

Table S2. Results of the stability selection performed with the 595 metabolite features in the SOLAR (discovery) cohort. The percentage of subsamples selected represents the percentage that a given metabolite feature was selected in each of the 5,000 LASSO regression analyses. Effect estimates are shown for the association between the metabolite features and Prediabetes/T2D calculated using linear regression and adjusting for all general and specific risk factors. Mean intensity represents the raw feature intensity from the LC-MS analysis before log transformation. The annotation confidence level indicates the confidence of metabolite annotation based on the criteria of Schymanski et al. (40), where level 1 represents the confirmed structure, level 2 represents the probable structure based on diagnostic evidence, level 3 represents tentative candidates, level 4 represents the unequivocal molecular structure, and level 5 represents the exact mass of interest. Level 4 and 5 annotations were generated using version 2 of the MS peaks to paths module from MetaboAnalyst v5.0. Level 1 annotations were obtained by comparison to a database of authentic standards analyzed on the same instrument using identical instrumental methods based upon mass error and retention difference of 10ppm and 20 seconds. Some metabolite features were mapped to multiple possible metabolites; a semicolon separates the possible metabolite names for these features. Level 5 annotations are indicated by the m/z and retention time only.

| m/z | Retention Time | Metabolite Name | Percentage of LASSO iterations selected | Mean Feature Intensity | Mode | Adduct | Confidence Level |
|----------|----------------|---|---|------------------------|----------------|-------------------------|------------------|
| 515.2872 | 215.2 | Taurocholic acid | 90.6% | 2101027.282 | HILIC Negative | M(C13)-H[-] | 1 |
| 214.0261 | 35.1 | Allylphenol sulfate | 90.3% | 19673198.57 | HILIC Negative | M(C13)-H[-] | 2 |
| 125.0974 | 58.1 | Caprylic acid | 87.0% | 7822326.224 | HILIC Negative | M-H ₂ O-H[-] | 1 |
| 132.0807 | 170.2 | 132.08071@170.2 | 81.5% | 635043.2692 | C18 Positive | - | 5 |
| 301.5323 | 22.4 | Guanosine diphosphate mannose | 76.8% | 4854818.013 | C18 Negative | M-2H[2-] | 3 |
| 425.252 | 66.5 | 5-oxo-prostaglandin E2-glyceryl ester | 76.4% | 3446135.724 | HILIC Positive | M+H[1+] | 3 |
| 134.0473 | 18.7 | Adenine | 74.6% | 3047477.901 | HILIC Negative | M-H[-] | 3 |
| 85.02953 | 137 | Gamma Hydroxybutyric Acid; 3R-hydroxy-butanoic acid; (S)-3-Hydroxybutyric acid; 2-Hydroxybutyric acid; (S)-3-Hydroxyisobutyric acid | 74.3% | 20195152.4 | HILIC Negative | M-H ₂ O-H[-] | 4 |
| 343.2241 | 69 | 343.2241@69 | 71.6% | 934233.5 | HILIC Positive | - | 5 |
| 184.0363 | 18.4 | 184.03633@18.4 | 70.0% | 4092200.128 | HILIC Negative | - | 5 |

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|----------|-------|---|-------|-------------|----------------|--------------------------|---|
| 101.0244 | 21.3 | Acetoacetate; Acetoacetic acid; 2-Oxobutanoate; 2-Oxobutyric acid | 66.4% | 25970235.15 | C18 Negative | M-H | 3 |
| 262.9755 | 22.1 | 262.97546@22.1 | 62.0% | 238428493.5 | C18 Negative | - | 5 |
| 87.04518 | 209.8 | Butyric acid | 60.8% | 4065969.484 | HILIC Negative | M-H[-] | 3 |
| 184.0735 | 110.1 | 184.07349@110.1 | 60.1% | 19548594.18 | HILIC Positive | - | 5 |
| 126.031 | 19.5 | 126.03099@19.5 | 57.0% | 2015198.34 | HILIC Negative | - | 5 |
| 331.248 | 254.7 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 54.1% | 2617213.288 | C18 Positive | M+H ₂ O+H[1+] | 4 |
| 174.0547 | 44.1 | 4-Quinolincarboxylate; 2-Quinolincarboxylate | 53.7% | 2659101.795 | C18 Positive | M+H | 3 |
| 120.9965 | 274.5 | 3-Mercaptolactic acid | 52.9% | 651380.8558 | HILIC Negative | M-H[-] | 3 |
| 227.0869 | 140.6 | Deoxycytidine | 51.6% | 16295073.13 | HILIC Negative | M(C13)-H[-] | 3 |
| 542.929 | 444.6 | Phosphoadenosine phosphosulfate | 51.6% | 89625386.9 | HILIC Negative | M+K-2H[-] | 3 |
| 135.926 | 225 | Thiosulfate | 49.8% | 4856108.545 | HILIC Positive | M+Na[1+] | 3 |
| 114.0198 | 53.9 | L-Aspartic acid; D-Aspartic acid | 49.6% | 52268792.66 | HILIC Negative | M-H ₂ O-H[-] | 4 |
| 147.0123 | 140.4 | 2-Oxo-4-methylthiobutanoic acid | 49.4% | 5496260.413 | HILIC Negative | M-H[-] | 3 |
| 331.191 | 223.3 | 17-beta Estradiol | 47.3% | 1847332.228 | C18 Negative | M+Hac-H | 1 |
| 145.0002 | 315 | 145.0002@315 | 47.1% | 451343.3301 | HILIC Negative | - | 5 |
| 377.1449 | 59 | 377.14492@59 | 45.6% | 699997.6058 | C18 Positive | - | 5 |
| 223.0564 | 20.2 | Allocystathionine; L-Cystathionine | 45.5% | 15081970.78 | C18 Negative | M(S34)-H[-] | 4 |
| 158.0823 | 256.4 | 5-Acetamidovalerate | 45.1% | 1280500.276 | HILIC Negative | M-H[-] | 3 |
| 132.0809 | 65.5 | 132.0809@65.5 | 44.5% | 12804375.05 | HILIC Positive | - | 5 |
| 123.0998 | 219.1 | N,N-Dimethylaniline; Phenylethylamine | 43.1% | 2110513.349 | HILIC Positive | M(C13)+H[1+] | 4 |
| 403.3581 | 54 | 3a,7a-Dihydroxy-5b-cholestane | 43.0% | 3272285.208 | HILIC Negative | M-H[-] | 3 |
| 173.0932 | 290.4 | N-Acetyloronithine | 42.8% | 938831.891 | HILIC Negative | M-H[-] | 3 |

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| 206.0578 | 72.1 | 206.05778@72.1 | 42.6% | 1957307.827 | HILIC Positive | - | 5 |
| 353.1571 | 66.8 | 353.15711@66.8 | 42.5% | 10926240.58 | HILIC Positive | - | 5 |
| 122.0248 | 18.8 | Nicotinic acid | 42.2% | 1560134.689 | C18 Negative | M-H | 1 |
| 129.0659 | 80.9 | 129.06594@80.9 | 42.2% | 5861203.984 | HILIC Positive | - | 5 |
| 99.00887 | 310.3 | 99.00887@310.3 | 40.7% | 10428337.5 | HILIC Negative | - | 5 |
| 449.3111 | 63.4 | 449.31109@63.4 | 40.1% | 22939638.55 | HILIC Negative | - | 5 |
| 208.0968 | 74.3 | N-Acetylphenylalanine | 39.9% | 2243943.679 | HILIC Positive | M+H | 1 |
| 143.0705 | 69.5 | 33-diMe-50-33-dimethylpentanedioate | 38.8% | 1525123.962 | HILIC Positive | M+H-H2O | 1 |
| 199.0441 | 285 | Allantoic acid | 38.6% | 1138156.045 | HILIC Positive | M+Na[1+] | 3 |
| 245.0483 | 17.7 | Allantoic acid | 38.6% | 1236740.894 | C18 Positive | M+HCOONa[1+] | 3 |
| 317.2497 | 367 | 317.24972@367 | 38.1% | 25546714.33 | C18 Negative | - | 5 |
| 273.185 | 66.2 | Estradiol-17Alpha | 38.1% | 2045619.907 | HILIC Positive | M+H | 1 |
| 140.1069 | 38.6 | 3-Methoxytyramine; Epinine | 37.9% | 2512859.994 | C18 Positive | M-CO+H[1+] | 4 |
| 350.2403 | 58.3 | Tetrahydrocorticosterone | 36.5% | 5828934.429 | HILIC Negative | M(C13)-H[-] | 3 |
| 154.0864 | 76 | L-Dopa | 36.1% | 2897412.317 | HILIC Positive | M-CO2+H[1+] | 3 |
| 243.2111 | 65.2 | Gamma-Linolenic acid; Alpha-Linolenic acid | 36.1% | 2923034.462 | HILIC Positive | M-H4O2+H[1+] | 4 |
| 395.1558 | 20.8 | Riboflavin | 35.5% | 8510759.769 | C18 Positive | M+H2O+H[1+] | 3 |
| 384.3124 | 54 | Pendtadenoyl carnitine | 33.9% | 5776794.673 | HILIC Negative | M-H[-] | 3 |
| 203.129 | 140.8 | 203.12897@140.8 | 33.3% | 4213292.734 | HILIC Negative | - | 5 |
| 411.2902 | 339.7 | 411.29022@339.7 | 32.9% | 1303569.647 | C18 Negative | - | 5 |
| 110.0271 | 266.2 | Hypotaourine | 31.0% | 4410941.006 | HILIC Positive | M+H | 1 |
| 314.2403 | 249.9 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 31.0% | 722465.9006 | C18 Positive | M(C13)+H[1+] | 4 |
| 144.0655 | 26.2 | 2-Oxobutyric acid | 30.0% | 4398574.131 | C18 Positive | M+ACN+H | 1 |

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| 171.1026 | 35.2 | 4-Hydroperoxy-2-nonenal | 29.7% | 2539024.888 | C18 Negative | M-H[-] | 3 |
| 175.9989 | 10 | L-Cysteinesulfinic acid | 29.0% | 1151638.154 | C18 Positive | M+Na | 1 |
| 386.3266 | 182.7 | Pendtadenoyl carnitine | 29.0% | 1870688.282 | HILIC Positive | M+H[1+] | 3 |
| 540.4987 | 372.5 | Hexacosanoyl Carnitine | 29.0% | 6694324.712 | C18 Positive | M+H[1+] | 3 |
| 101.0245 | 69.8 | 101.0245@69.8 | 28.1% | 354727145.9 | HILIC Negative | - | 5 |
| 510.4519 | 326.2 | Nervonyl carnitine | 27.8% | 2814262.436 | C18 Positive | M+H[1+] | 3 |
| 291.0064 | 22.5 | 291.00635@22.5 | 27.5% | 871722105.1 | C18 Negative | - | 5 |
| 195.1025 | 55.6 | Perillyl aldehyde | 27.4% | 998645.7404 | C18 Negative | M+HCOO[-] | 3 |
| 167.9972 | 444.4 | Cysteic acid | 27.2% | 25923734.96 | HILIC Negative | M-H[-] | 3 |
| 312.2258 | 252.8 | 312.22575@252.8 | 26.4% | 1513669.558 | C18 Negative | - | 5 |
| 101.0705 | 272 | 101.0705@272 | 26.1% | 641882677.6 | HILIC Positive | - | 5 |
| 182.0573 | 307.8 | 182.05725@307.8 | 26.0% | 6894096.314 | HILIC Negative | - | 5 |
| 137.9867 | 15.9 | Sulfate | 26.0% | 7502425.647 | HILIC Negative | M+ACN-H[-] | 3 |
| 129.1275 | 70.8 | 129.1275@70.8 | 25.7% | 859844.5641 | HILIC Positive | - | 5 |
| 413.3067 | 239.7 | 413.30669@239.7 | 25.3% | 1701165.657 | C18 Positive | - | 5 |
| 156.0304 | 19.5 | 156.03041@19.5 | 25.0% | 2021850.298 | HILIC Negative | - | 5 |
| 140.073 | 74.7 | Pantetheine | 24.9% | 7278219.631 | HILIC Positive | M+2H[2+] | 3 |
| 181.0859 | 237.9 | Metanephrene | 24.8% | 6454042.051 | C18 Positive | M-NH3+H[1+] | 3 |
| 187.0977 | 66 | 187.09767@66 | 24.8% | 11632684.49 | HILIC Negative | - | 5 |
| 170.0814 | 79.9 | 170.08135@79.9 | 24.3% | 1606449.183 | HILIC Positive | - | 5 |
| 198.0752 | 51.9 | L-Dopa | 24.1% | 2277596.404 | C18 Positive | M+H | 1 |
| 480.2779 | 242.1 | Taurocholic acid; Taurohyocholate | 22.9% | 1264909.388 | C18 Positive | M-H4O2+H[1+] | 4 |
| 185.0807 | 124.7 | 185.08074@124.7 | 22.8% | 2495814.641 | C18 Positive | - | 5 |
| 192.0668 | 197.7 | 192.06678@197.7 | 22.7% | 1970168.446 | HILIC Negative | - | 5 |

