## Sheet1
| Table S1. Significant associations between untargeted features and BMIz, 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; BCAA, branched chain amino acid; BMIz, BMI z-score; Cer, ceramide; DG, diglyceride; DiC, dicarboxylic group; FA, fatty acid; FDR, false discovery rate; N, negative ionization mode; OH, hydroxyl group; P, positive ionization mode; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PS, phosphatidylserine; 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 |
| 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 |
| isovalerylcarnitine | 245.1626 | 4.58061 | P | Amino Acid | Fatty Acid Metabolism(Acyl Carnitine) | 0.319782 | 0.08122 | 0.000082 | 0.012259 | 0.349901 | 0.11853 | 0.003157 | 0.153617 | 0.284339 | 0.112116 | 0.011209 | 0.362297 |
| isoleucine | 131.0954 | 1.502874 | P | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.31319 | 0.081984 | 0.000133 | 0.017624 | 0.419505 | 0.101874 | 0.000038 | 0.020854 | 0.153912 | 0.131902 | 0.243262 | 0.741044 |
| leucine | 131.0951 | 1.596301 | P | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.185769 | 0.082001 | 0.023485 | 0.353842 | 0.347824 | 0.102244 | 0.000669 | 0.091229 | -0.041678 | 0.127587 | 0.74392 | 0.94926 |
| valine | 117.0793 | 0.870426 | P | Amino Acid | Leucine, Isoleucine and Valine Metabolism | 0.261205 | 0.083949 | 0.001862 | 0.093713 | 0.363425 | 0.122944 | 0.003116 | 0.153617 | 0.18291 | 0.113121 | 0.105891 | 0.627226 |
| tyrosine | 181.0741 | 1.297716 | P | Amino Acid | Phenylalanine and Tyrosine Metabolism | 0.385234 | 0.084424 | 0.000005 | 0.002062 | 0.436145 | 0.141249 | 0.002017 | 0.130239 | 0.352615 | 0.104382 | 0.00073 | 0.077031 |
| 5-methylthioadenosine | 297.0898 | 4.448414 | P | Amino Acid | Polyamine Metabolism | 0.302482 | 0.085155 | 0.000382 | 0.037128 | 0.548998 | 0.140741 | 0.000096 | 0.027545 | 0.184508 | 0.10536 | 0.079907 | 0.586989 |
| D-lyxose | 150.0527 | 0.706673 | N | Carbohydrate | Pentose Metabolism | -0.315228 | 0.098893 | 0.001435 | 0.082363 | -0.222082 | 0.138557 | 0.108974 | 0.487574 | -0.410729 | 0.142491 | 0.003945 | 0.253121 |
| Cer t36:0(2OH) | 599.5055 | 24.486198 | N | Lipid | Ceramide | 0.334425 | 0.083748 | 0.000065 | 0.010156 | 0.258406 | 0.126834 | 0.041615 | 0.340411 | 0.372822 | 0.114132 | 0.001089 | 0.101762 |
| PE-Cer d32:3 | 628.4845 | 25.65966 | N | Lipid | Ceramide phosphoethanolamines | 0.234735 | 0.080057 | 0.003367 | 0.13114 | 0.035848 | 0.11765 | 0.760595 | 0.958655 | 0.420348 | 0.105288 | 0.000065 | 0.013866 |
