 0.000529 | 0.081865 |
| UNKNOWN [M+H] | 921.5418 | 24.26121 | P | NaN | NaN | -0.139572 | 0.130135 | 0.283488 | 0.85898 | -0.404341 | 0.125811 | 0.00131 | 0.08128 | 0.146776 | 0.220136 | 0.504929 | 0.97403 |
| UNKNOWN [M+H] | 934.6938 | 22.8985 | P | NaN | NaN | -0.40857 | 0.123881 | 0.000974 | 0.070785 | -0.367363 | 0.119472 | 0.002106 | 0.102064 | -0.447801 | 0.215857 | 0.038031 | 0.535273 |
| UNKNOWN [M-H] | 937.515 | 24.2434 | N | NaN | NaN | -0.46497 | 0.13018 | 0.000355 | 0.044629 | -0.118584 | 0.132392 | 0.370412 | 0.689021 | -0.840713 | 0.215932 | 0.000099 | 0.03561 |
| UNKNOWN [M+H] | 965.6468 | 27.96958 | P | NaN | NaN | -0.334691 | 0.126402 | 0.008101 | 0.211391 | -0.522222 | 0.125657 | 0.000032 | 0.01325 | -0.156326 | 0.211654 | 0.460156 | 0.963912 |
| UNKNOWN [M-H] | 968.6684 | 22.88444 | N | NaN | NaN | -0.229307 | 0.131083 | 0.080235 | 0.5953 | -0.487686 | 0.129547 | 0.000167 | 0.034122 | 0.000807 | 0.214005 | 0.996991 | 0.999434 |
| UNKNOWN [M+H] | 991.6704 | 28.15788 | P | NaN | NaN | -0.293298 | 0.122176 | 0.016368 | 0.306027 | -0.497813 | 0.139697 | 0.000366 | 0.04276 | -0.17455 | 0.182883 | 0.339865 | 0.943963 |
| UNKNOWN [M+H] | 1116.7264 | 22.272392 | P | NaN | NaN | -0.428203 | 0.133792 | 0.001372 | 0.081838 | 0.035455 | 0.156129 | 0.820356 | 0.938205 | -0.725865 | 0.197244 | 0.000233 | 0.054419 |
| UNKNOWN [M+H] | 1573.0428 | 24.039658 | P | NaN | NaN | -0.219436 | 0.130392 | 0.092395 | 0.639146 | -0.477515 | 0.135786 | 0.000437 | 0.045139 | -0.051926 | 0.206125 | 0.801105 | 0.995774 |
| UNKNOWN [M+H] | 1804.806 | 22.90585 | P | NaN | NaN | -0.476578 | 0.122081 | 0.000095 | 0.021697 | -0.336024 | 0.112117 | 0.002726 | 0.11449 | -0.667635 | 0.22707 | 0.00328 | 0.202256 |