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| 257.0123 | 202.6 | 257.01227@202.6 | 22.7% | 2659325.494 | C18 Negative | - | 5 |
| 157.1225 | 68.8 | 157.12251@68.8 | 21.9% | 2576102.699 | HILIC Positive | - | 5 |
| 209.0919 | 26.4 | Kynurenine | 21.8% | 27847033.51 | C18 Positive | M+H | 1 |
| 135.0442 | 69.5 | 3,4-Dihydroxyphenylglycol | 21.8% | 3222555.837 | HILIC Positive | M-H4O2+H[1+] | 3 |
| 149.1074 | 207.6 | Serotonin | 21.7% | 2968276.872 | HILIC Positive | M-CO+H[1+] | 3 |
| 183.0256 | 435.6 | Oxoadipic acid | 21.3% | 7688480.404 | C18 Positive | M+Na[1+] | 3 |
| 213.1132 | 250.7 | 213.11318@250.7 | 21.1% | 5072119.272 | HILIC Negative | - | 5 |
| 255.0973 | 34.8 | 255.0973@34.8 | 20.2% | 527116.8013 | C18 Positive | - | 5 |
| 111.0088 | 18.5 | Glutaconic acid; 2-Methylmaleate; Citraconic acid; Itaconate | 19.6% | 2901613.603 | C18 Negative | M-H2O-H | 3 |
| 397.2232 | 188.6 | Prostaglandin H2; Prostaglandin E2; Prostaglandin D2; Prostaglandin I2; Thromboxane A2; (13E)-11a-Hydroxy-9,15- dioxoprost-13-enoic acid; 13,14- Dihydro-15-keto-PGE2; 20- Hydroxy-leukotriene B4; Lipoxin A4; Lipoxin B4 | 18.9% | 1365606.429 | HILIC Negative | M+HCOO[-] | 4 |
| 201.035 | 145.8 | L-Fucose | 18.8% | 5441600.362 | HILIC Negative | M+Cl37[-] | 3 |
| 115.0501 | 23.4 | Dihydrouracil | 18.8% | 2307776.772 | C18 Positive | M+H | 1 |
| 241.1071 | 68 | Glycerophosphocholine | 18.7% | 3558589.676 | HILIC Positive | M-H2O+H[1+] | 3 |
| 301.2168 | 58.3 | Eicosapentaenoate | 18.1% | 53738174.86 | HILIC Negative | M-H | 1 |
| 192.0654 | 26.2 | 192.06538@26.2 | 18.0% | 3881620 | C18 Positive | - | 5 |
| 160.0604 | 26.1 | 2-Aminomuconic acid semialdehyde | 18.0% | 1021142.484 | C18 Positive | M+H2O+H[1+] | 3 |
| 295.2271 | 64.4 | 13-L-Hydroperoxylinoleic acid; 9(S)-HPODE | 17.8% | 7960879.413 | HILIC Positive | M-H2O+H[1+] | 4 |
| 183.0782 | 79 | Caprylic acid | 17.7% | 2405308.481 | HILIC Positive | M+K[1+] | 3 |
| 175.0249 | 140.8 | D-Glucuronolactone | 17.6% | 54151196.08 | HILIC Negative | M-H | 1 |

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| 142.051 | 41.3 | 142.05101@41.3 | 17.4% | 38484320.89 | HILIC Negative | - | 5 |
| 150.055 | 195.8 | 150.05495@195.8 | 16.9% | 754211.8462 | C18 Positive | - | 5 |
| 170.1177 | 229.8 | Metanephrine | 16.4% | 5382579.311 | HILIC Positive | M-CO+H[1+] | 3 |
| 776.6804 | 162.3 | Thyroxine | 16.2% | 1375623.529 | HILIC Negative | M(C13)-H[-] | 3 |
| 109.1011 | 254.6 | 109.10113@254.6 | 15.8% | 10305142.82 | C18 Positive | - | 5 |
| 149.0456 | 308 | D-Ribose; D-Xylose; L-Arabinose; D-Ribulose; D-Xylulose; L-Threo-2-pentulose; L-Ribulose | 15.6% | 48680149.85 | HILIC Negative | M-H[-] | 4 |
| 190.051 | 283.8 | 190.05103@283.8 | 15.4% | 3554595.212 | HILIC Negative | - | 5 |
| 112.9551 | 15.4 | Sulfate | 15.3% | 2660216.266 | HILIC Negative | M-H+O[-] | 3 |
| 263.237 | 290.9 | Linoleic acid | 15.1% | 8566460.91 | C18 Positive | M-H2O+H[1+] | 3 |
| 273.098 | 67.4 | 273.09803@67.4 | 14.9% | 15446695.38 | HILIC Negative | - | 5 |
| 200.0683 | 19.5 | Dihydroorotic acid | 14.8% | 7969238.66 | C18 Positive | M+ACN+H | 1 |
| 347.2214 | 240.3 | Cortexolone; Corticosterone | 14.5% | 443012.7308 | C18 Positive | M+H | 3 |
| 129.1023 | 167.1 | L-Lysine | 14.3% | 3530794.599 | HILIC Positive | M-H2O+H[1+] | 3 |
| 192.1136 | 246.1 | gamma-CEHC | 14.0% | 4294090.763 | HILIC Positive | M-C3H4O2+H[1+] | 3 |
| 191.0199 | 142.5 | 191.01985@142.5 | 14.0% | 24685013.17 | HILIC Negative | - | 5 |
| 352.2248 | 153.5 | 352.22481@153.5 | 14.0% | 1631128.311 | HILIC Positive | - | 5 |
| 312.2985 | 433.8 | Phytanic acid; Arachidic acid | 13.6% | 6546655.92 | C18 Negative | M(C13)-H[-] | 4 |
| 120.0443 | 35.9 | 5-Hydroxyindoleacetic acid; 5-Phenyl-1,3-oxazinane-2,4-dione | 13.4% | 4253433.285 | C18 Positive | M-C3H4O2+H[1+] | 4 |
| 213.1121 | 68.2 | Glycerophosphocholine | 13.3% | 3671840.686 | HILIC Positive | M-HCOOH+H[1+] | 3 |
| 229.0313 | 147.2 | 5-Phosphoribosylamine | 12.9% | 56895408.01 | HILIC Negative | M(C13)-H[-] | 3 |

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| 211.134 | 120.3 | (-)-trans-Carveol; Perillyl alcohol; Alpha-Pinene-oxide; (+)-trans-Carveol | 12.4% | 5027155.343 | HILIC Negative | M+CH ₃ COO ⁻ | 4 |
| 166.0591 | 144.1 | Homovanillin | 12.2% | 4396171.413 | HILIC Negative | M(C ₁₃)-H ⁻ | 3 |
| 228.028 | 146.8 | 5-Phosphoribosylamine | 12.0% | 952161193.7 | HILIC Negative | M-H ⁻ | 3 |
| 343.2277 | 64.9 | Docosahexaenoic acid | 11.9% | 932626.8141 | HILIC Negative | M-H+O ⁻ | 3 |
| 214.0258 | 198 | 214.02584@198 | 11.8% | 3541349.199 | C ₁₈ Negative | - | 5 |
| 190.0508 | 26.8 | 5-Hydroxyindoleacetate | 11.6% | 2193338.038 | C ₁₈ Negative | M-H | 1 |
| 118.0228 | 314.1 | Succinic acid; Methylmalonic acid | 11.5% | 7555198.891 | HILIC Negative | M(C ₁₃)-H ⁻ | 4 |
| 122.0965 | 218.6 | N,N-Dimethylaniline; Phenylethylamine | 11.5% | 35089307.13 | HILIC Positive | M+H ^[1+] | 4 |
| 437.2905 | 229.7 | Nordeoxycholic acid | 11.2% | 4049032.994 | C ₁₈ Negative | M+Hac-H | 1 |
| 206.0822 | 140.1 | Homovanillin | 11.0% | 6266131.804 | HILIC Negative | M+ACN-H ⁻ | 3 |
| 154.0587 | 20.3 | Creatine | 10.6% | 13541040.61 | C ₁₈ Positive | M+Na | 1 |
| 186.1125 | 21.9 | 3-Methoxytyramine; Epinine | 10.3% | 13340755.38 | C ₁₈ Positive | M+H ₂ O+H ^[1+] | 4 |
| 168.1021 | 74.5 | 168.10209@74.5 | 10.1% | 3077346.74 | HILIC Positive | - | 5 |
| 214.0721 | 125.1 | Pyridoxine; Norepinephrine | 10.0% | 1086840.151 | HILIC Negative | M+HCOO ⁻ | 4 |
| 201.1637 | 257.3 | Estradiol | 9.5% | 1958022.221 | C ₁₈ Positive | M- C ₃ H ₄ O ₂ +H ^[1+] | 3 |
| 327.1049 | 72 | Glycerophosphocholine | 9.5% | 1577644.481 | HILIC Positive | M+HCOONa ^[1+] | 3 |
| 168.0736 | 124.9 | Homovanillin | 9.2% | 685159.9808 | C ₁₈ Positive | M(C ₁₃)+H ^[1+] | 3 |
| 103.0595 | 325.9 | 103.0595@325.9 | 9.1% | 2133517.526 | HILIC Negative | - | 5 |
| 185.0568 | 19.1 | 185.05678@19.1 | 8.7% | 3006812.872 | HILIC Negative | - | 5 |
| 103.0402 | 214.6 | 2-Hydroxybutyrate | 8.6% | 1105713929 | HILIC Negative | M-H | 1 |
| 195.1389 | 240.5 | Chenodeoxycholic acid; Deoxycholic acid; Hyodeoxycholic acid | 8.5% | 5376408.026 | C ₁₈ Negative | M-2H ^[2-] | 4 |