| DG 32:0 | 568.5067 | 26.219461 | P | Lipid | Diacylglycerol | 0.382192 | 0.078682 | 0.000001 | 0.002062 | 0.298121 | 0.124332 | 0.016495 | 0.258 | 0.437857 | 0.100484 | 0.000013 | 0.005381 |
| DG 34:0 | 618.5204 | 27.634111 | P | Lipid | Diacylglycerol | 0.362284 | 0.080427 | 0.000007 | 0.002419 | 0.223631 | 0.144929 | 0.122821 | 0.504227 | 0.417481 | 0.095072 | 0.000011 | 0.005297 |
| DG 30:1 | 560.4423 | 24.64577 | P | Lipid | Diacylglycerol | 0.329851 | 0.081578 | 0.000053 | 0.009186 | 0.225884 | 0.130575 | 0.083644 | 0.432358 | 0.406334 | 0.102081 | 0.000069 | 0.013866 |
| DG 32:1 | 588.4736 | 25.42276 | P | Lipid | Diacylglycerol | 0.367956 | 0.080415 | 0.000005 | 0.002062 | 0.230878 | 0.122307 | 0.059067 | 0.37795 | 0.482765 | 0.103923 | 0.000003 | 0.002419 |
| DG 33:1 | 602.4901 | 25.90679 | P | Lipid | Diacylglycerol | 0.331743 | 0.081227 | 0.000044 | 0.009047 | 0.221899 | 0.121129 | 0.066963 | 0.396927 | 0.425641 | 0.107229 | 0.000072 | 0.013866 |
| DG 34:1 | 616.5049 | 26.494192 | P | Lipid | Diacylglycerol | 0.375883 | 0.079928 | 0.000003 | 0.002062 | 0.289084 | 0.126944 | 0.022771 | 0.285651 | 0.444129 | 0.101167 | 0.000011 | 0.005297 |
| DG 35:1 | 630.5215 | 27.154875 | P | Lipid | Diacylglycerol | 0.305878 | 0.081188 | 0.000165 | 0.019266 | 0.262376 | 0.140628 | 0.062077 | 0.383206 | 0.338095 | 0.097726 | 0.000541 | 0.06321 |
| DG 36:1 | 644.5369 | 28.001514 | P | Lipid | Diacylglycerol | 0.354307 | 0.081427 | 0.000014 | 0.004027 | 0.28924 | 0.138885 | 0.037289 | 0.332556 | 0.386736 | 0.099038 | 0.000094 | 0.017133 |
| DG 32:2 | 586.4577 | 24.862595 | P | Lipid | Diacylglycerol | 0.380458 | 0.079867 | 0.000002 | 0.002062 | 0.17611 | 0.130154 | 0.176027 | 0.586237 | 0.513102 | 0.096885 | 0.0 | 0.000387 |
| DG 34:2 | 614.4888 | 25.732864 | P | Lipid | Diacylglycerol | 0.336504 | 0.080013 | 0.000026 | 0.006356 | 0.1939 | 0.124897 | 0.120548 | 0.500548 | 0.449549 | 0.104049 | 0.000016 | 0.005658 |
| DG 35:2 | 628.5046 | 26.1662 | P | Lipid | Diacylglycerol | 0.389276 | 0.083565 | 0.000003 | 0.002062 | 0.293269 | 0.128961 | 0.02296 | 0.285651 | 0.455192 | 0.108091 | 0.000025 | 0.008311 |
| DG 34:3 | 612.4738 | 25.196987 | P | Lipid | Diacylglycerol | 0.340525 | 0.079934 | 0.00002 | 0.005572 | 0.172898 | 0.120838 | 0.152481 | 0.558697 | 0.478501 | 0.103399 | 0.000004 | 0.002419 |
