**Supplementary Tables:**

**Table S1** 272 compounds identified in PVSO under positive (ESI+) ion mode by UPLC-MS/MS.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **NameEN** | **Class** | **SMILES** | **Formula** | **mzmed** | **rtmed** | **ppm** | **ms2Adduct** | **MS2** | **Area** |
| Betaine | alkaloid | [O-1]C(=O)C[N+1](C)(C)C | C5H11NO2 | 118.0862 | 733.682 | 1.99323098289476 | [M+H]+ | 118.086;59.06;119.087;58.065;95.05 | 51601781.8 |
| BIOTIN | alkaloid | C1C2C(C(S1)CCCCC(=O)O)NC(=O)N2 | C10H16N2O3S | 245.0994 | 38.9802 | 1.47308288135547 | [M+H]+ | 245.1;246.102;173.077;81.071;55.055 | 38109268.07 |
| Hordenine | alkaloid | CN(C)CCc1ccc(cc1)O | C10H15NO | 166.1221 | 3.930577 | 0.609356294187035 | [M+H]+ | 166.123;167.071;93.07;43.018;107.086 | 7101516.227 |
| Indole | alkaloid | N1C=CC2=C1C=CC=C2 | C8H7N | 118.0649 | 41.7877 | 0.877814737450821 | [M+H]+ | 118.087;119.073;59.073;76.934;91.054 | 66115693.33 |
| Nicotinic acid | alkaloid | C1=CC(=CN=C1)C(=O)O | C6H5NO2 | 124.0391 | 33.7484 | 0.86941418623751 | [M+H] | 124.039;125.06;43.018;97.028;79.055 | 4894878.773 |
| Indoxyl | alkaloid | OC1=CNC2=CC=CC=C12 | C8H7NO | 134.0597 | 98.241 | 2.24180552554061 | [M+H]+ | 134.06;106.065;135.08;79.055;107.086 | 7780783.424 |
| Valine | alkaloid | CC(C)C(C(=O)O)N | C5H11NO2 | 118.086 | 660.426 | 0.286700737507923 | [M+H]+ | 118.086;59.061;95.048;119.088;58.065 | 26060815.17 |
| Austricine | alkaloid | CC1C2C(CC(=C3C(C2OC1=O)C(=CC3=O)C)C)O | C15H18O4 | 263.1248 | 260.588 | 0.91799788204488 | [M+H]+ | 263.125;175.11;111.005;264.132;95.085 | 20689456.89 |
| 3-Formylindole | alkaloid | c1ccc2c(c1)c(c[nH]2)C=O | C9H7NO | 146.0597 | 132.46 | 1.89585131445636 | [M+H]+ | 118.065;146.059;91.054;147.063;119.068 | 29472369.79 |
| DL-Coniine | alkaloid | CCCC1CCCCN1 | C8H17N | 128.1431 | 897.247 | 0.991041298819983 | [M+H]+ | 128.143;111.092;69.07;70.065;44.049 | 117979535.5 |
| 1-Piperidinecarboxaldehyde | alkaloid | O=CN1CCCCC1 | C6H11NO | 114.0911 | 49.995 | 0.477744563243366 | [M+H]+ | 114.091;72.937;69.069;115.094;90.947 | 14398364.02 |
| 4-Hydroxybenzoylcholine | alkaloid | C[N+](C)(C)CCOC(=O)C1=CC=C(C=C1)O | C12H18NO3 | 224.128 | 271.052 | 0.132546210501776 | [M]+ | 224.126;93.07;165.054;121.065;79.054 | 3258087.949 |
| 1-methoxyindole-3-carbaldehyde | alkaloid | CON1C=C(C2=CC=CC=C21)C=O | C10H9NO2 | 176.0703 | 42.7307 | 1.79783943271973 | [M+H]+ | 176.071;130.065;158.059;114.971;148.075 | 5356057.708 |
| Aconine | alkaloid | CCN1CC2(C(CC(C34C2C(C(C31)C5(C6C4CC(C6O)(C(C5O)OC)O)O)OC)OC)O)COC | C25H41NO9 | 500.2872 | 499.954 | 1.54522050209669 | [M+H] | 500.291;501.297;55.589;429.236;93.07 | 5924262.215 |
| Bullatine G | alkaloid | CCN1CC2(CCC(C34C2CC(C31)C56C4CC(=O)C(C5)C(=C)C6O)O)C | C22H31NO3 | 358.2347 | 704.75 | 0.827081530480296 | [M+H] | 358.238;359.238;81.071;340.188;83.086 | 43039891.48 |
| 3,4-Dimethoxybenzaldehyde | Aromaticity | O=CC1=CC=C(OC)C(OC)=C1 | C9H10O3 | 167.0698 | 109.245 | 1.07705072606637 | [M+H]+ | 43.018;167.071;107.086;149.097;125.06 | 30433489.88 |
| Phenethylacetate | Aromaticity | O=C(OCCC=1C=CC=CC1)C | C10H12O2 | 165.0909 | 193.818 | 0.697760037733774 | [M+H]+ | 165.092;137.097;119.085;43.018;123.081 | 5270165.096 |
| Phenylpropanolamine | Aromaticity | OC(C=1C=CC=CC1)C(N)C | C9H13NO | 152.1067 | 366.602 | 1.65762023412497 | [M+H]+ | 91.054;117.07;152.107;153.128;43.018 | 56008599.89 |
| 3-n-Butylphathlide | Aromaticity | CCCCC1C2=CC=CC=C2C(=O)O1 | C12H14O2 | 191.1063 | 403.6365 | 1.43670032620529 | [M+H] | 145.102;173.097;191.105;135.044;91.054 | 780711.1491 |
| alpha-Linolenic acid | Fatty acids | CCC=CCC=CCC=CCCCCCCCC(=O)O | C18H30O2 | 279.2317 | 564.099 | 2.62920735421201 | [M+H] | 81.071;67.055;95.085;279.233;109.102 | 611326955.9 |
| Linoleic acid | Fatty acids | CCCCC/C=C\C/C=C\CCCCCCCC(=O)O | C18H32O2 | 281.2471 | 594.953 | 0.395134906559388 | [M+H]+ | 69.07;83.086;245.225;263.238;81.07 | 25545530.46 |
| Arachidonic acid (not validated) | Fatty acids | CCCCC/C=C\C/C=C\C/C=C\C/C=C\CCCC(=O)O | C20H32O2 | 305.2474 | 579.668 | 1.18656058934185 | [M+H]+ | 305.195;81.07;93.069;121.101;79.054 | 5774412.999 |
| (+/-)-Jasmonic acid | Fatty acids | CCC=CCC1C(CCC1=O)CC(=O)O | C12H18O3 | 211.1329 | 473.7205 | 0.364394969275328 | [M+H]+ | 81.033;211.113;193.121;169.1;55.054 | 11562200.18 |
| Daidzein | flavonoids | C1=CC(=CC=C1C2=COC3=C(C2=O)C=CC(=C3)O)O | C15H10O4 | 255.0651 | 359.679 | 0.199541284909284 | [M+H] | 255.064;256.07;95.085;83.086;195.139 | 4190766.63 |
| Maltol | flavonoids | O=C1C=COC(=C1O)C | C6H6O3 | 127.0387 | 38.4143 | 2.42159451798851 | [M+H]+ | 127.039;109.028;128.143;43.018;81.071 | 11063872.25 |
| Pinocembrin | flavonoids | C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=CC=C3 | C15H12O4 | 257.08 | 369.516 | 0.0379193767483675 | [M+H]+ | 257.077;153.018;131.049;145.101;159.117 | 2347824.213 |
| Loureirin A | flavonoids | COC1=CC(=C(C=C1)CCC(=O)C2=CC=C(C=C2)O)OC | C17H18O4 | 287.1249 | 205.516 | 0.52112480626524 | [M+H] | 287.128;269.188;109.065;97.065;288.13 | 1830892.677 |
| 5-O-Demethylnobiletin | flavonoids | COC1=C(C=C(C=C1)C2=CC(=O)C3=C(C(=C(C(=C3O2)OC)OC)OC)O)OC | C20H20O8 | 389.1227 | 431.49 | 0.877105085894796 | [M+H] | 389.127;359.08;341.063;353.246;371.262 | 3662628.53 |
| Myrigalone H | flavonoids | COC1=C(C(=O)CCC2=CC=CC=C2)C(O)=C(C)C(O)=C1 | C17H18O4 | 287.1278 | 189.413 | 2.75962977126124 | [M+H]+ | 287.199;255.104;195.08;227.103;269.193 | 749096.0395 |
| 5-Methoxyflavanone | flavonoids | COC1=CC=CC2=C1C(=O)CC(O2)C3=CC=CC=C3 | C16H14O3 | 255.1017 | 348.365 | 2.69675231288451 | [M+H]+ | 255.103;199.076;81.07;227.109;186.068 | 1537560.156 |
| 5-hydroxy-7,8-dimethoxy-2-phenyl-2,3-dihydrochromen-4-one | flavonoids | COC1=CC(O)=C2C(=O)CC(OC2=C1OC)C3=CC=CC=C3 | C17H16O5 | 301.1068 | 267.321 | 2.72079188715217 | [M+H]+ | 197.045;301.107;182.022;283.242;131.048 | 1976832.249 |
| 6-Demethoxytangeretin | flavonoids | COC1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C=C3OC)OC)OC | C19H18O6 | 343.1177 | 374.861 | 1.9158634301862 | [M+H] | 343.114;313.071;282.09;299.091;328.096 | 3607462.048 |
| Artemetin | flavonoids | COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(C(=C(C=C3O2)OC)OC)O)OC)OC | C20H20O8 | 389.1228 | 377.16 | 0.58236917368095 | [M+H] | 389.127;331.078;356.093;353.247;371.261 | 4902777.075 |
| Farrerol | flavonoids | CC1=C(C(=C2C(=C1O)C(=O)CC(O2)C3=CC=C(C=C3)O)C)O | C17H16O5 | 301.1039 | 185.159 | 0.213157399564916 | [M+H] | 301.107;283.241;302.107;81.071;109.1 | 3315726.626 |
| Nobiletin | flavonoids | COC1=C(C=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C(=C3OC)OC)OC)OC)OC | C21H22O8 | 403.1373 | 373.114 | 1.81605736883542 | [M+H] | 403.135;373.088;388.116;105.034;152.108 | 45126369.79 |
| Licoflavone A | flavonoids | CC(=CCC1=CC2=C(C=C1O)OC(=CC2=O)C3=CC=C(C=C3)O)C | C20H18O4 | 323.1267 | 232.579 | 0.804514185378092 | [M+H] | 323.13;291.102;263.106;231.082;308.103 | 3379383.081 |
| Demethoxycurcumin | Phenols | COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC=C(C=C2)O)O | C20H18O5 | 339.12 | 344.343 | 0.0764506988406695 | [M+H] | 339.12;321.257;340.127;95.085;69.07 | 3721680.401 |