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|----------|-------|---|------|-------------|----------------|-------------|---|
| 281.0999 | 70.3 | Glycerophosphocholine | 8.4% | 6124498.426 | HILIC Positive | M+Na[1+] | 3 |
| 209.0301 | 18.9 | Saccharate; Galactarate | 8.4% | 3902899.045 | C18 Negative | M-H | 3 |
| 205.0354 | 89.5 | 205.03537@89.5 | 8.0% | 6832683.263 | HILIC Negative | - | 5 |
| 185.0456 | 63.8 | 185.04563@63.8 | 7.9% | 17986871.24 | HILIC Negative | - | 5 |
| 110.06 | 32.6 | 2-Aminophenol | 7.8% | 2107937.869 | C18 Positive | M+H | 1 |
| 363.2158 | 219.5 | Cortisol | 7.7% | 9575195.625 | C18 Positive | M+H | 1 |
| 198.9754 | 21.3 | 198.97542@21.3 | 7.1% | 58158875.71 | C18 Negative | - | 5 |
| 135.1169 | 64.7 | 135.11693@64.7 | 6.9% | 16591436.48 | HILIC Positive | - | 5 |
| 307.0019 | 21.7 | 307.00194@21.7 | 6.9% | 3030796.779 | C18 Negative | - | 5 |
| 311.2952 | 434.9 | Phytanic acid; Arachidic acid | 6.8% | 28466911.24 | C18 Negative | M-H[-] | 4 |
| 198.9757 | 23.2 | 198.97569@23.2 | 6.7% | 2186433.862 | HILIC Negative | - | 5 |
| 171.113 | 374.7 | N6-Acetyl-L-lysine | 6.7% | 1312803.76 | HILIC Positive | M-H2O+H[1+] | 3 |
| 305.2461 | 65.6 | 305.24611@65.6 | 6.5% | 2681101.872 | HILIC Positive | - | 5 |
| 140.1071 | 166.1 | 140.10707@166.1 | 6.4% | 3551995.205 | HILIC Positive | - | 5 |
| 331.2479 | 66.4 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 6.4% | 276643.891 | HILIC Positive | M+H2O+H[1+] | 4 |
| 194.0811 | 194.9 | 194.0811@194.9 | 6.4% | 623951.2051 | C18 Positive | - | 5 |
| 170.0326 | 21.8 | Creatine | 6.2% | 3145434.66 | C18 Positive | M+K[1+] | 3 |
| 201.1848 | 259.8 | Dodecanoic acid | 6.2% | 2248400.654 | C18 Positive | M+H[1+] | 3 |
| 335.2217 | 64.2 | 335.22172@64.2 | 6.0% | 5593897.651 | HILIC Negative | - | 5 |
| 349.2019 | 217.3 | 15-Keto-prostaglandin E2; Prostaglandin E3 | 6.0% | 91645.66987 | C18 Negative | M-H[-] | 4 |
| 221.0591 | 20.2 | Cystathionine | 5.9% | 6435839.577 | C18 Negative | M-H | 1 |
| 191.0196 | 18.7 | Citrate; Citric acid; Isocitrate | 5.7% | 67760955.89 | C18 Negative | M-H | 3 |
| 163.133 | 67.9 | 163.13303@67.9 | 5.6% | 3616099.981 | HILIC Positive | - | 5 |
| 253.0829 | 33.6 | 253.08293@33.6 | 5.5% | 24219078.66 | HILIC Negative | - | 5 |

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| 244.0365 | 36.3 | 244.03653@36.3 | 5.4% | 4309434.609 | HILIC Negative | - | 5 |
| 137.0962 | 64.9 | 137.09623@64.9 | 5.2% | 12876403.04 | HILIC Positive | - | 5 |
| 195.1027 | 66.3 | 195.10271@66.3 | 5.2% | 12403408.04 | HILIC Negative | - | 5 |
| 108.0126 | 335.6 | Hypotaurine | 5.1% | 555286.8205 | HILIC Negative | M-H | 1 |
| 175.0249 | 313.7 | 175.02485@313.7 | 5.1% | 19402599.91 | HILIC Negative | - | 5 |
| 211.1338 | 83.9 | (-)-trans-Carveol; Perillyl alcohol; Alpha-Pinene-oxide; (+)-trans-Carveol | 5.1% | 1843579.503 | C18 Negative | M+CH3COO[-] | 4 |
| 96.9601 | 18.2 | 96.9601@18.2 | 5.1% | 153605552.6 | C18 Negative | - | 5 |
| 245.1378 | 71.1 | 9-Hydroxy-10-O-D-glucuronoside-12Z-octadecenoate; 10-Hydroxy-octadec-12Z-enoate-9-beta-D-glucuronide; 12-hydroxy-13-O-D-glucuronoside-octadec-9Z-enoate; 12-O-D-Glucuronoside-13-hydroxyoctadec-9Z-enoate | 5.0% | 1552129.497 | HILIC Positive | M+2H[2+] | 4 |
| 178.0864 | 68.6 | 178.08643@68.6 | 4.9% | 2617426.019 | HILIC Positive | - | 5 |
| 165.0921 | 69.8 | 165.09214@69.8 | 4.8% | 52643856.16 | HILIC Negative | - | 5 |
| 328.236 | 57.7 | Docosaehaenoate | 4.8% | 90821059.38 | HILIC Negative | M-H _[-1] | 1 |
| 155.1068 | 64.5 | 4-Hydroperoxy-2-nonenal | 4.8% | 20659495.42 | HILIC Positive | M-H ₂ O+H[1+] | 3 |
| 363.2094 | 329 | Docosaehaenoic acid | 4.8% | 766249.0737 | C18 Negative | M+Cl _[-] | 3 |
| 291.1951 | 65.8 | Estradiol | 4.7% | 8016541.282 | HILIC Positive | M+H ₂ O+H[1+] | 3 |
| 165.0556 | 26.9 | 3-(4-hydroxyphenyl)propanoic acid | 4.7% | 4683992.968 | C18 Negative | M-H | 1 |
| 162.0761 | 22.5 | N-Methyl-L-glutamate; 2-Aminoadipic acid | 4.7% | 4105160.593 | C18 Positive | M+H | 3 |
| 209.0668 | 141.1 | L-Fucose | 4.7% | 10474542.46 | HILIC Negative | M+HCOO _[-] | 3 |
| 247.0391 | 19 | 3-(3-Methoxy-4hydroxyphenyl)lactate | 4.5% | 224514.7244 | C18 Negative | M+Cl | 1 |

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|----------|-------|--|------|-------------|----------------|--|---|
| 140.1071 | 228 | N,N-Dimethylaniline; Phenylethylamine | 4.4% | 4239288.016 | HILIC Positive | M+H ₂ O+H[1+] | 4 |
| 147.5159 | 16 | 147.51593@16 | 4.4% | 84084.39103 | C18 Positive | - | 5 |
| 296.9934 | 230.4 | 296.99341@230.4 | 4.3% | 13325233.32 | HILIC Positive | - | 5 |
| 264.1355 | 237.8 | gamma-CEHC | 4.3% | 1060065.997 | C18 Positive | M+H[1+] | 3 |
| 777.695 | 166.3 | Thyroxine | 4.3% | 2149589.888 | HILIC Positive | M+H | 1 |
| 221.0527 | 20.2 | 221.05269@20.2 | 4.2% | 1288682460 | C18 Negative | - | 5 |
| 433.1023 | 317.9 | Gama-glutamylglutathione | 4.2% | 3144696.76 | C18 Negative | M-H[-] | 3 |
| 260.9794 | 20.2 | 260.97936@20.2 | 4.2% | 11690348.83 | C18 Negative | - | 5 |
| 174.0407 | 18.4 | N-Acetylaspartate | 4.1% | 1340245.128 | C18 Negative | M-H | 1 |
| 179.0714 | 44.8 | Phenylacetaldehyde | 4.1% | 137372821.9 | HILIC Negative | M+CH ₃ COO[-] | 3 |
| 194.0811 | 107 | 2-Hydroxyphenylacetic acid | 4.1% | 576671.3942 | C18 Positive | M+ACN+H | 1 |
| 227.1025 | 26.9 | Porphobilinogen | 4.0% | 634300.8173 | C18 Positive | M+H | 1 |
| 106.0285 | 15.3 | Nicotinic acid | 3.9% | 975600.1891 | C18 Positive | M+H-H ₂ O | 1 |
| 515.2871 | 211.3 | Taurocholic acid; Taurohyocholate | 3.9% | 693919.4551 | C18 Negative | M(C13)-H[-] | 4 |
| 176.0282 | 314.5 | 176.02823@314.5 | 3.8% | 1331202.798 | HILIC Negative | - | 5 |
| 159.1026 | 62.6 | C80-3-Hydroxyoctanoic acid | 3.8% | 4471335.365 | C18 Negative | M-H | 1 |
| 574.2571 | 205.5 | Taurocholic acid; Taurohyocholate | 3.8% | 1075624.641 | HILIC Positive | M+NaCl[1+] | 4 |
| 381.2264 | 66.1 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 3.7% | 3793176.554 | HILIC Positive | M+HCOONa[1+] | 4 |
| 223.0967 | 66.5 | Glycerophosphocholine | 3.7% | 4297801.128 | HILIC Positive | M-H ₄ O ₂ +H[1+] | 3 |
| 139.0753 | 124 | 139.0753@124 | 3.6% | 2931090.843 | C18 Positive | - | 5 |
| 126.0914 | 94 | Pyridoxine; Norepinephrine | 3.6% | 41181824.13 | HILIC Positive | M-CO ₂ +H[1+] | 4 |
| 157.0138 | 315.1 | 157.0138@315.1 | 3.5% | 2584928.144 | HILIC Negative | - | 5 |
| 132.0768 | 22.8 | Creatine | 3.5% | 183844259.4 | C18 Positive | M+H | 1 |

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|----------|-------|--|------|-------------|----------------|--------------------------|---|
| 148.0617 | 347.8 | Gamma-Aminobutyric acid; Dimethylglycine; (R)-b-aminoisobutyric acid; L-Alpha-aminobutyric acid; (S)-b-aminoisobutyric acid; 3-Aminoisobutanoic acid | 3.4% | 2080262.574 | HILIC Negative | M+HCOO[-] | 4 |
| 175.0247 | 18.7 | D-Glucuronolactone; Ascorbate | 3.3% | 37355381.53 | C18 Negative | M-H | 3 |
| 194.0814 | 69.3 | 194.08139@69.3 | 3.2% | 912854.4647 | HILIC Positive | - | 5 |
| 100.0405 | 202.6 | L-Threonine; L-Allothreonine | 3.2% | 121670.2853 | HILIC Negative | M-H ₂ O-H[-] | 4 |
| 155.0464 | 16.4 | Methylimidazoleacetic acid | 3.2% | 3505726.301 | HILIC Negative | M-H+O[-] | 3 |
| 141.0658 | 23.6 | Methylimidazoleacetic acid | 3.1% | 3459205.788 | C18 Positive | M+H[1+] | 3 |
| 394.2957 | 249.2 | Myristoyl-L-carnitine | 3.0% | 1679898.285 | C18 Positive | M+Na | 1 |
| 195.1391 | 59.4 | 195.1391@59.4 | 2.9% | 48311452.63 | HILIC Negative | - | 5 |
| 243.0873 | 68.6 | 243.0873@68.6 | 2.9% | 19135804.34 | HILIC Negative | - | 5 |
| 124.1122 | 73.1 | 3-Methoxytyramine; Epinine | 2.8% | 5118174.933 | HILIC Positive | M-CO ₂ +H[1+] | 4 |
| 229.0119 | 147 | Glucuronic acid; 3-Dehydro-L-gulonate; Iduronic acid | 2.8% | 13814145.64 | HILIC Negative | M+Cl[-] | 4 |
| 168.0655 | 196 | 168.06549@196 | 2.7% | 1071312.151 | C18 Positive | - | 5 |
| 185.0714 | 310.2 | L-Tryptophan; D-Tryptophan | 2.6% | 13223289.8 | HILIC Negative | M-H ₂ O-H[-] | 4 |
| 312.2261 | 66.2 | 312.22612@66.2 | 2.6% | 2251812.449 | HILIC Negative | - | 5 |
| 138.0198 | 15.2 | 2-Aminomuconic acid | 2.4% | 14003658.67 | HILIC Negative | M-H ₂ O-H[-] | 3 |
| 373.2377 | 329.4 | Docosahexaenoic acid | 2.3% | 3001047.429 | C18 Negative | M+HCOO[-] | 3 |
| 180.102 | 213.8 | Metanephrine | 2.3% | 5958103.231 | HILIC Positive | M-H ₂ O+H[1+] | 3 |
| 179.0559 | 22.6 | Psicose; Tagatose; Allose; Alpha-D-Glucose; Galactose; Mannose; Myoinositol; Sorbose; Theobromine; Paraxanthine; Theophylline; Gulose | 2.3% | 182454647.3 | C18 Negative | M-H | 3 |
| 226.0125 | 161.4 | L-Glutamic acid 5-phosphate | 2.3% | 70952061.78 | HILIC Negative | M-H[-] | 3 |