| DG 35:3 | 626.49 | 25.472881 | P | Lipid | Diacylglycerol | 0.37383 | 0.080933 | 0.000004 | 0.002062 | 0.194533 | 0.121645 | 0.109781 | 0.487574 | 0.517995 | 0.105885 | 0.000001 | 0.001633 |
| DG 36:3 | 640.5052 | 25.970724 | P | Lipid | Diacylglycerol | 0.26248 | 0.085898 | 0.002245 | 0.106465 | 0.077879 | 0.12192 | 0.522969 | 0.888298 | 0.449063 | 0.119201 | 0.000165 | 0.027002 |
| DG 36:4 | 638.4888 | 25.322704 | P | Lipid | Diacylglycerol | 0.293716 | 0.083991 | 0.000471 | 0.04161 | 0.043979 | 0.152733 | 0.773388 | 0.960397 | 0.404072 | 0.097292 | 0.000033 | 0.00894 |
| AC 3:0 | 217.1321 | 1.629795 | P | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.250593 | 0.085893 | 0.003528 | 0.134245 | 0.601173 | 0.139598 | 0.000017 | 0.01357 | 0.093663 | 0.106147 | 0.377567 | 0.819755 |
| AC 8:1 | 285.1943 | 9.563584 | P | Lipid | Fatty Acid Metabolism (Acyl Carnitine) | 0.34502 | 0.085391 | 0.000053 | 0.009186 | 0.474896 | 0.12214 | 0.000101 | 0.027545 | 0.267371 | 0.117545 | 0.022928 | 0.461827 |
| AC 5:0 (OH) | 261.1578 | 1.981441 | P | Lipid | Leucine, Isoleucine and Valine Metabolism | 0.285465 | 0.086957 | 0.001028 | 0.067257 | 0.40274 | 0.132617 | 0.002391 | 0.139541 | 0.198784 | 0.114316 | 0.082052 | 0.587318 |
| FA 9:1 (DiC) | 186.0894 | 6.299434 | P | Lipid | Fatty Acid, Dicarboxylate | 0.229351 | 0.082805 | 0.00561 | 0.168394 | 0.483956 | 0.123333 | 0.000087 | 0.027545 | 0.0592 | 0.108706 | 0.586039 | 0.896109 |
| PC 34:0/PE 37:0 | 761.5923 | 25.413399 | N | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.202587 | 0.083149 | 0.014833 | 0.271145 | -0.342987 | 0.09977 | 0.000587 | 0.08832 | 0.025584 | 0.137641 | 0.852543 | 0.970456 |
| PC 31:5/PE 34:5 | 707.509 | 25.409264 | P | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | 0.267512 | 0.079845 | 0.000807 | 0.062866 | 0.12867 | 0.128373 | 0.316193 | 0.745026 | 0.359674 | 0.100115 | 0.000327 | 0.048689 |
| PC 35:5/PE 38:5 | 765.5672 | 25.150826 | P | Lipid | Phosphatidylcholine/Phosphatidylethanolamine | -0.301259 | 0.083237 | 0.000295 | 0.03118 | -0.487306 | 0.12455 | 0.000091 | 0.027545 | -0.149699 | 0.112321 | 0.182606 | 0.690837 |
| PE 36:2 | 620.5388 | 26.788805 | P | Lipid | Phosphoethanolamines | 0.27862 | 0.084548 | 0.000983 | 0.066997 | 0.150214 | 0.128312 | 0.241723 | 0.666878 | 0.382678 | 0.110129 | 0.000511 | 0.061948 |
| PS 35:4 | 769.496 | 24.213146 | P | Lipid | Phosphoserines | 0.242895 | 0.083178 | 0.003498 | 0.134245 | 0.378814 | 0.113559 | 0.00085 | 0.097883 | 0.113345 | 0.118801 | 0.340045 | 0.809194 |