| Anisic aldehyde | Phenols | COC1=CC=C(C=C1)C=O | C8H8O2 | 137.0593 | 47.0471 | 2.07193274883994 | [M+H] | 137.06;81.071;95.085;114.971;138.053 | 5978848.727 |
| Vanillin | Phenols | COC1=C(C=CC(=C1)C=O)O | C8H8O3 | 153.0543 | 92.7794 | 1.73442410239317 | [M+H] | 111.044;153.054;125.06;93.033;65.038 | 88089229.49 |
| p-Hydroxybenzaldehyde | Phenols | C1=CC(=CC=C1C=O)O | C7H6O2 | 123.0437 | 81.7324 | 2.0949404685327 | [M+H] | 123.044;95.049;124.038;81.071;67.055 | 3977120.981 |
| 2-Hydroxy-4-methoxybenzaldehyde | Phenols | COC1=CC(=C(C=C1)C=O)O | C8H8O3 | 153.0543 | 114.104 | 1.93338979628124 | [M+H] | 111.044;153.054;125.06;97.065;43.018 | 18061849.92 |
| shogaol | Phenols | O=C(C=CCCCCC)CCC1=CC=C(O)C(OC)=C1 | C17H24O3 | 277.1798 | 385.487 | 3.04201905648255 | [M+H]+ | 137.06;138.064;278.183;81.071;111.044 | 48750172.28 |
| 4-Methoxysalicylic acid | Phenols | COC1=CC(=C(C=C1)C(=O)O)O | C8H8O4 | 169.0491 | 62.1557 | 0.877060774943603 | [M+H] | 169.048;141.054;111.044;125.06;109.028 | 24090419.13 |
| Asarylaldehyde | Phenols | COC1=CC(=C(C=C1C=O)OC)OC | C10H12O4 | 197.0802 | 56.0255 | 1.01656979053223 | [M+H] | 151.039;73.027;179.071;197.081;125.06 | 7610926.106 |
| Thymol | Phenols | OC1=CC(=CC=C1C(C)C)C | C10H14O | 151.1113 | 589.962 | 2.01211244855378 | [M+H]+ | 81.035;53.039;151.097;67.055;69.069 | 64088631.82 |
| 3,5-Dimethoxy-4-hydroxybenzaldehyde | Phenols | COC1=CC(=CC(=C1O)OC)C=O | C9H10O4 | 183.065 | 100.051 | 0.212035802733756 | [M+H] | 123.044;95.049;155.069;183.064;140.046 | 6970570.228 |
| Guaiacol | Phenols | COC1=C(O)C=CC=C1 | C7H8O2 | 125.0596 | 92.7794 | 2.82857858297809 | [M+H]+ | 125.097;43.018;126.055;97.028;111.044 | 22668881.28 |
| Citropten | phenylpropanoids | O=C1OC2=CC(OC)=CC(OC)=C2C=C1 | C11H10O4 | 207.0647 | 306.292 | 1.36375322775669 | [M+H]+ | 207.066;147.117;192.042;161.133;123.08 | 3448757.441 |
| isoimperatorin | phenylpropanoids | O=C1OC=2C=C3OC=CC3=C(OCC=C(C)C)C2C=C1 | C16H14O4 | 309.2058 | 319.505 | 0.739509165687388 | M-H | 292.2;310.211;274.188;81.071;123.08 | 37329248.33 |
| Scopoletin | phenylpropanoids | O=C1OC=2C=C(O)C(OC)=CC2C=C1 | C10H8O4 | 193.0489 | 102.554 | 0.54511541828432 | [M+H]+ | 193.048;133.028;194.115;178.025;135.044 | 10036711.54 |
| Coumarin | phenylpropanoids | O=C1OC2=CC=CC=C2C=C1 | C9H6O2 | 147.0438 | 167.304 | 1.66758215848179 | [M+H]+ | 147.044;103.054;91.055;148.048;105.07 | 6584677.399 |
| Coniferyl aldehyde | phenylpropanoids | COC1=CC(C=CC=O)=CC=C1O | C10H10O3 | 179.0699 | 139.057 | 0.558153452671733 | [M+H]+ | 179.071;147.043;55.018;161.059;119.049 | 68058369.22 |
| Cinnamaldehyde | phenylpropanoids | C1=CC=C(C=C1)C=CC=O | C9H8O | 133.0644 | 246.628 | 4.374551523084 | [M+H] | 55.018;133.065;115.054;105.07;91.055 | 12636362.14 |
| Citrusal | phenylpropanoids | COC1=C(CC(C)(C)C=O)C2=C(C=CC(=O)O2)C=C1 | C15H16O4 | 261.1106 | 308.078 | 2.15768831667351 | [M+H]+ | 261.112;189.053;81.071;119.085;145.101 | 922390.7146 |
| Isomeranzin | phenylpropanoids | CC(C)C(=O)CC1=C(C=CC2=C1OC(=O)C=C2)OC | C15H16O4 | 261.1117 | 185.159 | 1.00077740029031 | [M+H] | 189.054;131.048;261.112;243.103;159.044 | 23484118.84 |
| (E/Z)-cinnamic acid | phenylpropanoids | OC(=O)C=CC1=CC=CC=C1 | C9H8O2 | 149.0595 | 225.874 | 3.62725394521423 | [M+H]+ | 131.05;103.055;149.096;121.101;107.086 | 1561399.369 |
| Isoferulic acid | phenylpropanoids | COC1=C(C=C(C=C1)C=CC(=O)O)O | C10H10O4 | 195.0647 | 103.157 | 1.65777055889351 | [M+H] | 177.054;145.029;117.034;149.059;195.065 | 7993131.002 |
| Coumaric acid | phenylpropanoids | O=C(O)C=CC1=CC=C(O)C=C1 | C9H8O3 | 147.0438 | 139.057 | 1.61346876314731 | [M+H-H2O]+ | 147.044;119.05;91.055;123.964;105.07 | 5431880.214 |
| 8-(2-hydroxy-3-methylbut-3-enyl)-7-methoxychromen-2-one | phenylpropanoids | COC1=CC=C2C=CC(=O)OC2=C1CC(O)C(C)=C | C15H16O4 | 243.1008 | 185.159 | 0.969469617548368 | [M-H2O+H]+ | 189.053;243.103;201.053;131.048;187.038 | 4486981.125 |
| 7-Methoxycoumarin | phenylpropanoids | COC1=CC2=C(C=C1)C=CC(=O)O2 | C10H8O3 | 177.0544 | 231.975 | 2.39523570322965 | [M+H] | 177.054;145.029;117.034;121.101;149.059 | 8933648.812 |
| Grandisin | phenylpropanoids | COC1=CC(=CC(OC)=C1OC)C2OC(C(C)C2C)C3=CC(OC)=C(OC)C(OC)=C3 | C24H32O7 | 415.2104 | 460.677 | 1.38872064022943 | [M-H2O+H]+ | 119.085;120.088;121.092;417.216;133.065 | 267009544.6 |
| 5-[6-(3-hydroxy-4-methoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan-3-yl]-2-methoxyphenol | phenylpropanoids | COC1=CC=C(C=C1O)C2OCC3C2COC3C4=CC=C(OC)C(O)=C4 | C20H22O6 | 341.1384 | 232.579 | 1.19342598058829 | [M-H2O+H]+ | 137.06;291.101;271.097;341.139;323.131 | 16615381.95 |
| alpha-Asarone | phenylpropanoids | CC=CC1=CC(=C(C=C1OC)OC)OC | C12H16O3 | 209.1169 | 79.8588 | 0.29920646681047 | [M+H] | 209.116;149.097;131.085;191.106;145.1 | 9318945.971 |
| Sclareapinone | quinones | CC(C)C1=CC2=C(C(=O)C1=O)C(CCC(=O)C(C)(C)O)=C(C)C=C2 | C20H24O4 | 329.1714 | 419.161 | 1.91759390659864 | [M+H]+ | 329.17;330.176;98.984;134.034;301.176 | 123728376.3 |
| Claussequinone | quinones | COc(c3)c(=O)cc(c(=O)3)C(C1)Cc(c2)c(cc(O)c2)O1 | C16H14O5 | 287.0915 | 332.644 | 1.56991920136152 | [M+H]+ | 255.064;287.093;227.071;269.081;199.076 | 8067094.835 |
| 5-O-Methylembelin | quinones | CCCCCCCCCCCC1=C(O)C(=O)C=C(OC)C1=O | C18H28O4 | 309.2059 | 539.5825 | 3.03696576107986 | [M+H]+ | 291.196;165.092;193.123;171.102;67.055 | 36834048.91 |
| 2,8-Dihydroxy-5,5,8-trimethyl-11-oxatetracyclo[7.3.1.0~1,9~.0~3,7~]tridecan-10-one | terpenoids | CC1(C)CC2C(O)C34COC(=O)C3(C4)C(C)(O)C2C1 | C15H22O4 | 249.1455 | 135.447 | 1.92294046563307 | [M-H2O+H]+ | 249.148;250.148;231.14;84.081;166.051 | 11418705.31 |
| Kaurane-17,18-dioic acid | terpenoids | CC12CCCC(C)(C1CCC34CC(CCC23)C(C4)C(O)=O)C(O)=O | C20H30O4 | 352.2475 | 395.861 | 1.39114259750844 | [M+NH4]+ | 289.178;353.238;271.171;352.252;81.071 | 12627672.04 |
| Lucidenic acid D2 | terpenoids | CC(CCC(O)=O)C1CC(=O)C2(C)C3=C(C(=O)C(OC(C)=O)C12C)C1(C)CCC(=O)C(C)(C)C1CC3=O | C29H38O8 | 515.2635 | 478.082 | 2.83101166483217 | [M+H]+ | 515.263;57.253;516.261;59.06;61.478 | 28923114.43 |
| Lucidone C | terpenoids | CC(=O)C1CC(O)C2(C)C3=C(C(=O)CC12C)C1(C)CCC(O)C(C)(C)C1CC3O | C24H36O5 | 405.2619 | 605.442 | 2.15345998660744 | [M+H]+ | 405.262;406.252;264.174;279.199;69.07 | 54134039.38 |
| Zizyberanalic acid | terpenoids | O=CC1C(O)C(C)(C)C2CCC3(C)C(CCC4C5C(C(=C)C)CCC5(C(=O)O)CCC43C)C12C | C30H46O4 | 471.3469 | 564.099 | 1.80432829912333 | [M+H]+ | 205.157;473.362;189.165;203.178;187.148 | 81009818.25 |
| Cycloastragenol | terpenoids | CC1(C(CCC23C1C(CC4C2(C3)CCC5(C4(CC(C5C6(CCC(O6)C(C)(C)O)C)O)C)C)O)O)C | C30H50O5 | 513.3538 | 650.042 | 0.454431487859292 | [M+Na] | 513.359;57.041;514.367;111.041;425.299 | 18505136.64 |
| Ganoderic acid Me | terpenoids | CC(CC\C=C(/C)C(O)=O)C1CC(OC(C)=O)C2(C)C3=CCC4C(C)(C)C(CCC4(C)C3=CCC12C)OC(C)=O | C34H50O6 | 555.365 | 776.91 | 0.0361012653252331 | [M+H]+ | 555.365;61.708;556.373;221.116;277.14 | 12068679.67 |
| Cryptomeridiol 11-rhamnoside | terpenoids | CC1OC(OC(C)(C)C2CCC3(C)CCCC(C)(O)C3C2)C(O)C(O)C1O | C21H38O6 | 387.2705 | 776.669 | 1.29847850724243 | [M+H]+ | 387.272;81.07;388.272;69.069;95.085 | 22119326.62 |