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|----------|-------|---|------|-------------|----------------|-------------|---|
| 416.3372 | 191.7 | 3-Hydroxyhexadecanoylcarnitine | 2.3% | 4789588.753 | HILIC Positive | M+H | 1 |
| 320.2311 | 65.1 | 320.23105@65.1 | 2.2% | 1158392.372 | HILIC Negative | - | 5 |
| 152.0706 | 37.5 | 152.07058@37.5 | 2.2% | 9363509.433 | C18 Positive | - | 5 |
| 144.0304 | 22.3 | 144.03039@22.3 | 2.2% | 3221460.59 | HILIC Negative | - | 5 |
| 423.2393 | 62.7 | 5-oxo-prostaglandin E2-glyceryl ester | 2.1% | 4599324.689 | HILIC Negative | M-H[-] | 3 |
| 140.1071 | 75.9 | 3-Methoxytyramine; Epinine | 2.1% | 5242080.763 | HILIC Positive | M-CO+H[1+] | 4 |
| 461.2731 | 66.6 | 9-Hydroxy-10-O-D-glucuronoside-12Z-octadecenoate; 10-Hydroxy-octadec-12Z-enoate-9-beta-D-glucuronide; 12-hydroxy-13-O-D-glucuronoside-octadec-9Z-enoate; 12-O-D-Glucuronoside-13-hydroxyoctadec-9Z-enoate | 2.0% | 22932384.15 | HILIC Positive | M-CO+H[1+] | 4 |
| 199.0376 | 145.7 | L-Fucose | 1.9% | 20283487.16 | HILIC Negative | M+Cl[-] | 3 |
| 232.9888 | 148 | 2-Oxo-4-methylthiobutanoic acid | 1.8% | 2448140.926 | HILIC Positive | M+HCOOK[1+] | 3 |
| 161.1285 | 369.3 | N6-Acetyl-L-lysine | 1.8% | 42021783.98 | HILIC Positive | M-CO+H[1+] | 3 |
| 126.0218 | 21.5 | Taurine | 1.8% | 6714006.298 | C18 Positive | M+H | 1 |
| 157.0367 | 15.8 | 157.03674@15.8 | 1.8% | 4588196.917 | HILIC Negative | - | 5 |
| 269.0431 | 67.6 | 269.04308@67.6 | 1.7% | 2026893.891 | HILIC Positive | - | 5 |
| 147.0299 | 20.1 | 3-Hydroxyglutarate; 2-Hydroxyglutaric acid; Citramalate | 1.7% | 14987385.54 | C18 Negative | M-H | 3 |
| 113.0598 | 66.1 | Sorbate | 1.7% | 7284221.997 | HILIC Positive | M+H | 1 |
| 119.0503 | 35.4 | Phenylacetaldehyde | 1.7% | 12424163.78 | HILIC Negative | M-H[-] | 3 |
| 136.0518 | 310.9 | 136.0518@310.9 | 1.7% | 57484140.89 | HILIC Negative | - | 5 |
| 143.1078 | 66.6 | 2-Me-70-2-Methylheptanoic acid; Caprylate | 1.7% | 60612089.34 | HILIC Negative | M-H | 3 |
| 181.0355 | 26.5 | Amino adipic acid | 1.7% | 4481646.032 | HILIC Negative | M+Na-2H[-] | 3 |

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|----------|-------|--|------|-------------|----------------|-------------|---|
| 115.0037 | 19 | Fumarate; Fumaric acid; Maleate | 1.7% | 2311978.567 | C18 Negative | M-H | 3 |
| 140.0355 | 18.5 | 2-Aminomuconic acid semialdehyde | 1.6% | 2030951.324 | HILIC Negative | M-H[-] | 3 |
| 127.0755 | 66 | 3,4-Dihydroxyphenylglycol | 1.6% | 4775967.696 | HILIC Positive | M-CO2+H[1+] | 3 |
| 190.0864 | 68.1 | Indole-3-propionic acid; Indole-3-Methyl Acetate | 1.6% | 4871820.288 | HILIC Positive | M+H | 3 |
| 143.1077 | 103.9 | Caprylic acid | 1.6% | 3496813.74 | C18 Negative | M-H[-] | 3 |
| 151.04 | 199.7 | Resorcinol Monoacetate; 24-Dihydroxyacetophenone | 1.6% | 5603950.436 | C18 Negative | M-H | 3 |
| 129.0194 | 20.2 | Glutaconic acid; 2-Methylmaleate; Citraconic acid; Itaconate | 1.6% | 10678469.2 | C18 Negative | M-H | 3 |
| 203.0523 | 20.8 | 203.05232@20.8 | 1.6% | 314153339.5 | C18 Positive | - | 5 |
| 137.0961 | 241.7 | 137.09608@241.7 | 1.5% | 5490682.298 | C18 Positive | - | 5 |
| 139.0515 | 19 | Methylimidazoleacetic acid | 1.5% | 1904054.064 | HILIC Negative | M-H[-] | 3 |
| 116.0706 | 22.1 | Proline | 1.5% | 370117790.5 | C18 Positive | M+H | 1 |
| 225.0317 | 254.8 | 225.03167@254.8 | 1.5% | 818879.7724 | C18 Negative | - | 5 |
| 451.3069 | 66.1 | Chenodeoxycholic acid; Deoxycholic acid; Hyodeoxycholic acid | 1.5% | 5371859.721 | HILIC Negative | M+CH3COO[-] | 4 |
| 195.0507 | 19.2 | Gluconate | 1.5% | 17891802.31 | C18 Negative | M-H | 1 |
| 167.0702 | 124.7 | 167.07019@124.7 | 1.5% | 8410413.679 | C18 Positive | - | 5 |
| 372.3471 | 285.1 | L-Palmitoylcarnitine | 1.5% | 4845119.542 | C18 Positive | M-CO+H[1+] | 3 |
| 191.0562 | 300.7 | Quinic acid; Quinic Acid | 1.5% | 2073337.577 | HILIC Negative | M-H | 3 |
| 295.2995 | 425.3 | Phytanic acid; Arachidic acid | 1.4% | 1058923.026 | C18 Positive | M-H2O+H[1+] | 4 |
| 183.0669 | 68.6 | 4-Hydroxy-3-Methoxyphenylglycol; Phosphorylcholine | 1.4% | 746956442.4 | HILIC Negative | M-H | 3 |
| 225.0614 | 21.2 | Sedoheptulose | 1.4% | 222194144.5 | C18 Negative | M-H+O[-] | 3 |

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| 311.2225 | 253.6 | 311.22251@253.6 | 1.4% | 4408807.147 | C18 Negative | - | 5 |
| 98.95591 | 18.2 | 98.95591@18.2 | 1.4% | 5997991.17 | C18 Negative | - | 5 |
| 189.0405 | 117 | Pyridoxine; Norepinephrine | 1.4% | 16300815.08 | HILIC Negative | M+Na-2H[-] | 4 |
| 498.2882 | 250.5 | Tauromuricholic acid; Tauro-beta-muricholic acid; Taurocholic acid | 1.4% | 1212076.798 | C18 Positive | M+H-H2O | 3 |
| 203.1287 | 48.1 | 203.12874@48.1 | 1.3% | 582243.9519 | C18 Negative | - | 5 |
| 261.2208 | 66.5 | Gamma-Linolenic acid; Alpha-Linolenic acid | 1.3% | 7203646.404 | HILIC Positive | M-H2O+H[1+] | 4 |
| 287.2371 | 69.3 | 287.23705@69.3 | 1.3% | 1839249.083 | HILIC Positive | - | 5 |
| 283.007 | 318.5 | L-Tryptophan; D-Tryptophan | 1.3% | 6909224.862 | HILIC Negative | M+Br[-] | 4 |
| 448.3053 | 240.8 | Glycocholic acid | 1.3% | 8222733.083 | C18 Positive | M+H-H2O | 1 |
| 303.232 | 65.2 | 303.23198@65.2 | 1.3% | 3054467.731 | HILIC Positive | - | 5 |
| 167.0704 | 70.6 | 3-(4-hydroxyphenyl)propanoic acid; 3-(2-Hydroxyphenyl)Propanoate | 1.2% | 5757086.173 | HILIC Positive | M+H | 3 |
| 217.0364 | 20.3 | sulfuric acid [4-(2-aminoethyl)phenyl] ester | 1.2% | 21551577.69 | C18 Negative | M(C13)-H[-] | 3 |
| 364.2193 | 219.4 | Cortisol; 18-Hydroxycorticosterone; 17a,21-Dihydroxy-5b-pregnane-3,11,20-trione; 11b,21-Dihydroxy-3,20-oxo-5b-pregnan-18-al | 1.2% | 2570346.026 | C18 Positive | M(C13)+H[1+] | 4 |
| 110.0601 | 24.7 | (S)-2,3,4,5-Tetrahydropiperidine-2-carboxylate; D-1-Piperidine-2-carboxylic acid | 1.1% | 1656707.683 | HILIC Positive | M-H2O+H[1+] | 4 |
| 189.975 | 7.6 | 3-Sulfinioalanine | 1.1% | 1367012.513 | C18 Negative | M+Cl37[-] | 3 |
| 114.0914 | 75.9 | 5-Acetamidovalerate | 1.1% | 22034281.94 | HILIC Positive | M-HCOOH+H[1+] | 3 |
| 116.1071 | 119.9 | 116.10705@119.9 | 1.1% | 11270960.36 | HILIC Positive | - | 5 |
| 143.1078 | 246.9 | 143.10779@246.9 | 1.1% | 7428685.731 | HILIC Negative | - | 5 |

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| 301.1184 | 72.7 | 301.11842@72.7 | 1.1% | 1254084.071 | HILIC Positive | - | 5 |
| 112.0504 | 25.6 | Cytosine | 1.1% | 2039004.09 | C18 Positive | M+H | 1 |
| 177.1022 | 207.7 | Serotonin | 1.1% | 290328.9904 | HILIC Positive | M+H[1+] | 3 |
| 149.0599 | 68.4 | Trans-Cinnamate | 1.0% | 2438578.452 | HILIC Positive | M+H | 1 |
| 247.2424 | 365.8 | 247.24237@365.8 | 1.0% | 34145188.78 | C18 Positive | - | 5 |
| 146.06 | 35 | 5-Hydroxyindoleacetic acid; 5-Phenyl-1,3-oxazinane-2,4-dione | 1.0% | 76777730.76 | C18 Positive | M-HCOOH+H[1+] | 4 |
| 118.0861 | 21.4 | 5-Aminovaleric acid; Norvaline; Betaine; Valine | 1.0% | 1645656976 | C18 Positive | M+H | 3 |
| 144.0301 | 19.7 | 2-Keto-glutaramic acid; 4-Oxoglutaramate | 1.0% | 1514563.378 | C18 Negative | M-H[-] | 4 |
| 159.03 | 308.2 | 2-Oxoadipic acid; Oxoadipate | 1.0% | 5761329.926 | HILIC Negative | M-H | 3 |
| 239.0925 | 70.5 | 239.09247@70.5 | 1.0% | 40188251.04 | HILIC Negative | - | 5 |
| 184.097 | 80.4 | 3-O-methyldopa | 1.0% | 1267894.353 | HILIC Positive | M-CO+H[1+] | 3 |
| 124.0757 | 84.9 | 124.07568@84.9 | 1.0% | 1228371.413 | C18 Positive | - | 5 |
| 127.1117 | 252.6 | 127.11168@252.6 | 0.9% | 2315756.971 | C18 Positive | - | 5 |
| 151.0755 | 65.3 | 3-Methoxytyramine; Epinine | 0.9% | 6383618.196 | HILIC Positive | M-NH3+H[1+] | 4 |
| 110.0361 | 17.5 | 110.03606@17.5 | 0.9% | 3548257.404 | HILIC Negative | - | 5 |
| 162.0919 | 71.8 | Indole-3-Ethanol | 0.9% | 3499087.125 | HILIC Positive | M+H | 1 |
| 191.0561 | 308.1 | 191.05605@308.1 | 0.9% | 3619447.41 | C18 Negative | - | 5 |
| 216.0345 | 20.9 | sulfuric acid [4-(2-aminoethyl)phenyl] ester | 0.9% | 119698856.7 | C18 Negative | M-H[-] | 3 |
| 297.2428 | 63 | Gamma-Linolenic acid; Alpha-Linolenic acid | 0.9% | 11434624.53 | HILIC Positive | M+H2O+H[1+] | 4 |
| 117.0193 | 18 | Methylmalonate; Methylmalonic acid; Succinate; Succinic acid | 0.9% | 14762956.29 | C18 Negative | M-H | 3 |
| 295.2274 | 279.3 | 295.22744@279.3 | 0.9% | 9002114.112 | C18 Negative | - | 5 |