| PS 42:6 | 863.5603 | 25.18495 | P | Lipid | Phosphoserines | -0.277941 | 0.083921 | 0.000927 | 0.066673 | -0.282273 | 0.133929 | 0.035063 | 0.32465 | -0.259952 | 0.107503 | 0.015602 | 0.425403 |
| PS 39:7 | 819.5096 | 24.150833 | P | Lipid | Phosphoserines | -0.155455 | 0.086207 | 0.071346 | 0.535572 | -0.435617 | 0.130431 | 0.000838 | 0.097883 | 0.029207 | 0.11313 | 0.796276 | 0.956818 |
| cortisone | 360.1939 | 13.359143 | N | Lipid | Steroid | -0.28984 | 0.081851 | 0.000399 | 0.037128 | -0.248765 | 0.12686 | 0.049886 | 0.361921 | -0.295937 | 0.109276 | 0.006766 | 0.284621 |
| glutamyl-phenylalanine | 294.1236 | 2.800813 | P | Peptide | Dipeptide | 0.266864 | 0.08484 | 0.001658 | 0.087005 | 0.245596 | 0.117936 | 0.037301 | 0.332556 | 0.311227 | 0.121488 | 0.010413 | 0.347679 |
| L-gamma-glutamyl-L-isoleucine | 260.1368 | 4.586305 | P | Peptide | Gamma-glutamyl Amino Acid | 0.286659 | 0.084061 | 0.000649 | 0.05182 | 0.466239 | 0.129656 | 0.000323 | 0.062204 | 0.164454 | 0.108815 | 0.130707 | 0.648971 |
| UNKNOWN [M+H] | 186.0643 | 1.041837 | P | NaN | NaN | 0.263605 | 0.080879 | 0.001117 | 0.07167 | 0.167563 | 0.123518 | 0.174913 | 0.583399 | 0.335067 | 0.108347 | 0.001984 | 0.158371 |
| UNKNOWN [M-H] | 214.8972 | 0.935251 | N | NaN | NaN | -0.324438 | 0.094436 | 0.000591 | 0.048379 | -0.541996 | 0.127341 | 0.000021 | 0.013604 | -0.111199 | 0.135468 | 0.411731 | 0.845499 |
| UNKNOWN [M-H] | 220.9893 | 1.570175 | N | NaN | NaN | 0.239872 | 0.087946 | 0.006382 | 0.179662 | 0.393071 | 0.117979 | 0.000863 | 0.097883 | 0.09023 | 0.126933 | 0.477179 | 0.868942 |
| UNKNOWN [M+H] | 224.0398 | 6.385331 | P | NaN | NaN | 0.223436 | 0.081495 | 0.006112 | 0.175417 | 0.550946 | 0.118491 | 0.000003 | 0.010878 | 0.012829 | 0.107114 | 0.904664 | 0.98595 |
| UNKNOWN [M-H] | 224.9258 | 0.859642 | N | NaN | NaN | -0.293364 | 0.085126 | 0.000568 | 0.047691 | -0.399566 | 0.131204 | 0.002324 | 0.139541 | -0.206831 | 0.111363 | 0.063274 | 0.577234 |
| UNKNOWN [M+H] | 230.0533 | 6.384756 | P | NaN | NaN | 0.236573 | 0.082618 | 0.00419 | 0.144327 | 0.532618 | 0.121275 | 0.000011 | 0.01357 | 0.045735 | 0.1084 | 0.673089 | 0.928163 |
| UNKNOWN [M+H] | 244.1781 | 5.107907 | P | NaN | NaN | 0.279973 | 0.085148 | 0.001009 | 0.067257 | 0.356021 | 0.136389 | 0.009045 | 0.231218 | 0.235627 | 0.108962 | 0.030582 | 0.500322 |
| UNKNOWN [M-H] | 280.1057 | 3.926439 | N | NaN | NaN | 0.247954 | 0.07466 | 0.000897 | 0.06667 | 0.380716 | 0.102167 | 0.000194 | 0.042307 | 0.13052 | 0.106025 | 0.21831 | 0.718042 |