| 3-Hydroxyurs-12-en-23-oic acid | terpenoids | CC1CCC2(C)CCC3(C)\C(=C/CC4C5(C)CCC(O)C(C)(C5CCC34C)C(O)=O)C2C1C | C30H48O3 | 479.349 | 746.776 | 1.99335964060386 | [M+Na]+ | 479.354;53.262;480.351;81.07;461.367 | 27803153.01 |
| (3beta,6beta)-Furanoeremophilane-3,6-diol | terpenoids | CC1C(O)CCC2CC3=C(C(O)C12C)C(C)=CO3 | C15H22O3 | 251.1634 | 362.114 | 2.26995337768185 | [M+H]+ | 251.167;81.069;95.085;67.054;109.101 | 14188246.48 |
| ent-16a-Hydroxy-17-acetoxy-19-kauranal | terpenoids | CC(=O)OCC1(O)CC23CC1CCC2C1(C)CCCC(C)(C=O)C1CC3 | C22H34O4 | 363.2504 | 579.668 | 1.18310884942955 | [M+H]+ | 363.251;86.06;364.258;85.076;81.071 | 17335957.14 |
| 2,3-Secoporrigenin | terpenoids | CC1C2C(CC3C4CC5OC(=O)CC5C(C)(CC(O)=O)C4CCC23C)OC11CCC(C)CO1 | C27H40O6 | 461.2858 | 701.028 | 0.500493176777705 | [M+H]+ | 461.294;51.255;462.296;95.085;81.07 | 15917189.74 |
| Abscisic acid | terpenoids | CC1=CC(=O)CC(C1(C=CC(=CC(=O)O)C)O)(C)C | C15H20O4 | 265.1424 | 212.349 | 1.47186519518493 | [M+H] | 265.14;247.135;81.069;69.07;83.086 | 10705474.48 |
| alpha-Cyperone | terpenoids | CC1=C2CC(CCC2(CCC1=O)C)C(=C)C | C15H22O | 219.1737 | 222.86 | 1.28734937650116 | [M+H]+ | 219.174;81.07;201.163;159.116;95.085 | 4533172.891 |
| Lucidenic acid M | terpenoids | CC(CCC(O)=O)C1CC(O)C2(C)C3=C(C(=O)CC12C)C1(C)CCC(O)C(C)(C)C1CC3O | C27H42O6 | 463.3025 | 660.426 | 1.06920851932519 | [M+H]+ | 463.299;51.479;464.306;111.041;127.036 | 501069333.8 |
| Reichsteins substance S | terpenoids | CC12CCC3C(CCC4=CC(=O)CCC34C)C2CCC1(O)C(=O)CO | C21H30O4 | 347.2195 | 555.128 | 1.37834226623933 | [M+H]+ | 347.218;348.222;81.071;95.085;69.07 | 7207756.362 |
| 7-hydroxy-1,4a-dimethyl-9-oxo-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthrene-1-carboxylic acid | terpenoids | O=C(O)C1(C)CCCC2(C)C3C(=CC(O)(CC3)C(C)C)C(=O)CC12 | C20H30O4 | 335.2194 | 469.945 | 1.07776382189793 | [M+H]+ | 335.218;336.219;83.049;81.071;195.1 | 112934915.9 |
| Cadabicilone | terpenoids | CC1C2CCC3(C)CCC(=O)C(C)C3C2OC1=O | C15H22O3 | 251.1621 | 196.265 | 0.234803836327575 | [M+H]+ | 251.162;233.153;147.117;145.1;205.158 | 3550945.377 |
| 9-Acetoxyfukinanolide | terpenoids | CC1CCCC2C(OC(C)=O)C3(CC12C)C(=C)COC3=O | C17H24O4 | 293.1728 | 263.079 | 0.531460413489619 | [M+H]+ | 293.175;275.199;81.071;107.085;93.07 | 4517702.019 |
| Mangiferonic acid | terpenoids | CC(CC\C=C(/C)C(O)=O)C1CCC2(C)C3CCC4C5(CC35CCC12C)CCC(=O)C4(C)C | C30H46O3 | 455.3509 | 749.002 | 2.38057471258847 | [M+H]+ | 455.356;50.596;437.347;205.157;203.178 | 37121437.78 |
| 1beta-Hydroxyalantolactone | terpenoids | CC1CCC(O)C2(C)CC3OC(=O)C(=C)C3C=C12 | C15H20O3 | 249.148 | 447.492 | 0.129687233400801 | [M+H]+ | 249.148;231.138;179.07;121.101;81.069 | 6604577.305 |
| Germacrone | terpenoids | CC1=CCC(=C(C)C)C(=O)CC(=CCC1)C | C15H22O | 219.1738 | 330.876 | 1.12176736202153 | [M+H] | 219.174;175.149;133.102;159.116;201.163 | 9270047.993 |
| 11,17,21-Trihydroxypregn-4-ene-3,20-dione | terpenoids | CC12CC(O)C3C(CCC4=CC(=O)CCC34C)C2CCC1(O)C(=O)CO | C21H30O5 | 363.2152 | 517.227 | 2.17077144884013 | [M+H]+ | 363.217;364.217;249.111;259.133;231.135 | 595328494 |
| Santalyl acetate | terpenoids | CC(=O)OCC(C)=CCCC1(C)C2CCC(C2)C1=C | C17H26O2 | 263.2002 | 339.095 | 0.603885076050323 | [M+H]+ | 263.202;121.101;81.07;93.069;79.054 | 5544696.946 |
| Cichoralexin | terpenoids | CC1C2CCC(C)C3C(C2OC1=O)C(C)=CC3=O | C15H20O3 | 249.1476 | 165.1855 | 1.44865807418319 | [M+H]+ | 249.148;231.14;149.097;189.129;105.07 | 3056732.966 |
| Beta-Caryophyllene Alcohol | terpenoids | OC12CCCC(C)(CCC3C1CC3(C)C)C2 | C15H26O | 240.2318 | 810.44 | 0.852024656930926 | [M+NH4]+ | 240.23;83.085;69.069;57.07;95.085 | 6434245.671 |
| Curcumenol | terpenoids | OC12OC3(CC1=C(C)C)C(C(=C2)C)CCC3C | C15H22O2 | 257.1503 | 898.389 | 1.22485247998464 | [M+Na]+ | 257.151;216.125;258.146;56.05;175.098 | 16062206.29 |
| (6beta,22E)-6-Hydroxystigmasta-4,22-dien-3-one | terpenoids | CCC(\C=C\C(C)C1CCC2C3CC(O)C4=CC(=O)CCC4(C)C3CCC12C)C(C)C | C29H46O2 | 427.3555 | 820.904 | 1.15900231900535 | [M+H]+ | 83.086;427.363;69.07;55.054;81.071 | 10202318.81 |
| Sideridiol | terpenoids | CC1=CC23CC1CCC2C1(C)CCCC(C)(CO)C1CC3O | C20H32O2 | 305.2472 | 553.417 | 0.709732784413776 | [M+H]+ | 305.195;217.196;81.07;259.207;133.102 | 6764608.332 |
| Loliolide | terpenoids | CC1(CC(CC2(C1=CC(=O)O2)C)O)C | C11H16O3 | 197.1168 | 131.869 | 0.949154144784456 | [M+H]+ | 197.118;179.105;135.116;107.086;133.102 | 241711808.5 |
| Spathulenol | terpenoids | CC1(C)C2CCC(=C)C3CCC(C)(O)C3C12 | C15H24O | 221.1895 | 325.488 | 2.20008277780735 | [M+H]+ | 203.179;221.19;147.116;95.085;107.086 | 11684978.91 |
| Camphor | terpenoids | CC1(C2CCC1(C(=O)C2)C)C | C10H16O | 153.127 | 633.036 | 0.29468544857372 | [M+H] | 153.113;55.018;69.069;112.087;93.069 | 6630890.655 |
| (+)-Alantolactone | terpenoids | CC1CCCC2(C1=CC3C(C2)OC(=O)C3=C)C | C15H20O2 | 233.1531 | 495.896 | 0.574617384427587 | [M+H]+ | 233.153;187.148;81.07;215.144;151.074 | 3088522.284 |
| Perillene | terpenoids | CC(=CCCC1=COC=C1)C | C10H14O | 151.1115 | 140.265 | 3.29367508464979 | [M+H] | 151.112;133.1;107.086;93.07;105.07 | 12577271.77 |
| Vulgarin | terpenoids | CC1C2CCC3(C)C(C2OC1=O)C(C)(O)C=CC3=O | C15H20O4 | 265.1424 | 240.453 | 2.42567030629656 | [M+H]+ | 265.14;191.07;247.135;81.07;229.123 | 4030143.023 |
| Oleanane -4H, + 2O | terpenoids | OCC2(C)(C(O)CCC3(C)(C4CC=C1C5CC(C=CC5(C)(CCC1(C)C4(C)(CCC23)))(C)C)) | C30H48O2 | 441.3719 | 628.411 | 2.52549840865296 | [M+H]+ | 441.327;95.085;81.071;109.102;107.086 | 11245364.4 |
| 3,19-Dihydroxyurs-12-ene-23,28-dioic acid | terpenoids | CC1CCC2(CCC3(C)\C(=C/CC4C5(C)CCC(O)C(C)(C5CCC34C)C(O)=O)C2C1(C)O)C(O)=O | C30H46O6 | 485.3231 | 776.523 | 0.287614856187281 | [M-H2O+H]+ | 485.323;53.926;486.326;59.06;87.092 | 11800781.29 |
| 22-Dehydroclerosterol | terpenoids | CCC(\C=C\C(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)=C | C29H46O | 411.3614 | 762.723 | 1.3827472094069 | [M+H]+ | 411.274;81.07;95.085;69.069;59.06 | 9402176.918 |
| Azuleno(5,6-c)furan-1(3H)-one, 4,4a,5,6,7,7a,8,9-octahydro-3,4,8-trihydroxy-6,6,8-trimethyl- | terpenoids | O=C1OC(O)C2=C1CC(O)(C)C3CC(C)(C)CC3C2O | C15H22O5 | 283.1535 | 205.516 | 1.65142214910319 | [M+H]+ | 227.129;163.11;283.157;81.07;135.116 | 2265816.861 |
| 2-(Methoxycarbonyl)-5-methyl-2,4-bis(3-methyl-2-butenyl)-6-(2-methyl-1-oxopropyl)-5-(4-methyl-3-pentenyl)cyclohexanone | terpenoids | COC(=O)C1(CC=C(C)C)CC(CC=C(C)C)C(C)(CCC=C(C)C)C(C(=O)C(C)C)C1=O | C29H46O4 | 459.3467 | 523.343 | 1.53552280836456 | [M+H]+ | 459.349;263.166;69.07;51.04;441.339 | 8330609.795 |
| (2E)-5-(2,3-Dimethyltricyclo[2.2.1.0~2,6~]hept-3-yl)-2-methyl-2-pentenoic acid | terpenoids | C\C(=C/CCC1(C)C2CC3C(C2)C13C)C(O)=O | C15H22O2 | 235.169 | 542.513 | 0.202293549086198 | [M+H]+ | 235.17;57.07;179.106;93.069;79.054 | 18505948.13 |
| Azuleno[5,6-c]furan-1(3H)-one, 4,4a,5,6,7,7a,8,9-octahydro-4,8-dihydroxy-6,6,8-trimethyl- | terpenoids | CC1(C)CC2C(O)C/3=C(CC(C)(O)C2C1)/C(=O)OC3 | C15H22O4 | 249.148 | 188.186 | 0.145991834962296 | [M-H2O+H]+ | 249.148;231.139;191.107;145.102;189.128 | 3638474.951 |