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| 226.0834 | 138.2 | Deoxycytidine | 0.8% | 6460579.404 | HILIC Negative | M-H[-] | 3 |
| 273.1847 | 250.8 | 17-beta Estradiol | 0.8% | 1363970.442 | C18 Positive | M+H | 1 |
| 241.1047 | 26.2 | 4-Hydroperoxy-2-nonenal | 0.8% | 4369515.651 | C18 Positive | M+HCOONa[1+] | 3 |
| 224.0554 | 46.7 | 224.05537@46.7 | 0.8% | 7591143.506 | HILIC Negative | - | 5 |
| 335.1467 | 67.2 | Lipoyllysine | 0.8% | 7977650.288 | HILIC Positive | M+H[1+] | 3 |
| 407.1677 | 66 | Chitobiose | 0.8% | 4389278.49 | HILIC Positive | M-H2O+H[1+] | 3 |
| 111.1169 | 72.5 | (E)-4-hydroxynon-2-enal; 3,4-Epoxy-nonanal | 0.8% | 1919452.99 | HILIC Positive | M-HCOOH+H[1+] | 4 |
| 122.0248 | 19.5 | 2-Aminomuconic acid semialdehyde | 0.8% | 3163318.676 | HILIC Negative | M-H2O-H[-] | 3 |
| 153.0548 | 68.2 | Resorcinol Monoacetate; 3-Hydroxyphenylacetate; 24-Dihydroxyacetophenone | 0.8% | 1684967.827 | HILIC Positive | M+H | 3 |
| 196.0228 | 288.2 | 196.02282@288.2 | 0.8% | 165995.4904 | HILIC Negative | - | 5 |
| 313.237 | 253.3 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 0.8% | 3890885.388 | C18 Positive | M+H[1+] | 4 |
| 135.1168 | 124 | (-)-trans-Carveol; Perillyl alcohol; Alpha-Pinene-oxide; (+)-trans-Carveol | 0.7% | 2121078.035 | C18 Positive | M-H2O+H[1+] | 4 |
| 167.0099 | 18.3 | 167.00991@18.3 | 0.7% | 2895185.042 | HILIC Negative | - | 5 |
| 184.0697 | 68.2 | 4-Hydroxy-3-Methoxyphenylglycol; Phosphorylcholine | 0.7% | 64212714.28 | HILIC Negative | M-H ₂ [-1] | 3 |
| 225.032 | 50.2 | 225.03196@50.2 | 0.7% | 4787480.913 | HILIC Negative | - | 5 |
| 327.2326 | 57.9 | Docosaheptaenoate | 0.7% | 432607583.2 | HILIC Negative | M-H | 1 |
| 377.1451 | 20.7 | Riboflavin | 0.7% | 7229909.08 | C18 Positive | M+H[1+] | 3 |
| 117.0911 | 74.6 | Azelaic acid | 0.7% | 2256037.958 | HILIC Positive | M-C3H4O2+H[1+] | 3 |
| 176.0282 | 140.7 | 176.02822@140.7 | 0.7% | 3891897.673 | HILIC Negative | - | 5 |

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| 400.3067 | 53.5 | Pendtadenoyl carnitine | 0.7% | 23719325.63 | HILIC Negative | M-H+O ^[-] | 3 |
| 140.1069 | 172.1 | 140.10692@172.1 | 0.7% | 1376734.34 | C18 Positive | - | 5 |
| 321.2425 | 64.8 | 321.24251@64.8 | 0.7% | 3433203.859 | HILIC Positive | - | 5 |
| 385.3101 | 232.1 | 385.31009@232.1 | 0.7% | 2024972.362 | C18 Positive | - | 5 |
| 211.0015 | 146.3 | 211.00154@146.3 | 0.7% | 22827748.56 | HILIC Negative | - | 5 |
| 215.0673 | 18.3 | N-Acetyl-L-aspartic acid; N-Formyl-L-glutamic acid; 2-amino-3-oxo-hexanedioic acid | 0.7% | 431671.5929 | C18 Negative | M+ACN-H ^[-] | 4 |
| 351.2193 | 368.7 | 351.21926@368.7 | 0.7% | 281050026 | C18 Negative | - | 5 |
| 186.0772 | 16.7 | 186.07719@16.7 | 0.6% | 6048480.013 | HILIC Negative | - | 5 |
| 122.0963 | 23.3 | 3-Methoxytyramine; Epinine | 0.6% | 6651149.311 | C18 Positive | M-HCOOH+H ^[1+] | 4 |
| 191.056 | 24 | Quinic acid | 0.6% | 951810.6699 | C18 Negative | M-H | 1 |
| 196.0727 | 299.7 | 196.07273@299.7 | 0.6% | 3615967.689 | C18 Negative | - | 5 |
| 145.0494 | 22.1 | 3-Methylglutaconate | 0.6% | 4323278.946 | C18 Positive | M+H | 1 |
| 145.0507 | 139.7 | L-Fucose | 0.6% | 9660179.5 | HILIC Negative | M-H ₂ O-H ^[-] | 3 |
| 167.9972 | 19.6 | 3-Sulfinioalanine | 0.6% | 2275417.234 | HILIC Negative | M-H+O ^[-] | 3 |
| 249.0877 | 33.4 | 249.0877@33.4 | 0.6% | 7350728.987 | C18 Negative | - | 5 |
| 159.0764 | 24 | N-Acetylglycine | 0.6% | 1687810.702 | C18 Positive | M+ACN+H | 1 |
| 217.1083 | 67.5 | 217.10827@67.5 | 0.6% | 7648522.218 | HILIC Negative | - | 5 |
| 118.0498 | 23.4 | N-Acetylglycine | 0.6% | 1503538.115 | C18 Positive | M+H | 1 |
| 142.0509 | 26.4 | N-Methylglutamate; Amino adipate | 0.6% | 2005433.708 | C18 Negative | M-H ₂ O-H | 3 |
| 152.0708 | 74.5 | 152.07076@74.5 | 0.5% | 3163837.019 | HILIC Positive | - | 5 |
| 180.0596 | 310 | Mannose; Gulose | 0.5% | 138460359.8 | HILIC Negative | M-H ^[-1] | 3 |
| 118.0652 | 66.1 | methyl (indol-3-yl)acetate | 0.5% | 42668384.11 | HILIC Positive | M-C ₃ H ₄ O ₂ +H ^[1+] | 3 |

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|----------|-------|---|------|-------------|----------------|--------------------------|---|
| 131.035 | 308.2 | Glutarate; Glutaric acid | 0.5% | 39669875.13 | HILIC Negative | M-H | 3 |
| 153.1273 | 123.9 | (-)-trans-Carveol; Perillyl alcohol; Alpha-Pinene-oxide; (+)-trans-Carveol | 0.5% | 2716654.561 | C18 Positive | M+H[1+] | 4 |
| 395.2447 | 55.2 | Tetrahydrocorticosterone | 0.5% | 10362646 | HILIC Negative | M+HCOO[-] | 3 |
| 425.1784 | 66.5 | Chitobiose | 0.5% | 4918829.218 | HILIC Positive | M+H[1+] | 3 |
| 159.1027 | 70.1 | C80-3-Hydroxyoctanoic acid | 0.5% | 22904600.4 | HILIC Negative | M-H | 1 |
| 270.2298 | 63.7 | 270.2298@63.7 | 0.5% | 6296022.176 | HILIC Positive | - | 5 |
| 335.2207 | 65 | 13-L-Hydroperoxylinoleic acid; 9(S)-HPODE | 0.5% | 3220056.234 | HILIC Positive | M+Na[1+] | 4 |
| 430.3166 | 189.2 | 430.31658@189.2 | 0.5% | 4207633.359 | HILIC Negative | - | 5 |
| 133.1013 | 64.5 | Perillyl aldehyde | 0.5% | 10281247.35 | HILIC Positive | M-H ₂ O+H[1+] | 3 |
| 160.0969 | 78.6 | 2-Methylbutyrylglycine | 0.5% | 6646389.897 | HILIC Positive | M+H | 1 |
| 187.057 | 18.9 | 187.05699@18.9 | 0.5% | 3431038.151 | C18 Positive | - | 5 |
| 372.3107 | 258.1 | Myristoyl-L-carnitine | 0.5% | 6541976.606 | C18 Positive | M+H | 1 |
| 173.1174 | 64.7 | 4-Hydroperoxy-2-nonenal | 0.4% | 6550023.705 | HILIC Positive | M+H[1+] | 3 |
| 194.0457 | 29 | 194.04567@29 | 0.4% | 833634.8622 | C18 Negative | - | 5 |
| 130.0499 | 23.3 | Pyroglutamate; 5-Oxoproline; Oxoproline | 0.4% | 75085012.69 | C18 Positive | M+H | 3 |
| 183.1743 | 259.6 | Dodecanoic acid | 0.4% | 3660520.179 | C18 Positive | M-H ₂ O+H[1+] | 3 |
| 421.2227 | 220.6 | 421.22265@220.6 | 0.4% | 2941520.035 | C18 Negative | - | 5 |
| 126.0197 | 17.4 | 2-Keto-glutaramic acid | 0.4% | 3998390.244 | HILIC Negative | M-H ₂ O-H[-] | 3 |
| 127.1119 | 64.5 | 127.11186@64.5 | 0.4% | 6331633.131 | HILIC Positive | - | 5 |
| 129.1023 | 291 | 129.10233@291 | 0.4% | 10361542.32 | HILIC Positive | - | 5 |

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|----------|-------|--|------|-------------|----------------|-------------------|---|
| 391.2852 | 236.6 | Murideoxycholic acid; Hyodeoxycholic acid; Deoxycholate; Chenodeoxycholate; Ursodeoxycholate | 0.4% | 23388267.82 | C18 Negative | M-H | 3 |
| 143.1068 | 68.7 | Azelaic acid | 0.4% | 3680291.048 | HILIC Positive | M- HCOOH+H[1+] | 3 |
| 165.0053 | 19.2 | 2-Keto-glutaramic acid; 4- Oxoglutaramate | 0.4% | 2879305.792 | C18 Negative | M+Na-2H[-] | 4 |
| 132.0384 | 313.5 | 2-Acetolactate; (S)-2-Acetolactate | 0.3% | 4581934.862 | HILIC Negative | M(C13)-H[-] | 4 |
| 144.1112 | 65.8 | Caprylic acid | 0.3% | 5428570.337 | HILIC Negative | M(C13)-H[-] | 3 |
| 165.1638 | 254.7 | Dodecanoic acid | 0.3% | 2456365.792 | C18 Positive | M-H4O2+H[1+] | 3 |
| 168.102 | 162.7 | 168.10197@162.7 | 0.3% | 3948907.631 | HILIC Positive | - | 5 |
| 195.051 | 310.9 | Gluconate | 0.3% | 27753035.29 | HILIC Negative | M-H | 1 |
| 199.0377 | 20.9 | L-Fucose | 0.3% | 26217650.9 | C18 Negative | M+Cl[-] | 3 |
| 125.0599 | 66.7 | 4-Methylcatechol; 3- Hydroxybenzyl Alcohol | 0.3% | 5932954.321 | HILIC Positive | M+H | 3 |
| 154.0717 | 22.3 | Adenine | 0.3% | 3444546.054 | C18 Positive | M+H2O+H[1+] | 3 |
| 199.0725 | 19.1 | Methylimidazoleacetic acid | 0.3% | 2914917.247 | HILIC Negative | M+CH3COO[-] | 3 |
| 398.3261 | 262.5 | 3-Hydroxyhexadecanoylcarnitine | 0.3% | 7967308.51 | C18 Positive | M+H-H2O | 1 |
| 451.3063 | 232.3 | Murideoxycholic acid; Hyodeoxycholic acid; Deoxycholate; Chenodeoxycholate; Ursodeoxycholate | 0.3% | 3998228.276 | C18 Negative | M+Hac-H | 3 |
| 114.0662 | 20.8 | Creatinine | 0.3% | 234529732 | C18 Positive | M+H | 1 |
| 407.2071 | 220.6 | 407.20708@220.6 | 0.3% | 1937976.958 | C18 Negative | - | 5 |
| 87.00881 | 142.9 | 87.00881@142.9 | 0.3% | 4068954144 | HILIC Negative | - | 5 |
| 127.1117 | 133.4 | Caprylic acid | 0.3% | 1640189.314 | C18 Positive | M-H2O+H[1+] | 3 |