| UNKNOWN [M+H] | 280.1062 | 3.935487 | P | NaN | NaN | 0.278925 | 0.08432 | 0.00094 | 0.066673 | 0.411956 | 0.125888 | 0.001066 | 0.099717 | 0.187779 | 0.111773 | 0.092957 | 0.613001 |
| UNKNOWN [M+H] | 294.1223 | 5.026446 | P | NaN | NaN | 0.277998 | 0.08547 | 0.001144 | 0.071959 | 0.424972 | 0.161168 | 0.008369 | 0.231218 | 0.212291 | 0.100515 | 0.034684 | 0.512285 |
| UNKNOWN [M+H] | 297.2669 | 19.4744 | P | NaN | NaN | 0.303069 | 0.085611 | 0.0004 | 0.037128 | 0.114734 | 0.145558 | 0.430557 | 0.836709 | 0.415189 | 0.103942 | 0.000065 | 0.013866 |
| UNKNOWN [M+H] | 304.1301 | 20.21629 | P | NaN | NaN | 0.279878 | 0.087348 | 0.001354 | 0.079139 | 0.4788 | 0.14418 | 0.000897 | 0.097883 | 0.180722 | 0.108386 | 0.095438 | 0.613969 |
| UNKNOWN [M-H] | 324.0871 | 0.655723 | N | NaN | NaN | -0.290207 | 0.087055 | 0.000857 | 0.065237 | -0.214245 | 0.118701 | 0.071089 | 0.408075 | -0.360809 | 0.127721 | 0.004728 | 0.261996 |
| UNKNOWN [M-H] | 351.1579 | 8.286208 | N | NaN | NaN | 0.185765 | 0.087954 | 0.03468 | 0.416263 | 0.525206 | 0.130392 | 0.000056 | 0.023016 | -0.008669 | 0.11498 | 0.9399 | 0.992154 |
| UNKNOWN [M-H] | 375.1422 | 8.384085 | N | NaN | NaN | 0.271076 | 0.084229 | 0.001289 | 0.076708 | 0.229371 | 0.110958 | 0.038716 | 0.333169 | 0.327358 | 0.127357 | 0.010158 | 0.34266 |
| UNKNOWN [M+H] | 394.1599 | 6.383765 | P | NaN | NaN | 0.229372 | 0.079191 | 0.003774 | 0.13571 | 0.493307 | 0.113246 | 0.000013 | 0.01357 | 0.042466 | 0.106128 | 0.68905 | 0.931256 |
| UNKNOWN [M-H] | 422.1749 | 23.14975 | N | NaN | NaN | 0.314448 | 0.078186 | 0.000058 | 0.00945 | 0.400305 | 0.11308 | 0.0004 | 0.070715 | 0.230084 | 0.10738 | 0.032137 | 0.50868 |
| UNKNOWN [M-H] | 423.1896 | 13.36019 | N | NaN | NaN | -0.282384 | 0.081372 | 0.00052 | 0.044764 | -0.226188 | 0.129813 | 0.081437 | 0.430882 | -0.299036 | 0.105301 | 0.004514 | 0.261996 |
| UNKNOWN [M-H] | 432.2028 | 23.16128 | N | NaN | NaN | 0.262987 | 0.08309 | 0.00155 | 0.085976 | 0.332508 | 0.105862 | 0.001684 | 0.117239 | 0.162152 | 0.129397 | 0.210158 | 0.708173 |
| UNKNOWN [M+H] | 450.2434 | 10.09085 | P | NaN | NaN | 0.293652 | 0.083081 | 0.000408 | 0.037128 | 0.171544 | 0.116287 | 0.140166 | 0.537657 | 0.442639 | 0.116023 | 0.000136 | 0.023443 |
| UNKNOWN [M-H] | 460.206 | 22.80973 | N | NaN | NaN | 0.303507 | 0.082108 | 0.000219 | 0.023847 | 0.381145 | 0.102721 | 0.000207 | 0.042307 | 0.162224 | 0.132583 | 0.221116 | 0.718042 |