| Procurcumadiol | terpenoids | CC(C)=C1CC2(O)C(CCC2(C)O)C(C)=CC1=O | C15H22O3 | 251.1626 | 278.7495 | 1.76343962307793 | [M+H]+ | 251.163;233.153;81.07;147.117;205.158 | 11087772.63 |
| Sugiol | terpenoids | CC(C)C1=CC2=C(C=C1O)C1(C)CCCC(C)(C)C1CC2=O | C20H28O2 | 301.2159 | 475.223 | 0.401018493253621 | [M+H]+ | 301.214;133.102;163.111;107.086;81.071 | 7345787.71 |
| Isoshyobunone | terpenoids | CC(C)C1CCC(C)(C=C)C(=C(C)C)C1=O | C15H24O | 221.1895 | 570.069 | 2.05954561339659 | [M+H]+ | 221.19;81.071;95.085;121.101;67.055 | 82922665.73 |
| Polyporusterone B | terpenoids | CC(C)C(=C)CC(O)C(C)(O)C1CCC2(O)C3=CC(=O)C4CC(O)C(O)CC4(C)C3CCC12C | C28H44O6 | 477.3188 | 703.091 | 1.72674329860086 | [M+H]+ | 477.319;53.036;478.323;111.041;127.036 | 73825162.16 |
| beta-Elemonic acid | terpenoids | CC(=CCCC(C1CCC2(C1(CCC3=C2CCC4C3(CCC(=O)C4(C)C)C)C)C)C(=O)O)C | C30H46O3 | 455.3508 | 551.679 | 0.448541528689872 | [M+H] | 81.07;455.356;95.085;409.349;109.101 | 55891144.22 |
| (22E,24R)-Stigmasta-4,22-diene-3,6-dione | terpenoids | CCC(\C=C\C(C)C1CCC2C3CC(=O)C4=CC(=O)CCC4(C)C3CCC12C)C(C)C | C29H44O2 | 425.3423 | 690.746 | 0.672355452185846 | [M+H]+ | 425.334;95.086;109.101;107.085;407.326 | 31631999.87 |
| 3,8a-Dihydroxy-5-isopropylidene-3,8-dimethyl-2,3,3a,4,5,8a-hexahydro-6(1H)-azulenone | terpenoids | CC(C)=C1CC2C(C)(O)CCC2(O)\C(=C/C1=O)C | C15H22O3 | 233.1532 | 426.435 | 0.901869765244595 | [M-H2O+H]+ | 233.153;215.144;187.149;107.049;105.07 | 18264169.19 |
| Curcumanolide A | terpenoids | CC1CCC(C(C)=C)C11CC(=C(C)C)C(=O)O1 | C15H22O2 | 235.169 | 707.44 | 0.185975660658201 | [M+H]+ | 235.17;121.101;93.07;79.055;189.163 | 59146060.1 |
| 6beta-Hydroxy-3-oxo-12-oleanen-28-oic acid | terpenoids | CC1(C)CCC2(CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5C(O)CC34C)C2C1)C(O)=O | C30H46O4 | 471.3471 | 528.295 | 2.27340144160838 | [M+H]+ | 471.307;81.07;201.163;453.341;107.086 | 19639239.38 |
| Curdione | terpenoids | CC1CCC=C(CC(=O)C(CC1=O)C(C)C)C | C15H24O2 | 237.1842 | 384.338 | 3.1869599638328 | [M+H] | 237.127;81.069;95.085;219.17;109.101 | 8020519.97 |
| (6beta,8alpha)-6-Hydroxy-7(11)-eremophilen-12,8-olide | terpenoids | CC1CCCC2CC3OC(=O)C(C)=C3C(O)C12C | C15H22O3 | 251.1634 | 329.6695 | 2.4801109469446 | [M+H]+ | 251.163;233.153;95.086;109.065;81.07 | 7097353.981 |
| Polyporusterone F | terpenoids | CC(C)C(C)CC(O)C(C)C1CCC2(O)C3=CC(=O)C4CC(O)C(O)CC4(C)C3CCC12C | C28H46O5 | 463.338 | 750.687 | 2.26495877740023 | [M+H]+ | 463.323;51.483;182.154;464.335;199.181 | 5031603.5 |
| beta-Bourbonene | terpenoids | CC(C)C1CCC2(C)C3CCC(=C)C3C12 | C15H24 | 205.1946 | 561.31 | 2.08674054685407 | [M+H]+ | 121.101;205.197;135.116;67.055;81.071 | 27314766.72 |
| 4-Androstene-3,17-dione | terpenoids | CC12CCC3C(CCC4=CC(=O)CCC34C)C1CCC2=O | C19H26O2 | 287.1998 | 32.0274 | 0.725250431949498 | [M+H]+ | 287.198;269.193;251.182;93.071;159.116 | 5043167.089 |
| Kessyl glycol | terpenoids | CC1CC(O)C2C1CC1C(O)CC2(C)OC1(C)C | C15H26O3 | 255.195 | 301.596 | 0.188905217929565 | [M+H]+ | 81.07;237.184;69.069;255.206;121.101 | 2073114.999 |
| 4,4,8,10,14-pentamethyl-17-(4,5,6-trihydroxy-6-methylheptan-2-yl)-2,5,6,7,9,15-hexahydro-1H-cyclopenta[a]phenanthrene-3,16-dione | terpenoids | CC(CC(O)C(O)C(C)(C)O)C1=C2C=CC3C4(C)CCC(=O)C(C)(C)C4CCC3(C)C2(C)CC1=O | C30H46O5 | 509.3224 | 756.587 | 1.18338251214357 | [M+Na]+ | 509.319;56.593;510.328;69.07;95.085 | 23286582.36 |
| 8-Acetoxy-4-acoren-3-one | terpenoids | CC(C)C1C(CC(C)C11CC=C(C)C(=O)C1)OC(C)=O | C17H26O3 | 279.1951 | 403.632 | 3.96326681994897 | [M+H]+ | 81.07;279.194;67.054;95.085;109.101 | 10237546.67 |
| Cyperolone | terpenoids | CC(=C)C1CCC2(C)CCC(O)C2(C1)C(C)=O | C15H24O2 | 237.1843 | 373.114 | 1.19032946129127 | [M+H]+ | 237.127;95.086;177.072;81.07;109.101 | 4263704.14 |
| 1a,5,7a-Trimethyl-2,2a,6,6a,7a,8,9,9a-octahydrobisoxireno[4,5:8,9]cyclodeca[1,2-b]furan-4(1aH)-one | terpenoids | CC\1=C2/CC3OC3(C)CCC4OC4(C)CC2OC1=O | C15H20O4 | 265.1435 | 384.338 | 1.84748632648214 | [M+H]+ | 247.135;121.029;81.07;135.044;67.055 | 1652370.31 |
| Furanofukinin | terpenoids | COC1C2=C(CC3CCCC(C)C13C)OC=C2C | C16H24O2 | 249.1845 | 500.542 | 1.99435846514478 | [M+H]+ | 249.186;71.086;81.07;95.085;79.054 | 11807128.48 |
| Camelledionol | terpenoids | CC1(C)CCC2(O)C(C1)C1=CCC3C4(C)CCC(=O)C(C)(C)C4CCC3(C)C1(C)CC2=O | C29H44O3 | 441.336 | 620.305 | 0.0304373778678262 | [M+H]+ | 441.338;95.085;81.071;109.102;107.086 | 4682548.661 |
| Saussurea lactone | terpenoids | CC1C2CCC(C)(C=C)C(C2OC1=O)C(C)=C | C15H22O2 | 235.1689 | 408.824 | 0.350786298176339 | [M+H]+ | 235.17;93.07;121.101;107.086;81.07 | 11911397.61 |
| (1beta,4alpha,5alpha,6beta,8alpha,10b)-1,10:4,5-Diepoxy-6-hydroxy-7(11)-germacren-12,8-olide | terpenoids | CC1=C2C(CC3(C)OC3CCC3(C)OC3C2O)OC1=O | C15H20O5 | 281.1359 | 159.924 | 0.215483524363134 | [M+H]+ | 281.137;193.119;192.112;263.125;83.086 | 3249382.292 |
| 17-Hydroxy-15,16-epoxykauran-18-oic acid | terpenoids | CC12CCCC(C)(C1CCC34CC(CCC23)C5(CO)OC45)C(O)=O | C20H30O4 | 317.21 | 352.6 | 0.045595777756422 | [M-H2O+H]+ | 317.208;213.127;275.166;318.215;163.076 | 6487189.834 |
| beta-Costic acid | terpenoids | CC12CCCC(=C)C1CC(CC2)C(=C)C(O)=O | C15H22O2 | 235.1687 | 318.3555 | 1.12874885987544 | [M+H]+ | 235.17;217.159;119.085;133.1;107.086 | 9520542.933 |
| 3,8-dihydroxy-3,8-dimethyl-5-propan-2-ylidene-1,2,3a,4,7,8a-hexahydroazulen-6-one | terpenoids | O=C1C(=C(C)C)CC2C(CCC2(O)C)C(O)(C)C1 | C15H24O3 | 253.179 | 294.367 | 0.183756585053287 | [M+H]+ | 81.07;67.054;235.17;95.085;207.137 | 4350190.821 |
| 3-Hydroxy-5-isopropylidene-3,8-dimethyl-2,3,3a,4,5,8a-hexahydro-6(1H)-azulenone | terpenoids | CC(C)=C1CC2C(CCC2(C)O)\C(=C/C1=O)C | C15H22O2 | 217.158 | 331.465 | 0.205984385601468 | [M-H2O+H]+ | 217.158;199.146;159.116;157.101;119.085 | 3815998.963 |
| Bryonolic acid | terpenoids | CC1(C)C(O)CCC2(C)C1CCC1=C2CCC2(C)C3CC(C)(CCC3(C)CCC12C)C(O)=O | C30H48O3 | 457.3675 | 709.317 | 1.02308195444366 | [M+H]+ | 457.37;203.178;81.07;191.178;189.163 | 257310958 |
| Ursonic acid | terpenoids | CC1CCC2(CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5CCC34C)C2C1C)C(O)=O | C30H46O3 | 455.3512 | 579.126 | 0.488820187530904 | [M+H]+ | 409.348;205.158;203.179;455.345;189.163 | 22224603.19 |
| alpha-Amyrone | terpenoids | CC1CCC2(C)CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5CCC34C)C2C1C | C30H48O | 425.3767 | 587.692 | 0.701744420811061 | [M+H]+ | 109.101;95.085;425.376;81.071;135.118 | 13411987.73 |
| beta-Elemolic acid | terpenoids | CC(C)=CCCC(C1CCC2(C)C3=C(CCC12C)C1(C)CCC(O)C(C)(C)C1CC3)C(O)=O | C30H48O3 | 457.3675 | 739.65 | 1.12031324459921 | [M+H]+ | 457.335;81.071;95.085;411.365;107.086 | 30964224.88 |
| Methyl lucidenate F | terpenoids | COC(=O)CCC(C)C1CC(=O)C2(C)C3=C(C(=O)CC12C)C1(C)CCC(=O)C(C)(C)C1CC3=O | C28H38O6 | 471.2732 | 518.895 | 0.49714447148377 | [M+H]+ | 177.054;471.291;145.028;81.069;95.085 | 3181853.776 |
| Urocortisone | terpenoids | CC12CCC(CC1CCC3C2C(=O)CC4(C3CCC4(C(=O)CO)O)C)O | C21H32O5 | 365.2307 | 364.993 | 1.97732827538272 | [M+H]+ | 365.233;319.15;113.059;291.195;149.057 | 12260529.42 |
| Isoglabrolide | terpenoids | CC12CC3(OC1=O)C1=CC(=O)C4C5(C)CCC(O)C(C)(C)C5CCC4(C)C1(C)CCC3(C)CC2 | C30H44O4 | 469.3319 | 484.616 | 1.8612357826362 | [M+H]+ | 469.345;81.07;451.329;175.149;423.328 | 5587993.975 |