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|----------|-------|---|------|-------------|----------------|---------------|---|
| 129.0656 | 263.9 | 129.06563@263.9 | 0.3% | 101434900.2 | HILIC Positive | - | 5 |
| 212.0321 | 14.6 | (S)-2,3,4,5-Tetrahydropiperidine-2-carboxylate; D-1-Piperidine-2-carboxylic acid | 0.3% | 1094408.135 | C18 Positive | M+HCOOK[1+] | 4 |
| 600.2624 | 201.3 | Taurocholic acid; Taurohyocholate | 0.3% | 16102660.43 | HILIC Positive | M+HCOOK[1+] | 4 |
| 135.0452 | 33 | 135.04515@33 | 0.3% | 3170553.737 | C18 Negative | - | 5 |
| 165.0408 | 317.9 | D-Ribose; D-Xylose; L-Arabinose; D-Ribulose; D-Xylulose; L-Threo-2-pentulose; L-Ribulose | 0.3% | 58799859.85 | C18 Negative | M-H+O[-] | 4 |
| 269.0428 | 79.8 | 269.0428@79.8 | 0.3% | 2301595.923 | C18 Positive | - | 5 |
| 102.0562 | 329 | Alpha-aminobutyric acid; 2-Aminoisobutyrate; N-Methyl-Alanine; Gamma-Aminobutyrate; Aminoisobutanoate | 0.2% | 42520666.87 | HILIC Negative | M-H | 3 |
| 130.0653 | 68.5 | Indoleacetic acid; 5-Hydroxyindoleacetaldehyde | 0.2% | 5820038.811 | HILIC Positive | M-HCOOH+H[1+] | 4 |
| 134.06 | 115.4 | 134.05999@115.4 | 0.2% | 33732307.03 | C18 Positive | - | 5 |
| 142.0864 | 81.7 | 142.08642@81.7 | 0.2% | 4694747.391 | HILIC Positive | - | 5 |
| 145.1223 | 133.7 | Caprylic acid | 0.2% | 547390.1667 | C18 Positive | M+H[1+] | 3 |
| 155.1079 | 65.4 | 155.10792@65.4 | 0.2% | 14636169.03 | HILIC Negative | - | 5 |
| 165.0558 | 145.3 | Homovanillin | 0.2% | 34443473.85 | HILIC Negative | M-H[-] | 3 |
| 186.1126 | 75.2 | 3-Methoxytyramine; Epinine | 0.2% | 3718795.785 | HILIC Positive | M+H2O+H[1+] | 4 |
| 257.103 | 70.4 | 257.10301@70.4 | 0.2% | 17397331.66 | HILIC Negative | - | 5 |
| 319.2273 | 65.6 | 319.2273@65.6 | 0.2% | 7652238.365 | HILIC Negative | - | 5 |
| 112.0517 | 23.2 | Creatinine | 0.2% | 21193138 | C18 Negative | M-H | 1 |
| 121.0647 | 24.7 | Phenylacetaldehyde | 0.2% | 2845185.183 | C18 Positive | M+H | 1 |
| 147.044 | 22.5 | Phenylpyruvic acid | 0.2% | 4121708.686 | C18 Positive | M+H-H2O | 1 |

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|----------|-------|--|------|-------------|----------------|--------------|---|
| 165.0546 | 22.4 | Phenylpyruvic acid | 0.2% | 20577376.77 | C18 Positive | M+H | 1 |
| 183.0784 | 246.1 | 183.07838@246.1 | 0.2% | 4951511.349 | HILIC Positive | - | 5 |
| 214.0486 | 24.2 | Glucosamine | 0.2% | 2060087.997 | C18 Negative | M+Cl[-] | 3 |
| 467.3193 | 234.5 | Glycocholic acid | 0.2% | 3451453.724 | C18 Positive | M(C13)+H[1+] | 3 |
| 608.4881 | 376.2 | Hexacosanoyl Carnitine | 0.2% | 3679297.029 | C18 Positive | M+HCOONa[1+] | 3 |
| 169.1225 | 65.7 | Perillyl aldehyde | 0.2% | 6036558.449 | HILIC Positive | M+H2O+H[1+] | 3 |
| 137.1326 | 64.5 | (+)-Limonene; Polylimonene; D-Limonene; (+)-a-Pinene | 0.2% | 5798418.513 | HILIC Positive | M+H[1+] | 4 |
| 167.035 | 204.4 | p-Hydroxyphenylacetic acid; 3,4-Dihydroxyphenylacetaldehyde; Ortho-Hydroxyphenylacetic acid; 4-Hydroxyphenyl acetate | 0.2% | 5139036.74 | HILIC Negative | M-H+O[-] | 4 |
| 114.0549 | 24.8 | Cis-4-Hydroxy-D-Proline; N-Acetylalanine; Aminolevulinic acid; Trans-4-Hydroxy-L-Proline | 0.2% | 2938841.413 | C18 Positive | M+H-H2O | 3 |
| 176.0708 | 70.2 | Indole-3-Acetate | 0.2% | 3306336.535 | HILIC Positive | M+H | 1 |
| 89.02441 | 19.8 | Glyceraldehyde; Lactate | 0.2% | 599093484.8 | C18 Negative | M-H | 3 |
| 117.0194 | 313.1 | Succinic acid; Succinate | 0.1% | 186870886.7 | HILIC Negative | M-H | 3 |
| 121.1013 | 64.4 | (E)-4-hydroxynon-2-enal; 3,4-Epoxyxynonanal | 0.1% | 17747767.06 | HILIC Positive | M-H4O2+H[1+] | 4 |
| 143.562 | 242.5 | gamma-CEHC | 0.1% | 3518722.663 | C18 Positive | M+H+Na[2+] | 3 |
| 180.0656 | 73.8 | Hippurate; Hippuric acid | 0.1% | 35071623.87 | HILIC Positive | M+H | 3 |
| 191.105 | 246.3 | 191.10501@246.3 | 0.1% | 58202537.57 | HILIC Positive | - | 5 |
| 311.2228 | 66.6 | 311.22276@66.6 | 0.1% | 20625329.54 | HILIC Negative | - | 5 |
| 111.1167 | 69.8 | 111.1167@69.8 | 0.1% | 1616020.804 | C18 Positive | - | 5 |
| 163.0614 | 139.9 | L-Fucose | 0.1% | 4930825.506 | HILIC Negative | M-H[-] | 3 |
| 171.1014 | 65.5 | Azelaic acid | 0.1% | 8395562.849 | HILIC Positive | M-H2O+H[1+] | 3 |
| 180.0867 | 25.6 | Galactosamine | 0.1% | 4220994.042 | C18 Positive | M+H | 1 |

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|----------|-------|---|------|-------------|----------------|---------------------|---|
| 183.0353 | 265.2 | 183.03528@265.2 | 0.1% | 58908841.82 | HILIC Negative | - | 5 |
| 215.0562 | 68.3 | 215.05622@68.3 | 0.1% | 13353150.47 | HILIC Negative | - | 5 |
| 277.2172 | 59.2 | Palmitate | 0.1% | 227657400 | HILIC Negative | M+Na-2H | 1 |
| 278.2206 | 59.3 | Gamma-Linolenic acid; Alpha-Linolenic acid | 0.1% | 41869282.87 | HILIC Negative | M(C13)-H[-] | 4 |
| 279.232 | 63.8 | C183-9E11Z13E-Octadecatrienoic acid; C182-11-Octadecen-9-ynoic acid; Gamma-Linolenate | 0.1% | 43014562.57 | HILIC Positive | M+H | 3 |
| 334.1392 | 65.4 | 334.13916@65.4 | 0.1% | 333107.1378 | C18 Positive | - | 5 |
| 414.3003 | 63.1 | 414.30029@63.1 | 0.1% | 86260166.04 | HILIC Positive | - | 5 |
| 465.3051 | 255 | Glycocholic acid; Glycocholate | 0.1% | 5153516.853 | HILIC Negative | M-H _[-1] | 3 |
| 129.1273 | 69.9 | 129.12733@69.9 | 0.1% | 522326.7692 | C18 Positive | - | 5 |
| 139.1119 | 64.6 | C184-Stearidonic acid | 0.1% | 7318816.112 | HILIC Positive | M+2H | 1 |
| 147.0664 | 217.5 | Mevalonate | 0.1% | 10607467.79 | HILIC Negative | M-H | 1 |
| 148.0604 | 22 | N-Acetylserine; O-Acetylserine; N-Methyl-D-aspartic acid; Glutamate | 0.1% | 12429308.76 | C18 Positive | M+H | 3 |
| 168.1018 | 28 | 3-Methoxytyramine | 0.1% | 5749450.41 | C18 Positive | M+H | 1 |
| 179.0705 | 69.2 | 179.07046@69.2 | 0.1% | 1705275.554 | HILIC Positive | - | 5 |
| 218.1033 | 258.5 | Pantothenate | 0.1% | 6352067.824 | HILIC Negative | M-H | 1 |
| 229.0717 | 71.6 | 229.07169@71.6 | 0.1% | 16081907.45 | HILIC Negative | - | 5 |
| 243.1237 | 68.6 | 243.12371@68.6 | 0.1% | 16742172.92 | HILIC Negative | - | 5 |
| 249.0878 | 283.6 | 249.08784@283.6 | 0.1% | 6545025.369 | HILIC Negative | - | 5 |
| 292.0104 | 22.5 | 292.01038@22.5 | 0.1% | 55847221.11 | C18 Negative | - | 5 |
| 373.3138 | 258.1 | O-tetradecanoyl-(R)-carnitine | 0.1% | 1623008.532 | C18 Positive | M(C13)+H[1+] | 3 |
| 466.3162 | 232.2 | Glycocholic acid | 0.1% | 12484003.87 | C18 Positive | M+H | 1 |

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|----------|-------|--|------|-------------|----------------|--------------------------|---|
| 472.3036 | 69.8 | Glycohyodeoxcholic acid; Glycochenodeoxycholate | 0.1% | 6363774.987 | HILIC Positive | M+Na | 3 |
| 185.081 | 72.3 | 185.08099@72.3 | 0.1% | 3676912.737 | HILIC Positive | - | 5 |
| 118.0511 | 338 | Allothreonine; Threonine; Homoserine | 0.0% | 151570831.4 | HILIC Negative | M-H | 3 |
| 175.0477 | 24.5 | 26-Dihydroxypyridine; Deoxycytidine Monophosphate | 0.0% | 8650481.606 | C18 Positive | M+ACN+Na; M+ACN+2H | 3 |
| 217.0718 | 206.8 | Metanephrene | 0.0% | 7974986.66 | HILIC Negative | M+Na-2H[-] | 3 |
| 313.2373 | 65.9 | 13-L-Hydroperoxylinoic acid; 9(S)-HPODE | 0.0% | 3675784.279 | HILIC Positive | M+H[1+] | 4 |
| 379.1729 | 66.3 | Chitobiose | 0.0% | 9716029.192 | HILIC Positive | M- HCOOH+H[1+] | 3 |
| 87.02005 | 19.6 | 87.02005@19.6 | 0.0% | 2082207.33 | HILIC Negative | - | 5 |
| 113.0245 | 309.9 | 2-Acetolactate; (S)-2-Acetolactate | 0.0% | 556013265.1 | HILIC Negative | M-H ₂ O-H[-] | 4 |
| 130.05 | 94 | L-Glutamine; D-Glutamine; Ureidoisobutyric acid | 0.0% | 39705495.94 | HILIC Positive | M-NH ₃ +H[1+] | 4 |
| 133.1011 | 252.1 | 133.10114@252.1 | 0.0% | 3959295.272 | C18 Positive | - | 5 |
| 136.0756 | 25.4 | 136.07559@25.4 | 0.0% | 27242634.28 | C18 Positive | - | 5 |
| 141.0911 | 66.4 | 141.09112@66.4 | 0.0% | 7685678.244 | HILIC Positive | - | 5 |
| 146.0811 | 25.4 | 5-Hydroxyisoleucic acid; 4- Acetamidobutyric acid | 0.0% | 5905902.506 | C18 Positive | M+H | 3 |
| 151.0402 | 62 | 2-Hydroxyphenylacetic acid; Resorcinol Monoacetate; 24- Dihydroxyacetophenone; Vanillin; 2-Hydroxyphenylacetate; Mandelate | 0.0% | 34457318.43 | HILIC Negative | M-H | 3 |
| 160.0757 | 177.9 | 5-Hydroxytryptophol; 1,2- dehydrosalsolinol | 0.0% | 703557.5673 | C18 Positive | M-H ₂ O+H[1+] | 4 |
| 165.0405 | 309.5 | D-Ribose; D-Xylose; L- Arabinose; D-Ribulose; D- | 0.0% | 34380466.62 | HILIC Negative | M-H+O[-] | 4 |