| UNKNOWN [M-H] | 468.3793 | 22.82681 | N | NaN | NaN | -0.270887 | 0.086202 | 0.001675 | 0.087005 | -0.265763 | 0.120076 | 0.026877 | 0.300786 | -0.259471 | 0.123189 | 0.03518 | 0.512285 |
| UNKNOWN [M-H] | 488.2329 | 23.13435 | N | NaN | NaN | 0.269953 | 0.081738 | 0.000958 | 0.066673 | 0.20267 | 0.113631 | 0.074493 | 0.418101 | 0.325235 | 0.117292 | 0.005557 | 0.263491 |
| UNKNOWN [M-H] | 500.1831 | 23.1173 | N | NaN | NaN | 0.258465 | 0.085943 | 0.002635 | 0.1181 | 0.372747 | 0.113002 | 0.000972 | 0.099717 | 0.097084 | 0.129711 | 0.454177 | 0.859472 |
| UNKNOWN [M+H] | 514.0347 | 1.304331 | P | NaN | NaN | 0.34224 | 0.088198 | 0.000104 | 0.014839 | 0.380039 | 0.154198 | 0.013716 | 0.253425 | 0.321254 | 0.10816 | 0.002976 | 0.220679 |
| UNKNOWN [M-H] | 516.4114 | 23.23958 | N | NaN | NaN | -0.106121 | 0.090646 | 0.241714 | 0.732305 | -0.422603 | 0.12305 | 0.000594 | 0.08832 | 0.22574 | 0.125537 | 0.072146 | 0.58057 |
| UNKNOWN [M-H] | 548.1896 | 22.90553 | N | NaN | NaN | 0.188943 | 0.078582 | 0.016199 | 0.285701 | 0.418487 | 0.102666 | 0.000046 | 0.021398 | -0.066868 | 0.113418 | 0.555476 | 0.891383 |
| UNKNOWN [M-H] | 549.306 | 22.63429 | N | NaN | NaN | 0.250995 | 0.08209 | 0.002232 | 0.106465 | 0.077808 | 0.137147 | 0.570487 | 0.908114 | 0.347555 | 0.099828 | 0.000499 | 0.061948 |
| UNKNOWN [M+H] | 562.4572 | 25.22002 | P | NaN | NaN | 0.329975 | 0.079843 | 0.000036 | 0.007817 | 0.208306 | 0.123171 | 0.090799 | 0.451337 | 0.424844 | 0.102293 | 0.000033 | 0.00894 |
| UNKNOWN [M-H] | 584.265 | 23.20711 | N | NaN | NaN | -0.191651 | 0.07737 | 0.013247 | 0.257998 | 0.067318 | 0.127761 | 0.598262 | 0.917461 | -0.32608 | 0.095955 | 0.000678 | 0.073965 |
| UNKNOWN [M-H] | 594.4843 | 22.83466 | N | NaN | NaN | -0.117951 | 0.084077 | 0.160648 | 0.675578 | -0.447461 | 0.116841 | 0.000128 | 0.032297 | 0.168657 | 0.112831 | 0.134973 | 0.651308 |
| UNKNOWN [M-H] | 595.4051 | 22.8058 | N | NaN | NaN | 0.268532 | 0.083073 | 0.001227 | 0.075758 | 0.249216 | 0.113632 | 0.028293 | 0.302503 | 0.277818 | 0.121882 | 0.022643 | 0.460898 |
| UNKNOWN [M-H] | 596.501 | 23.11186 | N | NaN | NaN | -0.165648 | 0.084913 | 0.051081 | 0.48166 | -0.383375 | 0.117157 | 0.001067 | 0.099717 | 0.069755 | 0.119832 | 0.560498 | 0.891383 |
| UNKNOWN [M-H] | 600.5137 | 22.55868 | N | NaN | NaN | 0.233898 | 0.082743 | 0.004702 | 0.150821 | 0.036226 | 0.13037 | 0.78111 | 0.962563 | 0.373009 | 0.103664 | 0.00032 | 0.048689 |