| Pomonic acid | terpenoids | CC1CCC2(CCC3(C)C(=CCC4C5(C)CCC(=O)C(C)(C)C5CCC34C)C2C1(C)O)C(O)=O | C30H46O4 | 471.3469 | 632.46 | 1.90267081426771 | [M+H]+ | 471.352;189.162;119.085;95.085;81.07 | 24196384.26 |
| (1alpha,6alpha,7alphaH)-2,4(15)-Copadiene | terpenoids | CC(C)C1CCC2(C)C3C=CC(=C)C2C13 | C15H22 | 203.1794 | 559.625 | 1.7973475685211 | [M+H]+ | 203.179;147.116;133.102;95.085;105.07 | 19353025.66 |
| Bisacurone epoxide | terpenoids | CC(CC(=O)C=C(C)C)C1CC(O)C(C)(O)C2OC12 | C15H24O4 | 269.1739 | 433.751 | 0.266191530475325 | [M+H]+ | 269.177;67.054;81.07;69.07;93.07 | 4849158.32 |
| Vulgarole | terpenoids | CC(=O)OC1C(O)C2CCC1(C)C2(C)C | C12H20O3 | 213.1483 | 287.074 | 1.44019955097866 | [M+H]+ | 213.131;81.07;95.085;163.149;69.07 | 7913210.776 |
| Actinidic acid | terpenoids | CC1C2C3=CCC4C5(C)CC(O)C(O)C(C)(CO)C5CCC4(C)C3(C)CCC2(CCC1=C)C(O)=O | C30H46O5 | 487.3402 | 451.658 | 1.60976399247819 | [M+H]+ | 487.341;187.147;205.16;123.044;469.332 | 14468301.02 |
| Epoxyganoderiol C | terpenoids | CC(CCC1OC1(C)CO)C1CCC2(C)C3=CCC4C(C)(C)C(O)CCC4(C)C3=CCC12C | C30H48O3 | 457.3672 | 751.071 | 1.65745446871568 | [M+H]+ | 457.358;81.07;439.359;421.352;109.101 | 30226812.52 |
| 1-Naphthalenecarboxylic acid, 5-[2-(2,5-dihydro-2-oxo-3-furanyl)ethyl]decahydro-1,4a-dimethyl-6-methylene- | terpenoids | CC12CCCC(C)(C1CCC(=C)C2CC/C3=C/COC3=O)C(O)=O | C20H28O4 | 333.2036 | 538.626 | 1.93066683074616 | [M+H]+ | 333.201;334.196;133.1;105.07;119.085 | 61332133.32 |
| Ganoderol A | terpenoids | CC(CC\C=C(/C)CO)C1CCC2(C)C3=CCC4C(C)(C)C(=O)CCC4(C)C3=CCC12C | C30H46O2 | 439.3573 | 787.593 | 0.664330339691746 | [M+H]+ | 439.352;81.071;95.085;421.351;109.101 | 11898709.94 |
| Cafestol | terpenoids | CC12CCC3=C(C1CCC45C2CCC(C4)C(C5)(CO)O)C=CO3 | C20H28O3 | 317.2083 | 516.4245 | 2.18384242511868 | [M+H]+ | 317.209;299.197;271.203;69.07;281.229 | 9310008.959 |
| 6-Hydroxy-5a-methyl-3,9-bis(methylene)decahydronaphtho[1,2-b]furan-2(3H)-one | terpenoids | CC12CCC3C(OC(=O)C3=C)C1C(=C)CCC2O | C15H20O3 | 231.1349 | 899.53 | 0.375598107595447 | [M-H2O+H]+ | 231.135;190.109;148.087;189.113;232.156 | 57930088.46 |
| Ixocarpalactone B | terpenoids | CC1C(C)C2(OC1=O)OC1CC3C4CC5OC55C(O)C=CC(=O)C5(C)C4CCC3(C)C1C(C)(O)C2O | C28H38O8 | 503.265 | 441.499 | 1.90017420458578 | [M+H]+ | 59.06;503.342;194.119;105.034;485.319 | 41396914.22 |
| Ganoderiol F | terpenoids | CC(CCC=C(CO)CO)C1CCC2(C)C3=CCC4C(C)(C)C(=O)CCC4(C)C3=CCC12C | C30H46O3 | 455.3495 | 655.063 | 1.07626634567511 | [M+H]+ | 59.061;455.345;58.065;81.07;95.085 | 79636999.88 |
| Maslinic acid | terpenoids | CC1(C)CCC2(CCC3(C)C(=CCC4C5(C)CC(O)C(O)C(C)(C)C5CCC34C)C2C1)C(O)=O | C30H48O4 | 473.3624 | 544.006 | 2.9344868605422 | [M+H]+ | 409.348;473.367;203.178;191.181;189.163 | 22817951.91 |
| Ganoderic acid DM | terpenoids | CC(CC\C=C(/C)C(O)=O)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(=O)C(C)(C)C1CC3=O | C30H44O4 | 469.3294 | 530.892 | 1.21664884768578 | [M+H]+ | 469.339;405.311;201.163;119.085;187.148 | 14780135.43 |
| 1alpha-Hydroxyarbusculin A | terpenoids | CC1(O)CCC(O)C2(C)CCC3C(OC(=O)C3=C)C12 | C15H22O4 | 267.1571 | 140.333 | 0.31622082255731 | [M+H]+ | 267.158;249.145;81.07;69.07;95.085 | 1977709.882 |
| Auxin b | terpenoids | CCC(C)C1CC(C(C)CC)C(=C1)C(O)CC(=O)CC(O)=O | C18H30O4 | 311.2213 | 485.203 | 2.14326442402118 | [M+H]+ | 293.211;81.07;95.085;275.199;67.054 | 13868164.34 |
| Corosolic acid | terpenoids | CC1CCC2(CCC3(C)C(=CCC4C5(C)CC(O)C(O)C(C)(C)C5CCC34C)C2C1C)C(O)=O | C30H48O4 | 473.3624 | 579.668 | 0.831515477959404 | [M+H]+ | 427.353;205.158;207.173;189.162;473.35 | 27753830.18 |
| Progesterone | terpenoids | CC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C | C21H30O2 | 315.2313 | 951.005 | 1.00705358392143 | [M+H]+ | 315.23;297.218;95.085;50.008;107.086 | 2174740.391 |
| Betulin | terpenoids | CC(=C)C1CCC2(CO)CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC34C)C12 | C30H50O2 | 425.3787 | 757.99 | 1.66337338570308 | [M+H-H2O]+ | 425.383;191.178;81.07;95.085;109.101 | 229099656.8 |
| Ergosterol peroxide | terpenoids | CC(C)C(C)\C=C\C(C)C1CCC2C1(C)CCC1C3(C)CCC(O)CC33OOC21C=C3 | C28H44O3 | 429.3351 | 836.977 | 0.164723564089272 | [M+H]+ | 167.07;429.314;69.069;83.084;81.07 | 2844665.32 |
| gamma-Eudesmol rhamnoside | terpenoids | CC1OC(OC(C)(C)C2CCC3(C)CCCC(C)=C3C2)C(O)C(O)C1O | C21H36O5 | 369.2632 | 523.916 | 0.637697307494091 | [M+H]+ | 81.07;351.257;277.216;57.034;95.085 | 62162160.86 |
| Sebiferic acid | terpenoids | CC(=C)C1CCC2(C)C1CCC1(C)C2CCC2C(C)(CCC(O)=O)C(CCC12C)C(C)=C | C30H48O2 | 441.372 | 776.523 | 2.18870667289833 | [M+H]+ | 441.378;81.07;423.363;95.085;109.101 | 73988417.64 |
| Bufalin | terpenoids | CC12CCC(CC1CCC3C2CCC4(C3(CCC4C5=COC(=O)C=C5)O)C)O | C24H34O4 | 387.2496 | 710.197 | 0.974617889887377 | [M+H] | 387.254;388.254;108.044;81.07;369.237 | 28993634.95 |
| Panaxadiol | terpenoids | CC12CCC(C1C(O)CC1C3(C)CCC(O)C(C)(C)C3CCC21C)C1(C)CCCC(C)(C)O1 | C30H52O3 | 461.3986 | 676.358 | 0.792914458187282 | [M+H]+ | 81.07;109.101;95.085;107.086;127.111 | 14796755.2 |
| (10E,12E)-9-hydroxyoctadeca-10,12-dienoic acid |  | CCCCC\C=C\C=C\C(O)CCCCCCCC(O)=O | C18H32O3 | 279.2317 | 705.949 | 2.35177638815997 | [M-H2O+H]+ | 81.071;280.233;67.055;95.085;82.074 | 5292355769 |
| Azelaic acid |  | C(CCCC(=O)O)CCCC(=O)O | C9H16O4 | 189.1119 | 410.472 | 0.608145743976095 | [M+H] | 189.163;133.1;119.085;105.07;147.117 | 11812022.58 |
| LYSINE |  | O=C(O)C(N)CCCCN | C6H14N2O2 | 147.1166 | 362.693 | 4.3660330461924 | [M+H]+ | 147.116;105.07;119.085;91.054;123.964 | 8040295.005 |
| monoolein |  | O=C(OCC(O)CO)CCCCCCCC=CCCCCCCCC | C21H40O4 | 379.2816 | 755.165 | 1.06226291507151 | [M+Na]+ | 379.282;81.07;95.085;67.055;380.284 | 3339489.504 |
| (-)-12-Hydroxyjasmonic acid |  | O=C(O)CC1CCC(=O)C1(CC=CCCO) | C12H18O4 | 227.1275 | 79.8588 | 2.05619226122285 | [M+H]+ | 85.064;209.117;191.106;149.097;227.125 | 8934802.332 |
| Ginkgolic acid (C13:0) |  | CCCCCCCCCCCCCC1=C(C(=CC=C1)O)C(=O)O | C20H32O3 | 321.24 | 670.435 | 0.00609342548214592 | [M+H] | 321.242;81.07;95.085;322.239;67.054 | 15075636.02 |
| Carveol |  | CC1=CCC(CC1O)C(=C)C | C10H16O | 135.1165 | 112.329 | 3.34229508774432 | [M+H-H2O]- | 135.044;107.086;93.07;79.054;136.075 | 5736440.484 |
| cuminyl alcohol |  | OCC1=CC=C(C=C1)C(C)C | C10H14O | 133.1008 | 135.447 | 1.15941665281191 | [M+H-H2O]- | 133.1;105.07;91.055;134.105;131.086 | 26862542.46 |
| [12]-Gingerdione |  | CCCCCCCCCCCC(=O)CC(=O)CCC1=CC(OC)=C(O)C=C1 | C23H36O4 | 377.2655 | 709.0695 | 1.2057194724488 | [M+H]+ | 377.268;378.272;335.232;81.07;83.086 | 57563086.35 |
| 18-Nor-4(19),8,11,13-abietatetraene |  | CC(C)C1=CC2=C(C=C1)C1(C)CCCC(=C)C1CC2 | C19H26 | 255.2104 | 925.112 | 1.64111022940861 | [M+H]+ | 255.211;256.263;83.086;69.069;145.1 | 1672040.183 |
| 9-Hydroxycalabaxanthone |  | COC1=C(O)C=C2OC3=C(C(O)=C4C=CC(C)(C)OC4=C3)C(=O)C2=C1CC=C(C)C | C24H24O6 | 409.1618 | 397.301 | 0.605473140221155 | [M+H]+ | 409.159;410.164;289.109;119.085;81.071 | 79681625.26 |