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|----------|-------|--|------|-------------|----------------|----------------|---|
| | | Xylulose; L-Threo-2-pentulose; L-Ribulose | | | | | |
| 166.0862 | 27.4 | Phenylalanine | 0.0% | 1082880978 | C18 Positive | M+H | 1 |
| 178.0862 | 170.6 | 5-Hydroxytryptophol; 1,2-dehydrosalsolinol | 0.0% | 1134355 | C18 Positive | M+H[1+] | 4 |
| 179.0564 | 105.2 | Paraxanthine; Theophylline | 0.0% | 204626608.5 | HILIC Negative | M-H | 3 |
| 197.0566 | 24.9 | Urocanate | 0.0% | 3114952.846 | C18 Negative | M+Hac-H | 1 |
| 199.0611 | 63.8 | 199.06111@63.8 | 0.0% | 8675177.814 | HILIC Negative | - | 5 |
| 201.0354 | 20.9 | L-Fucose | 0.0% | 7963031.91 | C18 Negative | M+C137[-] | 3 |
| 209.0666 | 22 | D-Sedoheptulose | 0.0% | 51150783.32 | C18 Negative | M-H | 1 |
| 223.0821 | 22.2 | 223.08214@22.2 | 0.0% | 45615348.66 | C18 Negative | - | 5 |
| 293.2123 | 64.1 | 293.21229@64.1 | 0.0% | 9332254.683 | HILIC Negative | - | 5 |
| 328.3207 | 268.5 | L-Palmitoylcarnitine | 0.0% | 2052204.497 | C18 Positive | M-C3H4O2+H[1+] | 3 |
| 399.3295 | 262.6 | Hexadecenoyl carnitine; (2E)-hexadecenoylcarnitine | 0.0% | 1856417.333 | C18 Positive | M(C13)+H[1+] | 4 |
| 400.3418 | 274.1 | Palmitoylcarnitine | 0.0% | 41483367.81 | C18 Positive | M+H | 1 |
| 106.0649 | 64.4 | 5-Hydroxytryptophol; 1,2-dehydrosalsolinol | 0.0% | 5742917.311 | HILIC Positive | M-C3H4O2+H[1+] | 4 |
| 108.0659 | 22.3 | 108.06585@22.3 | 0.0% | 3373794.808 | C18 Positive | - | 5 |
| 109.1011 | 134 | Caprylic acid | 0.0% | 2083998.772 | C18 Positive | M-H4O2+H[1+] | 3 |
| 109.1013 | 64.4 | 109.10125@64.4 | 0.0% | 71220542.3 | HILIC Positive | - | 5 |
| 111.0917 | 216.4 | 111.09173@216.4 | 0.0% | 22152786.84 | HILIC Positive | - | 5 |
| 118.0413 | 310.6 | 118.0413@310.6 | 0.0% | 844583843 | HILIC Negative | - | 5 |

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| 121.9997 | 18.7 | 3-methyl pyruvic acid; Acetoacetic acid; Succinic acid semialdehyde; 2-Methyl-3-oxopropanoic acid; (S)-Methylmalonic acid semialdehyde | 0.0% | 14172677.79 | HILIC Negative | M+Na-2H[-] | 4 |
| 123.1169 | 65.1 | Perillyl aldehyde | 0.0% | 17572030.67 | HILIC Positive | M-CO+H[1+] | 3 |
| 129.1023 | 220.1 | 129.1023@220.1 | 0.0% | 4329768.436 | HILIC Positive | - | 5 |
| 131.035 | 300.9 | 131.03498@300.9 | 0.0% | 5262836.34 | C18 Negative | - | 5 |
| 132.0655 | 23.7 | Cis-4-Hydroxy-D-Proline; N-Acetylalanine; Aminolevulinic acid; Trans-4-Hydroxy-L-Proline | 0.0% | 17397450.12 | C18 Positive | M+H | 3 |
| 132.0807 | 34.1 | 3-Methoxytyramine; Epinine | 0.0% | 24535539.29 | C18 Positive | M-H4O2+H[1+] | 4 |
| 133.08 | 20.6 | Creatine | 0.0% | 4570755.321 | C18 Positive | M(C13)+H[1+] | 3 |
| 133.9919 | 16.7 | 3-Sulfinioalanine | 0.0% | 1285892.301 | HILIC Negative | M-H2O-H[-] | 3 |
| 134.0601 | 80.8 | Pyridoxine; Norepinephrine | 0.0% | 37941544.25 | HILIC Positive | M-H4O2+H[1+] | 4 |
| 139.0755 | 66.4 | 139.07546@66.4 | 0.0% | 10933115.62 | HILIC Positive | - | 5 |
| 145.0142 | 18.5 | Oxoglutarate; 2-Oxoglutaric acid | 0.0% | 28764325.77 | C18 Negative | M-H | 3 |
| 146.1176 | 238.4 | O-propanoyl-(R)-carnitine | 0.0% | 268341970.6 | HILIC Positive | M-C3H4O2+H[1+] | 3 |
| 147.0765 | 283 | Glutamine | 0.0% | 5022415206 | HILIC Positive | M+H | 1 |
| 150.0489 | 306.5 | D-Ribose; D-Xylose; L-Arabinose; D-Ribulose; D-Xylulose; L-Threo-2-pentulose; L-Ribulose | 0.0% | 4099494.631 | HILIC Negative | M(C13)-H[-] | 4 |
| 151.1119 | 64.8 | Perillyl aldehyde | 0.0% | 7334176.801 | HILIC Positive | M+H[1+] | 3 |
| 152.1071 | 65.9 | 152.10714@65.9 | 0.0% | 8647492.362 | HILIC Positive | - | 5 |
| 153.0912 | 64.4 | Azelaic acid | 0.0% | 54293736.6 | HILIC Positive | M-H4O2+H[1+] | 3 |
| 154.1227 | 222.1 | Metanephrene | 0.0% | 2992688.237 | HILIC Positive | M-CO2+H[1+] | 3 |
| 159.0301 | 129.6 | Oxoadipic acid | 0.0% | 50534697.44 | HILIC Negative | M-H[-] | 3 |

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| 161.0456 | 308.7 | 2-Oxobutyric acid; 3-Hydroxyadipic acid; 2-Hydroxyadipic acid; 3-Hydroxymethylglutarate; 3-Hydroxy-3-methylglutaric acid | 0.0% | 320519055 | HILIC Negative | M+Hac-H; M-H | 3 |
| 163.0612 | 22.3 | Rhamnose; Fucose; 2-Deoxy-D-Glucose | 0.0% | 5749249.494 | C18 Negative | M-H | 3 |
| 165.0558 | 69.4 | 3-(2-Hydroxyphenyl)Propanoate | 0.0% | 26495034.9 | HILIC Negative | M-H | 1 |
| 165.1276 | 64.6 | Docosaheptaenoate | 0.0% | 6776667.42 | HILIC Positive | M+2H | 1 |
| 169.0871 | 63.9 | 169.08709@63.9 | 0.0% | 26972616.99 | HILIC Negative | - | 5 |
| 171.0412 | 284.6 | Carglumic acid | 0.0% | 1684463.202 | HILIC Negative | M-H ₂ O-H[-] | 3 |
| 171.1026 | 439.2 | 171.10262@439.2 | 0.0% | 7867573.679 | C18 Negative | - | 5 |
| 172.0881 | 112.7 | (-)-trans-Carveol; Perillyl alcohol; Alpha-Pinene-oxide; (+)-trans-Carveol | 0.0% | 8339554.817 | HILIC Negative | M+Na-2H[-] | 4 |
| 172.1333 | 230 | O-propanoyl-(R)-carnitine | 0.0% | 18935845.54 | HILIC Positive | M-HCOOH+H[1+] | 3 |
| 174.149 | 227.7 | O-propanoyl-(R)-carnitine | 0.0% | 23984022.92 | HILIC Positive | M-CO ₂ +H[1+] | 3 |
| 177.1021 | 22.2 | 5-Hydroxy-L-tryptophan | 0.0% | 939285.891 | C18 Positive | M-CO ₂ +H[1+] | 3 |
| 178.0509 | 26.6 | Hippurate; Hippuric acid | 0.0% | 91377450.52 | C18 Negative | M-H | 3 |
| 179.0562 | 310.6 | Mannose; Gulose | 0.0% | 2159044475 | HILIC Negative | M-H | 3 |
| 181.0711 | 22.5 | Sorbitol; Galactitol | 0.0% | 6699968.699 | C18 Negative | M-H | 3 |
| 182.0809 | 22.8 | Tyrosine | 0.0% | 159331272.2 | C18 Positive | M+H | 1 |
| 182.1178 | 231.3 | O-propanoyl-(R)-carnitine | 0.0% | 1908405.997 | HILIC Positive | M-H ₄ O ₂ +H[1+] | 3 |
| 189.0404 | 19.7 | C80-Dihydrolipoate | 0.0% | 6351725.551 | C18 Negative | M-H ₂ O-H | 1 |
| 190.1438 | 221.6 | O-propanoyl-(R)-carnitine | 0.0% | 10288947.04 | HILIC Positive | M-CO+H[1+] | 3 |
| 191.0663 | 278.2 | Carglumic acid | 0.0% | 4988483.619 | HILIC Positive | M+H[1+] | 3 |