| UNKNOWN [M+H] | 606.4627 | 26.22056 | P | NaN | NaN | 0.373502 | 0.077149 | 0.000001 | 0.002062 | 0.246888 | 0.123458 | 0.045525 | 0.351319 | 0.458609 | 0.096826 | 0.000002 | 0.002373 |
| UNKNOWN [M-H] | 612.5332 | 24.05289 | N | NaN | NaN | -0.126866 | 0.085728 | 0.13891 | 0.64526 | -0.382847 | 0.1168 | 0.001046 | 0.099717 | 0.130555 | 0.119128 | 0.273111 | 0.771046 |
| UNKNOWN [M-H] | 614.463 | 22.86675 | N | NaN | NaN | -0.093784 | 0.083375 | 0.26065 | 0.747186 | -0.408453 | 0.115606 | 0.000411 | 0.070715 | 0.209945 | 0.113631 | 0.064661 | 0.577834 |
| UNKNOWN [M-H] | 634.3934 | 21.67741 | N | NaN | NaN | -0.163865 | 0.079705 | 0.039792 | 0.435965 | -0.418926 | 0.112554 | 0.000198 | 0.042307 | 0.059894 | 0.108979 | 0.582602 | 0.894721 |
| UNKNOWN [M-H] | 644.3779 | 21.6784 | N | NaN | NaN | 0.325937 | 0.086313 | 0.000159 | 0.019266 | 0.304104 | 0.120179 | 0.011393 | 0.248891 | 0.336494 | 0.12301 | 0.006229 | 0.278703 |
| UNKNOWN [M-H] | 652.4844 | 25.24636 | N | NaN | NaN | 0.161245 | 0.085242 | 0.05854 | 0.497517 | -0.075303 | 0.120516 | 0.532078 | 0.893817 | 0.386043 | 0.117042 | 0.000973 | 0.093603 |
| UNKNOWN [M-H] | 660.4454 | 23.04231 | N | NaN | NaN | -0.14761 | 0.088754 | 0.096285 | 0.603867 | -0.37682 | 0.107291 | 0.000445 | 0.072723 | 0.200322 | 0.140327 | 0.153425 | 0.669342 |
| UNKNOWN [M+H] | 684.4939 | 26.49437 | P | NaN | NaN | 0.350211 | 0.079542 | 0.000011 | 0.003496 | 0.263902 | 0.12251 | 0.03123 | 0.314414 | 0.419863 | 0.102724 | 0.000044 | 0.010985 |
| UNKNOWN [M+H] | 690.5221 | 26.09373 | P | NaN | NaN | 0.273547 | 0.084836 | 0.001262 | 0.076486 | 0.23881 | 0.116336 | 0.040095 | 0.333818 | 0.308185 | 0.123026 | 0.012244 | 0.36791 |
| UNKNOWN [M-H] | 712.1862 | 23.20823 | N | NaN | NaN | -0.2024 | 0.081399 | 0.012901 | 0.257975 | 0.091678 | 0.134568 | 0.495696 | 0.879672 | -0.356371 | 0.100318 | 0.000382 | 0.052038 |
| UNKNOWN [M-H] | 713.2542 | 21.68026 | N | NaN | NaN | -0.16107 | 0.078178 | 0.03937 | 0.435459 | -0.370227 | 0.111051 | 0.000857 | 0.097883 | 0.029971 | 0.107902 | 0.781195 | 0.952432 |
| UNKNOWN [M+H] | 716.5787 | 24.2146 | P | NaN | NaN | 0.260777 | 0.082288 | 0.001529 | 0.085976 | 0.277626 | 0.116133 | 0.016822 | 0.259482 | 0.245522 | 0.115145 | 0.032983 | 0.510665 |
| UNKNOWN [M-H] | 718.5264 | 23.34345 | N | NaN | NaN | 0.208459 | 0.083163 | 0.012189 | 0.254026 | 0.045852 | 0.128467 | 0.721153 | 0.948036 | 0.358261 | 0.106398 | 0.000759 | 0.077654 |