| Asperhenamate\_120258 |  | C1=CC=C(C=C1)CC(COC(=O)C(CC2=CC=CC=C2)NC(=O)C3=CC=CC=C3)NC(=O)C4=CC=CC=C4 | C32H30N2O4 | 529.2081 | 559.054 | 1.62910773719032 | [M+Na]+ | 529.204;292.093;238.125;530.216;117.07 | 4725341.701 |
| Edulan I |  | CC1CC=C2C(C)(C)CC=CC2(C)O1 | C13H20O | 193.1584 | 227.679 | 1.86663445466703 | [M+H]+ | 193.158;194.118;135.116;133.101;175.149 | 9089636.067 |
| Glyceryl linolenate |  | O=C(OCC(O)CO)CCCCCCCC=CCC=CCC=CCC | C21H36O4 | 375.2501 | 646.102 | 0.186242462254756 | [M+Na]+ | 375.252;376.258;249.111;122.232;165.692 | 462069337.6 |
| p-Cymene |  | CC(C)C1=CC=C(C)C=C1 | C10H14 | 135.1166 | 746.5655 | 3.22890083177404 | [M+H]+ | 135.116;136.087;107.086;93.07;79.055 | 34109019.12 |
| Phthalic anhydride |  | O=c(o1)c(c2)c(ccc2)c(=O)1 | C8H4O3 | 149.0229 | 318.318 | 0.402249391818714 | [M+H]+ | 149.022;121.028;93.07;107.086;65.038 | 5635008.57 |
| Rishitin |  | CC1C(O)C(O)CC2=C1CC(CC2)C(C)=C | C14H22O2 | 223.1691 | 214.8 | 0.481241473123336 | [M+H]+ | 223.171;224.13;149.096;205.158;187.148 | 3928722.871 |
| Santene |  | CC1=C(C)C2CCC1C2 | C9H14 | 123.1167 | 563.565 | 2.4031332960203 | [M+H]+ | 81.07;124.086;123.081;67.055;42.034 | 24189766.02 |
| 3-Methylbenzaldehyde |  | CC1=CC(C=O)=CC=C1 | C8H8O | 121.0646 | 397.301 | 4.72402790488017 | [M+H]+ | 93.07;121.065;122.07;91.054;95.049 | 11402855.5 |
| Panaquinquecol 2 |  | CCCCCCCC1OC1C(O)C#CC#CC(O)C=C | C17H24O3 | 277.1771 | 307.482 | 0.522350008598513 | [M+H]+ | 277.178;95.085;107.086;278.182;81.07 | 8404671.164 |
| 1,4,5-Naphthalenetriol |  | OC1=CC=CC2=C(O)C=CC(O)=C12 | C10H8O3 | 177.0544 | 332.055 | 2.34016499142556 | [M+H]+ | 145.028;177.054;117.034;186.056;149.059 | 26263197.38 |
| Hydroxytyrosol 1-O-glucoside |  | OCC1OC(OCCC2=CC(O)=C(O)C=C2)C(O)C(O)C1O | C14H20O8 | 317.1197 | 50.5909 | 0.867914397894323 | [M+H]+ | 317.12;245.099;299.234;318.126;281.225 | 4617845.431 |
| Diethyltoluamide |  | CCN(CC)C(=O)c1cccc(c1)C | C12H17NO | 192.1382 | 315.338 | 1.14212601027451 | [M+H]+ | 119.049;192.137;72.045;100.075;193.158 | 9092351.818 |
| alpha-Methylstyrene |  | CC(=C)C1=CC=CC=C1 | C9H10 | 119.0852 | 460.677 | 1.83606728429565 | [M+H]+ | 119.085;91.054;59.06;120.089;44.049 | 44222098.36 |
| alpha-Phellandrene |  | CC(C)C1CC=C(C)C=C1 | C10H16 | 137.1321 | 705.949 | 1.03242226335073 | [M+H]+ | 81.071;95.085;67.055;137.133;138.102 | 84399982.24 |
| 2-Phenylethanol |  | OCCC1=CC=CC=C1 | C8H10O | 105.0696 | 397.301 | 4.119243559868 | [M+H-H2O]+ | 105.07;79.054;106.073;103.054;95.049 | 92253192.62 |
| p-Mentha-1,3,5,8-tetraene |  | CC(=C)C1=CC=C(C)C=C1 | C10H12 | 133.1009 | 112.329 | 1.05333236168092 | [M+H]+ | 133.1;105.07;134.06;91.055;41.529 | 4791539.829 |
| 2,4-Dimethylbenzaldehyde |  | CC1=CC(C)=C(C=O)C=C1 | C9H10O | 135.0802 | 79.252 | 1.58458503720967 | [M+H]+ | 91.054;135.08;107.085;136.075;93.07 | 4423686.84 |
| p-Xylene |  | CC1=CC=C(C)C=C1 | C8H10 | 107.0853 | 512.807 | 2.42047946600099 | [M+H]+ | 107.086;79.055;91.055;108.056;105.07 | 9685724.258 |
| Linolenic acid ethyl ester |  | CCC=CCC=CCC=CCCCCCCCC(=O)OCC | C20H34O2 | 307.263 | 790.362 | 0.089727336298258 | [M+H] | 81.071;95.085;67.055;307.267;109.102 | 11424880.25 |
| Melilotocarpan C |  | COC1=C(O)C2=C(C=C1)C1OC3=C(C=CC(OC)=C3OC)C1CO2 | C18H18O6 | 331.1142 | 287.074 | 2.54716215308105 | [M+H]+ | 331.114;313.217;295.204;93.07;81.07 | 2962619.581 |
| 2',4'-Dimethylacetophenone |  | CC(=O)C1=C(C)C=C(C)C=C1 | C10H12O | 149.0956 | 163.049 | 2.6861899233655 | [M+H]+ | 149.097;93.07;121.101;107.086;150.102 | 6811403.216 |
| Myristicin |  | COC1=CC(CC=C)=CC2=C1OCO2 | C11H12O3 | 193.0858 | 202.459 | 4.10321147226018 | [M+H]+ | 193.087;69.034;105.07;194.116;91.054 | 1892281.501 |
| (4Z,7Z)-5,9,9-Trimethyl-11-oxabicyclo[8.2.1]trideca-1(13),4,7-triene-6,12-dione |  | C\C1=C\CC\C2=C/C(OC2=O)C(C)(C)\C=C/C1=O | C15H18O3 | 247.1322 | 384.338 | 0.801285524771 | [M+H]+ | 247.135;121.029;201.163;135.044;107.048 | 7076314.152 |
| 3-Ethylphenol |  | CCC1=CC(O)=CC=C1 | C8H10O | 123.0803 | 344.343 | 2.13708862428074 | [M+H]+ | 123.081;43.018;81.071;95.085;124.039 | 9371520.083 |
| 1-(2-Furanyl)-1-propanone |  | CCC(=O)C1=CC=CO1 | C7H8O2 | 125.0592 | 13.07352 | 1.88338010377055 | [M+H]+ | 125.06;43.018;79.054;97.065;81.07 | 14817084.82 |
| p-Mentha-1,3,8-triene |  | CC(=C)C1=CC=C(C)CC1 | C10H14 | 135.1166 | 302.756 | 2.84135217503449 | [M+H]+ | 135.116;107.086;93.07;79.054;136.022 | 8069189.597 |
| (R)-Carvotanacetone |  | CC(C)C1CC=C(C)C(=O)C1 | C10H16O | 153.1271 | 260.588 | 0.55993097874086 | [M+H]+ | 153.126;97.065;83.049;55.054;43.018 | 44185544.77 |
| 2'-Hydroxyacetophenone |  | CC(=O)C1=CC=CC=C1O | C8H8O2 | 137.0593 | 90.9787 | 2.53949076745433 | [M+H]+ | 137.06;43.018;81.07;95.085;114.971 | 14135963.43 |
| Paraldehyde |  | CC1OC(C)OC(C)O1 | C6H12O3 | 133.0856 | 36.1131 | 2.84094631401708 | [M+H]+ | 45.033;89.06;133.065;42.034;105.07 | 5367168.14 |
| 2,3-dihydroxypropyl hexadecanoate |  | CCCCCCCCCCCCCCCC(=O)OCC(O)CO | C19H38O4 | 331.2838 | 745.1785 | 0.662063348116115 | [M+H]+ | 57.07;71.086;313.277;95.085;239.236 | 48299341.87 |
| Gingerol |  | CCCCCC(O)CC(=O)CCC1=CC=C(O)C(OC)=C1 | C17H26O4 | 295.1896 | 174.125 | 5.47804952654917 | [M+H]+ | 295.186;277.216;59.049;83.086;67.055 | 699793.2442 |
| Cuminaldehyde |  | [H]C(=O)C1=CC=C(C=C1)C(C)C | C10H12O | 149.0957 | 542.882 | 1.78265151173754 | [M+H]+ | 149.097;107.049;79.054;93.07;43.054 | 30155613.52 |
| Diisobutyl phthalate |  | CC(C)COC(=O)C1=CC=CC=C1C(=O)OCC(C)C | C16H22O4 | 279.1564 | 242.976 | 2.32115595895476 | [M+H]+ | 279.155;81.07;95.085;67.055;149.022 | 1444028.272 |
| (R)-Campholenic aldehyde |  | CC1=CCC(CC=O)C1(C)C | C10H16O | 153.127 | 1.17496 | 0.0592286431935431 | [M+H]+ | 153.126;43.018;97.065;107.086;93.07 | 30555951.79 |
| Cuscohygrine |  | CN1CCCC1CC(=O)CC1CCCN1C | C13H24N2O | 225.1956 | 349.555 | 1.94715095202095 | [M+H]+ | 225.198;100.112;83.085;61.04;143.118 | 4120330.192 |
| Falcarindiol |  | CCCCCCC\C=C/C(O)C#CC#CC(O)C=C | C17H24O2 | 261.1844 | 395.861 | 2.30243696452488 | [M+H]+ | 261.188;81.07;79.054;133.102;105.07 | 6238073.579 |
| Ethylbenzene |  | CCC1=CC=CC=C1 | C8H10 | 107.0853 | 542.882 | 2.73431693869087 | [M+H]+ | 107.086;79.054;91.054;105.07;42.034 | 36572008.3 |
| Chavicol |  | OC1=CC=C(CC=C)C=C1 | C9H10O | 135.0803 | 460.677 | 1.97932523526286 | [M+H]+ | 107.086;135.08;79.055;93.07;91.055 | 7376472.347 |
| 2-Methylbenzaldehyde |  | CC1=CC=CC=C1C=O | C8H8O | 121.0646 | 648.522 | 3.09304340813756 | [M+H]+ | 121.065;93.07;95.049;103.054;105.044 | 134911211.4 |
| 3,4-Dimethylbenzoic acid |  | CC1=C(C)C=C(C=C1)C(O)=O | C9H10O2 | 151.0751 | 303.926 | 0.340888025477234 | [M+H]+ | 151.075;57.034;123.081;105.07;95.085 | 6702352.521 |
| 2-Propylphenol |  | CCCC1=CC=CC=C1O | C9H12O | 137.0958 | 313.55 | 1.11825052119603 | [M+H]+ | 81.07;137.097;95.085;67.055;109.1 | 2862367.398 |
| Dihydroactinidiolide |  | CC12CCCC(C)(C)C1=CC(=O)O2 | C11H16O2 | 181.1218 | 302.756 | 1.2335432229546 | [M+H]+ | 181.123;135.116;163.111;107.086;121.101 | 337600988.4 |
| 2-Pentylfuran |  | CCCCCC1=CC=CO1 | C9H14O | 139.1117 | 166.084 | 2.35718971717775 | [M+H]+ | 139.112;69.069;81.071;121.101;43.018 | 22427255.18 |