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| 197.1538 | 65.5 | Hyodeoxycholic acid; Deoxycholate; Chenodeoxycholate | 0.0% | 7084330.853 | HILIC Positive | M+2H | 3 |
| 200.0103 | 145.2 | 200.01028@145.2 | 0.0% | 2123969.795 | C18 Negative | - | 5 |
| 200.1281 | 228.1 | O-propanoyl-(R)-carnitine | 0.0% | 24967231.42 | HILIC Positive | M-H ₂ O+H[1+] | 3 |
| 203.0814 | 27.8 | 203.08138@27.8 | 0.0% | 13813487.28 | C18 Positive | - | 5 |
| 217.0485 | 20.1 | Dihydroorotate; Dihydroorotic acid | 0.0% | 1661798.247 | C18 Negative | M+Hac-H | 3 |
| 218.1388 | 218.3 | Propanoylcarnitine; Propionyl-L- carnitine | 0.0% | 100289636.4 | HILIC Positive | M+H | 3 |
| 219.0458 | 20.2 | Sorbitol; Mitobronitol; Galactitol | 0.0% | 2656047.968 | C18 Negative | M+Cl ₃₇ [-] | 4 |
| 219.1418 | 217.9 | O-propanoyl-(R)-carnitine | 0.0% | 8969921.779 | HILIC Positive | M(C ₁₃)+H[1+] | 3 |
| 221.0919 | 26.5 | 5-Hydroxy-L-Tryptophan | 0.0% | 2578217.343 | C18 Positive | M+H | 1 |
| 225.0616 | 310.5 | Sedoheptulose | 0.0% | 2360435376 | HILIC Negative | M-H+O[-] | 3 |
| 239.2367 | 360 | Palmitic acid | 0.0% | 6673039.426 | C18 Positive | M-H ₂ O+H[1+] | 3 |
| 241.0915 | 24.3 | Sorbitol; Mitobronitol; Galactitol | 0.0% | 2838184.279 | C18 Negative | M+CH ₃ COO[-] | 4 |
| 247.2426 | 64.4 | Oleic acid | 0.0% | 12149604.56 | HILIC Positive | M-H ₄ O ₂ +H[1+] | 3 |
| 253.2524 | 325.2 | 13S-hydroxyoctadecadienoic acid; 9,10-Epoxyoctadecenoic acid; 12,13-EpOME | 0.0% | 3770173.753 | C18 Positive | M-CO ₂ +H[1+] | 4 |
| 255.2326 | 367.7 | 14-Me-150-Isopalmitic acid | 0.0% | 12541173713 | C18 Negative | M-H | 1 |
| 255.2329 | 58.5 | Palmitate | 0.0% | 4140781695 | HILIC Negative | M-H | 1 |
| 256.236 | 367.6 | Palmitic acid | 0.0% | 2173978846 | C18 Negative | M(C ₁₃)-H[-] | 3 |
| 256.2363 | 58.6 | Palmitic acid | 0.0% | 745500771.6 | HILIC Negative | M(C ₁₃)-H[-] | 3 |
| 257.1128 | 24.5 | 257.11281@24.5 | 0.0% | 966792.4487 | C18 Positive | - | 5 |
| 265.2524 | 365.7 | Oleic acid | 0.0% | 90915003.9 | C18 Positive | M-H ₂ O+H[1+] | 3 |
| 265.2527 | 64.5 | Hexadecanol | 0.0% | 33388473.26 | HILIC Positive | M+Na | 1 |

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| 269.2262 | 63.9 | 269.22624@63.9 | 0.0% | 29441900.5 | HILIC Positive | - | 5 |
| 271.2277 | 66.6 | Palmitic acid | 0.0% | 59608168.49 | HILIC Negative | M-H+O[-] | 3 |
| 274.3104 | 233.2 | Phytosphingosine | 0.0% | 259819.1186 | C18 Positive | M-CO2+H[1+] | 3 |
| 277.2164 | 65.2 | C184-Stearidonic acid | 0.0% | 10793713.32 | HILIC Positive | M+H | 1 |
| 277.2167 | 323.5 | C182-11-Octadecen-9-ynoic acid | 0.0% | 196077673.6 | C18 Negative | M-H | 1 |
| 278.2203 | 323.9 | C182-11-Octadecen-9-ynoic acid | 0.0% | 34863535.83 | C18 Negative | M-H_-[-1] | 1 |
| 280.235 | 63.4 | C183-9E11Z13E-Octadecatrienoic acid; C182-11-Octadecen-9-ynoic acid; Gamma-Linolenate | 0.0% | 7675586.596 | HILIC Positive | M+H_[+1] | 3 |
| 281.2475 | 288 | Linoleic acid | 0.0% | 24925024.89 | C18 Positive | M+H[1+] | 3 |
| 281.2483 | 377.1 | C181-11-Octadecenoic acid; C181-6-Octadecenoic acid | 0.0% | 11096890198 | C18 Negative | M-H | 3 |
| 281.2485 | 58.7 | C181-11-Octadecenoic acid; C181-6-Octadecenoic acid; Elaidate; Oleate; Petroselinat | 0.0% | 3880606093 | HILIC Negative | M-H | 3 |
| 282.2512 | 58.3 | C181-11-Octadecenoic acid; C181-6-Octadecenoic acid; Elaidate; Oleate; Petroselinat | 0.0% | 722180673.3 | HILIC Negative | M-H_-[-1] | 3 |
| 282.2516 | 374.9 | Oleic acid | 0.0% | 2100932618 | C18 Negative | M(C13)-H[-] | 3 |
| 283.0936 | 19.9 | 283.09356@19.9 | 0.0% | 1487042.481 | C18 Negative | - | 5 |
| 283.2633 | 378.3 | Oleate | 0.0% | 4898999.231 | C18 Positive | M+H | 1 |
| 291.2093 | 368.6 | 14-Me-150-Isopalmitic acid | 0.0% | 3150998.192 | C18 Negative | M+Cl | 1 |
| 291.2097 | 59.1 | Palmitic acid | 0.0% | 4208513.375 | HILIC Negative | M+Cl[-] | 3 |
| 296.2309 | 282.7 | 13S-hydroxyoctadecadienoic acid; 9,10-Epoxyoctadecenoic acid; 12,13-EpOME | 0.0% | 1975306.792 | C18 Negative | M(C13)-H[-] | 4 |
| 297.2424 | 315.4 | 297.24235@315.4 | 0.0% | 1070926.304 | C18 Positive | - | 5 |
| 297.2428 | 62.4 | C181-12-hydroxy-9-cis-octadecenoic acid | 0.0% | 79339014.64 | HILIC Negative | M-H | 1 |

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| 297.2432 | 399.7 | 297.24315@399.7 | 0.0% | 11133737.69 | C18 Negative | - | 5 |
| 301.2381 | 366.7 | Palmitic acid | 0.0% | 82503550.43 | C18 Negative | M+HCOO[-] | 3 |
| 301.2383 | 59.6 | Glycerol-Myristate | 0.0% | 174970698 | HILIC Negative | M-H | 1 |
| 305.2482 | 356.3 | C203-5Z8Z11Z Eicosatrienoic acid | 0.0% | 453076175.9 | C18 Negative | M-H | 1 |
| 306.2514 | 355.8 | 8,11,14-Eicosatrienoic acid | 0.0% | 91581386.56 | C18 Negative | M(C13)-H[-] | 3 |
| 315.2534 | 368.6 | 14-Me-150-Isopalmitic acid | 0.0% | 89709195.01 | C18 Negative | M+Hac-H | 1 |
| 315.2536 | 58.9 | Palmitate | 0.0% | 31353844.68 | HILIC Negative | M+Hac-H | 1 |
| 317.2246 | 373.9 | Oleic acid; Elaidic acid | 0.0% | 13175996.89 | C18 Negative | M+Cl[-] | 4 |
| 317.2253 | 57.6 | C181-11-Octadecenoic acid; C181-6-Octadecenoic acid; Elaidate; Oleate; Petroselinat | 0.0% | 7081068.135 | HILIC Negative | M+Cl | 3 |
| 318.3 | 242.2 | Phytosphingosine | 0.0% | 3443646.946 | C18 Positive | M+H[1+] | 3 |
| 319.222 | 374.1 | Oleic acid; Elaidic acid | 0.0% | 3405865.221 | C18 Negative | M+Cl37[-] | 4 |
| 327.2321 | 329.6 | Docosahexaenoic acid | 0.0% | 260539967 | C18 Negative | M-H[-] | 3 |
| 327.2537 | 374 | Oleic acid; Elaidic acid | 0.0% | 83644573.79 | C18 Negative | M+HCOO[-] | 4 |
| 327.2541 | 58 | Oleic acid; Elaidic acid | 0.0% | 128730968.9 | HILIC Negative | M+HCOO[-] | 4 |
| 328.2358 | 329.8 | Docosahexaenoic acid | 0.0% | 62017327.13 | C18 Negative | M(C13)-H[-] | 3 |
| 335.2219 | 181.3 | Prostaglandin H2; Prostaglandin E2; Prostaglandin D2; Prostaglandin I2; Thromboxane A2; (13E)-11a-Hydroxy-9,15-dioxoprost-13-enoic acid; 13,14-Dihydro-15-keto-PGE2; 20-Hydroxy-leukotriene B4; Lipoxin A4; Lipoxin B4 | 0.0% | 2851159.058 | C18 Positive | M-H2O+H[1+] | 4 |
| 336.2542 | 271.1 | 13S-hydroxyoctadecadienoic acid; 9,10-Epoxyoctadecenoic acid; 12,13-EpOME | 0.0% | 242253.1795 | C18 Negative | M+ACN-H[-] | 4 |

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| 341.2248 | 355.5 | 8,11,14-Eicosatrienoic acid | 0.0% | 245066.516 | C18 Negative | M+Cl ⁻ | 3 |
| 341.2692 | 374.2 | Oleic acid; Elaidic acid | 0.0% | 51420000.2 | C18 Negative | M+CH ₃ COO ⁻ | 4 |
| 341.2695 | 58.1 | C181-11-Octadecenoic acid; C181-6-Octadecenoic acid; Elaidate; Oleate; Petroselinate | 0.0% | 29043687.45 | HILIC Negative | M+Hac-H | 3 |
| 351.2529 | 65.2 | Tetrahydrocorticosterone | 0.0% | 2969280.5 | HILIC Positive | M+H ^[1+] | 3 |
| 351.2535 | 356.2 | 8,11,14-Eicosatrienoic acid | 0.0% | 4498819.199 | C18 Negative | M+HCOO ⁻ | 3 |
| 353.2328 | 226.2 | 353.2328@226.2 | 0.0% | 695270.4199 | C18 Negative | - | 5 |
| 356.3519 | 276.9 | L-Palmitoylcarnitine | 0.0% | 4344243.439 | C18 Positive | M-CO ₂ +H ^[1+] | 3 |
| 370.1771 | 221.9 | 15-Keto-prostaglandin E2; Prostaglandin E3 | 0.0% | 30227230.38 | C18 Negative | M+Na-2H ⁻ | 4 |
| 398.2081 | 224.4 | 398.2081@224.2 | 0.0% | 10050966.23 | C18 Negative | - | 5 |
| 398.3266 | 182.8 | Hexadecenoyl carnitine; (2E)- hexadecenoylcarnitine | 0.0% | 10458915.47 | HILIC Positive | M+H ^[1+] | 4 |
| 399.33 | 182.3 | Hexadecenoyl carnitine; (2E)- hexadecenoylcarnitine | 0.0% | 2444602.631 | HILIC Positive | M(C13)+H ^[1+] | 4 |
| 401.3451 | 274.1 | L-Palmitoylcarnitine | 0.0% | 9967483.439 | C18 Positive | M(C13)+H ^[1+] | 3 |
| 403.3203 | 233.4 | 403.32033@233.4 | 0.0% | 1470849.423 | C18 Positive | - | 5 |
| 430.2949 | 234.2 | Glycocholic acid | 0.0% | 10257653.07 | C18 Positive | M-H ₄ O ₂ +H ^[1+] | 3 |
| 432.311 | 65.8 | Glycohyodeoxcholic acid; Glycochenodeoxycholate | 0.0% | 38483146.82 | HILIC Positive | M+H-H ₂ O | 3 |
| 438.3216 | 249.2 | 3-Hydroxyhexadecanoylcarnitine | 0.0% | 558194.2083 | C18 Positive | M+Na | 1 |
| 450.321 | 69.8 | Glycohyodeoxcholic acid; Glycochenodeoxycholate | 0.0% | 42483058.61 | HILIC Positive | M+H | 3 |
| 451.3245 | 69.8 | 451.32451@69.8 | 0.0% | 11740651.51 | HILIC Positive | - | 5 |
| 464.3014 | 256.2 | Glycocholic acid; Glycocholate | 0.0% | 33124880.38 | HILIC Negative | M-H | 3 |
| 505.9789 | 446.4 | Phosphoadenosine phosphosulfate | 0.0% | 25782079.23 | HILIC Negative | M-H ⁻ | 3 |
| 514.2833 | 212.1 | Taurocholic acid | 0.0% | 2149478.436 | C18 Negative | M-H | 1 |

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| 514.2847 | 206.1 | Tauromuricholic acid; Taurocholic acid | 0.0% | 5151631 | HILIC Negative | M-H | 3 |
| 87.00873 | 20.8 | Pyruvate | 0.0% | 35629688.47 | C18 Negative | M-H | 1 |
| 87.02002 | 285.4 | 87.02002@285.4 | 0.0% | 3549408.381 | HILIC Negative | - | 5 |