| UNKNOWN [M-H] | 764.5648 | 23.36646 | N | NaN | NaN | -0.230626 | 0.085489 | 0.006982 | 0.190365 | -0.389794 | 0.118562 | 0.00101 | 0.099717 | -0.062008 | 0.1208 | 0.607736 | 0.905571 |
| UNKNOWN [M-H] | 765.394 | 26.4027 | N | NaN | NaN | 0.306332 | 0.084835 | 0.000305 | 0.031197 | 0.358583 | 0.120557 | 0.002936 | 0.153617 | 0.260111 | 0.11807 | 0.027593 | 0.499839 |
| UNKNOWN [M-H] | 788.4726 | 23.14285 | N | NaN | NaN | 0.262839 | 0.0835 | 0.001645 | 0.087005 | 0.342805 | 0.118636 | 0.003858 | 0.168851 | 0.166853 | 0.117484 | 0.155543 | 0.669655 |
| UNKNOWN [M+H] | 811.6095 | 25.31489 | P | NaN | NaN | 0.348517 | 0.083064 | 0.000027 | 0.006356 | 0.298447 | 0.122619 | 0.014935 | 0.253676 | 0.397466 | 0.111237 | 0.000353 | 0.050176 |
| UNKNOWN [M+H] | 815.2758 | 22.37897 | P | NaN | NaN | -0.159899 | 0.083301 | 0.054918 | 0.486772 | -0.399026 | 0.119846 | 0.00087 | 0.097883 | 0.058816 | 0.11507 | 0.609257 | 0.905571 |
| UNKNOWN [M-H] | 824.6405 | 22.80646 | N | NaN | NaN | 0.250043 | 0.080587 | 0.001917 | 0.095047 | 0.192322 | 0.115201 | 0.09503 | 0.456612 | 0.290602 | 0.112527 | 0.009809 | 0.338224 |
| UNKNOWN [M-H] | 827.5686 | 24.13148 | N | NaN | NaN | -0.191947 | 0.086174 | 0.025919 | 0.373598 | -0.400527 | 0.117137 | 0.000628 | 0.089317 | 0.040426 | 0.123063 | 0.742537 | 0.948314 |
| UNKNOWN [M+H] | 863.6035 | 26.31528 | P | NaN | NaN | -0.308021 | 0.082087 | 0.000175 | 0.019762 | -0.382809 | 0.133283 | 0.004077 | 0.168851 | -0.242363 | 0.106053 | 0.022296 | 0.458819 |
| UNKNOWN [M+H] | 903.463 | 10.14332 | P | NaN | NaN | 0.302118 | 0.079405 | 0.000142 | 0.017863 | 0.244026 | 0.113215 | 0.031129 | 0.314361 | 0.377602 | 0.109805 | 0.000584 | 0.065913 |
| UNKNOWN [M+H] | 943.3523 | 4.415214 | P | NaN | NaN | 0.334865 | 0.082514 | 0.000049 | 0.009186 | 0.267839 | 0.126318 | 0.033975 | 0.324483 | 0.387933 | 0.109906 | 0.000416 | 0.054456 |
| UNKNOWN [M+H] | 965.6468 | 27.96958 | P | NaN | NaN | -0.249764 | 0.079928 | 0.001779 | 0.090942 | -0.283946 | 0.118587 | 0.016647 | 0.25815 | -0.196925 | 0.110767 | 0.075431 | 0.58057 |
| UNKNOWN [M+H] | 969.5642 | 25.31959 | P | NaN | NaN | 0.26467 | 0.083763 | 0.001579 | 0.08611 | 0.211725 | 0.126193 | 0.093389 | 0.455572 | 0.341019 | 0.111535 | 0.002232 | 0.17387 |
| UNKNOWN [M+H] | 997.273 | 4.414908 | P | NaN | NaN | 0.317935 | 0.083278 | 0.000135 | 0.017624 | 0.253231 | 0.125973 | 0.04441 | 0.348857 | 0.371441 | 0.112128 | 0.000924 | 0.091628 |