| 2,4,6-Trimethylphenol |  | CC1=CC(C)=C(O)C(C)=C1 | C9H12O | 137.0959 | 224.067 | 0.818182075107642 | [M+H]+ | 137.097;81.071;95.085;122.072;109.1 | 7523808.243 |
| Curzerenone |  | CC(=C)C1C(=O)C2=C(CC1(C)C=C)OC=C2C | C15H18O2 | 231.1378 | 630.739 | 0.766733210783639 | [M+H]+ | 231.139;175.074;69.07;161.059;129.07 | 6848415.882 |
| Kojic Acid |  | C1=C(OC=C(C1=O)O)CO | C6H6O4 | 143.0337 | 42.7307 | 1.86057019401115 | [M+H]+ | 143.034;125.023;98.984;69.069;43.018 | 15281615.09 |
| 2-Cyclohexen-1-one, 4-hydroxy-4-(3-hydroxybutyl)-3,5,5-trimethyl- |  | CC(O)CCC1(O)\C(=C/C(=O)CC1(C)C)C | C13H22O3 | 209.1533 | 229.228 | 1.39580712936032 | [M-H2O+H]+ | 191.143;151.112;209.153;109.102;107.086 | 8983735.408 |
| Panaquinquecol 1 |  | CCCCCCCC(OC)C(O)CC#CC#CC(O)C=C | C18H28O3 | 293.2107 | 490.478 | 0.968357203373488 | [M+H]+ | 293.211;275.199;294.214;81.071;151.112 | 66500279.32 |
| Acetylpanaxydol |  | CCCCCCCC1OC1CC#CC#CC(OC(C)=O)C=C | C19H26O3 | 303.1943 | 0.570827 | 1.11511901610147 | [M+H]+ | 303.195;285.187;267.173;81.071;245.154 | 2603234.47 |
| Furfuryl acetate |  | CC(=O)OCC1=CC=CO1 | C7H8O3 | 141.0545 | 51.2275 | 3.66777787549609 | [M+H]+ | 141.054;126.031;123.081;113.964;95.085 | 17835945.45 |
| Pterosin N |  | CC1=CC2=C(C(=O)C(C)(O)C2)C(C)=C1CCO | C14H18O3 | 235.1321 | 180.26 | 0.223779397221878 | [M+H]+ | 235.131;217.124;81.07;133.102;119.085 | 3053107.693 |
| 2-Methoxy-4-methylphenol |  | COC1=C(O)C=CC(C)=C1 | C8H10O2 | 139.0748 | 23.8688 | 1.40122672697035 | [M+H]+ | 139.076;43.018;97.065;111.044;93.07 | 35219854.75 |
| Methylisoeugenol |  | COC1=C(OC)C=C(\C=C/C)C=C1 | C11H14O2 | 179.1067 | 112.329 | 3.64508230481206 | [M+H]+ | 179.106;133.1;161.096;107.086;105.07 | 35637735.57 |
| [10]-Paradol |  | CCCCCCCCCCCC(=O)CCC1=CC(OC)=C(O)C=C1 | C21H34O3 | 335.2582 | 688.717 | 0.623627312799242 | [M+H]+ | 335.255;81.07;67.054;95.085;109.101 | 36376804.48 |
| (S)-Bilobanone |  | CC(C)CC1=CC(=CO1)C1CC=C(C)C(=O)C1 | C15H20O2 | 233.1533 | 478.663 | 1.17748322238034 | [M+H]+ | 233.153;119.085;215.144;187.148;105.07 | 5864798.018 |
| Acetylpterosin C |  | CC1C(O)C2=C(C1=O)C(C)=C(CCOC(C)=O)C(C)=C2 | C16H20O4 | 277.1409 | 265.506 | 0.228346626652567 | [M+H]+ | 277.139;81.069;125.097;93.07;95.085 | 2106870.797 |
| 2-Phenylethyl octanoate |  | CCCCCCCC(=O)OCCC1=CC=CC=C1 | C16H24O2 | 249.1845 | 314.742 | 1.99215710797542 | [M+H]+ | 249.186;121.101;79.054;93.069;107.086 | 4167191.472 |
| 4-Butyl-gamma-butyrolactone |  | CCCCC1CCC(=O)O1 | C8H14O2 | 143.1062 | 284.121 | 1.4590835768318 | [M+H]+ | 143.034;125.023;71.048;43.018;69.07 | 17192606.54 |
| (E)-3-(2-Hydroxyphenyl)-2-propenal |  | OC1=CC=CC=C1\C=C\C=O | C9H8O2 | 149.0595 | 120.808 | 3.4498546077793 | [M+H]+ | 149.059;131.048;55.018;103.053;121.064 | 10702127.96 |
| Benzenepropanamide, N-[2-(acetyloxy)-1-(phenylmethyl)ethyl]-alpha-(benzoylamino)- |  | CC(=O)OCC(CC1=CC=CC=C1)NC(=O)C(CC2=CC=CC=C2)NC(=O)C3=CC=CC=C3 | C27H28N2O4 | 445.2113 | 461.879 | 0.765570176942946 | [M+H]+ | 105.034;194.119;224.106;117.07;134.096 | 577890041.5 |
| 2-(3,7-Dimethyl-2,6-octadienyl)-4-hydroxy-6-methoxyacetophenone |  | COC1=C(C(C)=O)C(C\C=C(/C)CCC=C(C)C)=CC(O)=C1 | C19H26O3 | 303.1949 | 31.5571 | 0.1868568102866 | [M+H]+ | 303.195;285.187;267.173;159.08;109.065 | 2959534.138 |
| Ginsenoyne D |  | CCCCCCCC1OC1CC#CC#CC(O)CC | C17H26O2 | 263.2001 | 497.653 | 0.342742260930646 | [M+H]+ | 263.238;81.07;93.069;121.101;95.085 | 5152510.96 |
| Petroselinic acid |  | CCCCCCCCCCCC=CCCCCC(O)=O | C18H34O2 | 283.2635 | 799.471 | 1.6508024984036 | [M+H]+ | 57.07;69.069;71.086;81.07;83.085 | 133164422.6 |
| 1,2-Dehydro-alpha-cyperone |  | CC(=C)C1CCC2(C)C=CC(=O)C(C)=C2C1 | C15H20O | 217.158 | 367.5965 | 0.0310645143841245 | [M+H]+ | 217.158;81.07;199.147;119.085;105.07 | 15629483.12 |
| 3,4-Dihydrocadalene |  | CC(C)C1CC=C(C)C2=C1C=C(C)C=C2 | C15H20 | 201.1637 | 284.121 | 1.43098223295024 | [M+H]+ | 201.129;145.102;77.006;159.116;95.085 | 17587733.79 |
| alpha-Irone |  | CC1CC=C(C)C(\C=C\C(C)=O)C1(C)C | C14H22O | 207.1738 | 424.5 | 1.00781036919676 | [M+H]+ | 207.173;189.163;81.071;95.085;67.055 | 14830016.71 |
| 2-Methoxybenzaldehyde |  | COC1=CC=CC=C1C=O | C8H8O2 | 137.0595 | 186.966 | 3.6532097695585 | [M+H]+ | 137.06;109.065;81.071;95.085;94.041 | 4589342.066 |
| 2,6,6-Trimethyl-2-cyclohexene-1,4-dione |  | CC1=CC(=O)CC(C)(C)C1=O | C9H12O2 | 153.0907 | 79.252 | 2.23189020655623 | [M+H]+ | 153.09;43.018;135.08;93.07;107.086 | 7923593.451 |
| Moracin I |  | COC1=CC(O)=CC(C2=CC3=C(O2)C=C(O)C=C3)=C1CC=C(C)C | C20H20O4 | 325.1429 | 581.393 | 0.174919662826091 | [M+H]+ | 325.141;297.151;267.1;199.076;293.115 | 56955332.45 |
| beta-Ionone |  | CC(=O)\C=C\C1=C(C)CCCC1(C)C | C13H20O | 193.1584 | 279.333 | 2.26281861464209 | [M+H]+ | 135.116;193.158;175.149;133.1;194.118 | 4154307.805 |
| Panaxytriol |  | CCCCCCCC(O)C(O)CC#CC#CC(O)C=C | C17H26O3 | 279.1953 | 422.051 | 1.03749722762652 | [M+H]+ | 279.194;81.07;123.08;67.054;95.085 | 11487315.63 |
| (S)-gamma-Calacorene |  | CC(C)C1=CCC(C)C2=C1C=C(C)C=C2 | C15H20 | 201.1636 | 528.252 | 2.98999994313714 | [M+H]+ | 201.163;119.085;145.102;131.086;159.116 | 5874614.533 |
| 1-Nonen-3-ol |  | CCCCCCC(O)C=C | C9H18O | 143.1427 | 26.8005 | 2.04353328318185 | [M+H]+ | 69.069;57.07;55.054;43.018;83.084 | 3857287.402 |
| 2-Methyl-3-heptanone |  | CCCCC(=O)C(C)C | C8H16O | 129.1271 | 9.87293 | 0.891092904354319 | [M+H]+ | 69.069;55.054;59.049;83.085;43.018 | 6654849.311 |
| Moracin N |  | CC(C)=CCC1=CC2=C(OC(=C2)C2=CC(O)=CC(O)=C2)C=C1O | C19H18O4 | 311.1277 | 533.099 | 2.1658841292988 | [M+H]+ | 311.131;199.076;283.134;293.211;111.044 | 30649957.02 |
| 2,3-Pentanedione |  | CCC(=O)C(C)=O | C5H8O2 | 101.0594 | 25.0428 | 4.10415452112092 | [M+H]+ | 55.054;59.049;57.07;101.059;45.033 | 18859974.05 |
| 1,7-Dihydroxy-3-methoxy-2-prenylxanthone |  | COC1=CC2=C(C(O)=C1CC=C(C)C)C(=O)C1=C(O2)C=CC(O)=C1 | C19H18O5 | 327.1229 | 563.565 | 2.79701788259437 | [M+H]+ | 327.122;285.111;215.071;257.116;81.07 | 16067563.86 |
| Cyclo(leucylprolyl) |  | O=C1NC(C(=O)N2CCCC12)CC(C)C | C11H18N2O2 | 211.1438 | 97.6355 | 3.90891646326419 | [M+H]+ | 211.144;86.096;70.066;98.06;179.071 | 4309416.068 |
| (R)-2,5,11-Bisabolatriene |  | CC(CCCC(C)=C)C1=CCC(C)=CC1 | C15H24 | 205.1946 | 28.5588 | 2.83624257719343 | [M+H]+ | 205.196;149.131;121.101;107.086;135.118 | 2727940.41 |
| (R)-Pterosin B |  | CC1CC2=C(C1=O)C(C)=C(CCO)C(C)=C2 | C14H18O2 | 219.1376 | 200.279 | 1.74683993962627 | [M+H]+ | 219.139;175.076;159.116;173.132;131.086 | 3570399.353 |
| 8-Nonen-2-one |  | CC(=O)CCCCCC=C | C9H16O | 141.127 | 242.976 | 0.0931678433544574 | [M+H]+ | 141.127;71.085;99.08;112.087;81.071 | 10296110.34 |
| Isophorone |  | CC1=CC(=O)CC(C)(C)C1 | C9H14O | 139.1116 | 353.782 | 2.74414945902229 | [M+H]+ | 139.112;69.07;81.071;121.101;43.018 | 19217893.62 |
| 1-Heptadecene-4,6-diyne-3,9-diol |  | CCCCCCCCC(O)CC#CC#CC(O)C=C | C17H26O2 | 263.2004 | 543.438 | 1.51068854612215 | [M+H]+ | 81.07;263.202;67.054;133.102;217.196 | 6917950.72 |
| Valerophenone |  | CCCCC(=O)C1=CC=CC=C1 | C11H14O | 163.1115 | 147.66 | 3.25407724696807 | [M+H]+ | 163.111;139.982;145.102;121.101;93.07 | 10985452.52 |
| 2-Hexyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan |  | CCCCCCC1=CC=C(CCC2=CC(OC)=C(O)C=C2)O1 | C19H26O3 | 303.1943 | 560.151 | 2.20530577525097 | [M+H]+ | 303.182;275.199;177.09;57.07;81.07 | 4630457.391 |
| dihydrodamascenone |  | CC(=O)CCC1=C(C)C=CCC1(C)C | C13H20O | 193.1584 | 529.734 | 2.28797064506732 | [M+H]+ | 193.158;109.065;175.149;135.116;133.1 | 7425310.026 |
| Hypogeic acid |  | CCCCCCCC\C=C/CCCCCC(O)=O | C16H30O2 | 255.2316 | 579.126 | 1.50414942657815 | [M+H]+ | 69.069;81.07;57.07;83.084;255.211 | 5434417.222 |
| Citronellyl formate |  | CC(CCOC=O)CCC=C(C)C | C11H20O2 | 185.1533 | 479.245 | 1.79346720520655 | [M+H]+ | 69.069;185.154;157.123;117.98;139.111 | 3241523.269 |
| Civetone |  | O=C1CCCCCCC\C=C\CCCCCCC1 | C17H30O | 251.2362 | 631.895 | 3.07624069110645 | [M+H]+ | 251.234;69.07;83.086;153.127;55.018 | 42736235.42 |
| 4-Ethyl-2-methoxyphenol |  | CCC1=CC(OC)=C(O)C=C1 | C9H12O2 | 153.0908 | 589.962 | 1.1750310102127 | [M+H]+ | 125.097;153.113;93.069;79.054;107.086 | 24628021.5 |
| 7-methyl-3-methylidene-6-(3-oxobutyl)-4,7,8,8a-tetrahydro-3aH-cyclohepta[b]furan-2-one |  | CC1CC2OC(=O)C(=C)C2CC=C1CCC(C)=O | C15H20O3 | 266.1744 | 372.528 | 2.39793681431543 | [M+NH4]+ | 189.091;185.133;231.139;143.085;145.102 | 3203214 |
| L-2,3-DIAMINOPROPIONIC ACID |  | C(C(C(=O)O)N)N | C3H8N2O2 | 105.0696 | 4.222592 | 3.77047121645339 | [M+H]+ | 105.07;91.055;106.078;79.055;103.054 | 96466277.06 |
| Methoxyeugenol |  | COC1=CC(CC=C)=CC(OC)=C1O | C11H14O3 | 195.1012 | 142.182 | 0.954372418915234 | [M+H]+ | 195.1;177.091;149.096;135.08;121.101 | 19922065.09 |
| Methylgingerol |  | CCCCCC(O)CC(=O)CCC1=CC=C(OC)C(OC)=C1 | C18H28O4 | 309.2061 | 460.115 | 0.231060233212951 | [M+H]+ | 291.196;70.04;309.203;107.049;57.07 | 50778377.21 |
| Theaspirone A |  | CC1CCC2(O1)C(C)=CC(=O)CC2(C)C | C13H20O2 | 209.1533 | 145.831 | 1.31201929679783 | [M+H]+ | 209.153;55.018;177.054;191.143;99.08 | 13002726.38 |

**Table S2** 79 compounds identified in PVSO under positive (ESI-) ion mode by UPLC-MS/MS.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **NameEN** | **Class** | **SMILES** | **Formula** | **mzmed** | **rtmed** | **ppm** | **ms2Adduct** | **MS2** | **Area** |
| Methyl hexadecanoate | Aliphatic acyl | CCCCCCCCCCCCCCCC(=O)OC | C17H34O2 | 315.2555 | 650.056 | 1.67617885608297 | [M+HCOO] | 315.257;316.26;297.244;313.237;59.014 | 3309145.33 |
| Sebacic acid | Aliphatic acyl | OC(=O)CCCCCCCCC(O)=O | C10H18O4 | 201.1136 | 211.646 | 1.8595400142653 | [M-H]- | 201.115;139.113;183.102;57.035;201.802 | 20533374.3 |
| Azelaic acid | Aliphatic acyl | O=C(O)CCCCCCCC(=O)O | C9H16O4 | 187.0981 | 152.445 | 0.50016142969303 | [M-H]- | 125.097;187.099;97.066;57.035;169.088 | 299364603 |
| Ethyl myristate | Aliphatic acyl | O=C(OCC)CCCCCCCCCCCCC | C16H32O2 | 255.2332 | 751.266 | 3.08698643695328 | [M-H]- | 255.235;82.041;228.089;65.014;186.077 | 5646923.72 |
| Nicotinic acid | alkaloid | C1=CC(=CN=C1)C(=O)O | C6H5NO2 | 122.0253 | 39.11175 | 2.54228455084862 | [M-H] | 122.025;94.03;123.01;95.014;41.999 | 3075213.96 |
| Dihydrocapsaicin | alkaloid | CC(C)CCCCCCC(=O)NCc(c1)cc(OC)c(O)c1 | C18H29NO3 | 306.2078 | 528.825 | 0.757737328430935 | [M-H]- | 306.208;288.2;136.113;262.22;307.215 | 7728402.46 |
| Diethyl-phthalate | Aromaticity | CCOC(=O)C1=CC=CC=C1C(=O)OCC | C12H14O4 | 221.0828 | 318.028 | 3.68130561914171 | [M-H]- | 71.05;221.084;69.036;121.029;177.093 | 5476845.92 |
| 3-hydroxybenzoic acid | Aromaticity | O=C(O)c1cccc(O)c1 | C7H6O3 | 137.0249 | 51.5969 | 0.666332346939506 | [M-H]- | 137.025;93.035;138.029;136.018;109.031 | 9622955.37 |
| Methyl eugenol | Aromaticity | COC1=C(C=C(C=C1)CC=C)OC | C11H14O2 | 177.0562 | 139.089 | 1.15112965040675 | [M-H] | 162.033;177.057;134.038;163.036;59.014 | 18516938.1 |
| PHENYLACETIC ACID | Aromaticity | C1=CC=C(C=C1)CC(=O)O | C8H8O2 | 135.0456 | 90.7609 | 2.61864389201041 | [M-H]- | 135.046;93.035;120.022;92.027;136.051 | 9246314.12 |
| Linoelaidic acid | Fatty acids | CCCCC/C=C/C/C=C/CCCCCCCC(=O)O | C18H32O2 | 279.2338 | 772.563 | 0.78199525383374 | [M-H]- | 279.233;280.238;106.041;213.089;107.037 | 20669637.7 |
| a-Linolenic acid | Fatty acids | OC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC | C18H30O2 | 277.2179 | 536.593 | 0.522908861752971 | [M-H]- | 277.216;278.222;59.014;52.747;134.038 | 3630848.32 |
| 9E, 11E-Linoleic acid | Fatty acids | CCCCCC/C=C/C=C/CCCCCCCC(=O)O | C18H32O2 | 279.2337 | 749.288 | 1.12297285122293 | [M-H]- | 279.233;280.239;59.014;52.085;261.223 | 397146039 |
| Palmitic acid | Fatty acids | OC(=O)CCCCCCCCCCCCCCC | C16H32O2 | 255.2333 | 773.476 | 1.11895394961834 | [M-H]- | 255.235;256.237;82.042;65.014;106.041 | 39138770.3 |
| Stearic acid | Fatty acids | CCCCCCCCCCCCCCCCCC(=O)O | C18H36O2 | 283.2645 | 804.282 | 1.74863892870369 | [M-H]- | 283.265;284.268;65.014;106.041;66.009 | 3855530.63 |
| Trans-Vaccenic acid | Fatty acids | CCCCCC/C=C/CCCCCCCCCC(=O)O | C18H34O2 | 281.2488 | 778.061 | 0.79567115648759 | [M-H]- | 281.25;282.255;106.041;94.936;82.041 | 110358308 |
| (+/-)-Jasmonic acid | Fatty acids | CCC=CCC1C(CCC1=O)CC(=O)O | C12H18O3 | 209.1186 | 410.67 | 1.90719029191788 | [M-H]- | 209.12;83.051;163.113;210.122;165.13 | 21238945.3 |
| Pentadecanoic acid | Fatty acids | CCCCCCCCCCCCCCC(=O)O | C15H30O2 | 241.2179 | 13.2663 | 0.554136515715423 | [M-H]- | 241.216;59.014;57.035;52.432;50.799 | 837337.459 |
| Oleic acid | Fatty acids | O=C(O)CCCCCCCC=CCCCCCCCC | C18H34O2 | 281.2489 | 692.357 | 0.208715128952212 | [M-H]- | 281.25;94.936;282.255;197.041;96.961 | 2705441.84 |
| 12,13-EODE | Fatty acids | CCCCCC(O1)C(CC=CCCCCCCCC(O)=O)1 | C18H32O3 | 295.2287 | 540.949 | 0.883035837269976 | [M-H]- | 295.228;183.141;277.216;223.17;296.23 | 151179610 |
| Myristic acid | Fatty acids | CCCCCCCCCCCCCC(=O)O | C14H28O2 | 227.2024 | 14.6045 | 1.81518249578552 | [M-H]- | 227.203;183.14;209.12;59.014;71.014 | 815106.295 |
| Apigenin | flavonoids | C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O | C15H10O5 | 269.0461 | 446.22 | 0.396000404452037 | [M-H]- | 269.044;225.055;270.049;226.064;254.059 | 3230628.56 |
| Naringenin chalcone | flavonoids | C1=CC(=CC=C1C=CC(=O)C2=C(C=C(C=C2O)O)O)O | C15H12O5 | 271.0616 | 254.347 | 1.55931330867481 | [M-H] | 271.064;116.929;253.051;100.934;125.025 | 1824150.99 |
| Pinocembrin | flavonoids | O=C2C3=C(O)C=C(O)C=C3(OC(C1=CC=CC=C1)C2) | C15H12O4 | 255.0669 | 369.203 | 0.515786706523206 | [M-H]- | 255.069;219.845;213.056;151.005;83.014 | 11562826.7 |
| Calycosin | flavonoids | COC1=C(C=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3)O)O | C16H12O5 | 283.0626 | 399.045 | 2.14016176123822 | [M-H] | 283.06;268.04;239.036;211.039;240.042 | 4490740.47 |
| Isoxanthohumol | flavonoids | CC(=CCc1c(cc(c2c1OC(CC2=O)c3ccc(cc3)O)OC)O)C | C21H22O5 | 353.1426 | 734.065 | 1.24858208001153 | [M-H]- | 353.142;116.929;100.934;84.939;99.926 | 11756490.6 |
| Licochalcone B | flavonoids | COC1=C(C=CC(=C1O)O)C=CC(=O)C2=CC=C(C=C2)O | C16H14O5 | 285.0775 | 332.291 | 1.60401653738087 | [M-H] | 285.077;270.054;253.051;241.05;269.044 | 12491337.8 |
| Flavokawain A | flavonoids | COC1=CC=C(C=C1)C=CC(=O)C2=C(C=C(C=C2OC)OC)O | C18H18O5 | 313.1095 | 270.144 | 1.54479234970713 | [M-H] | 313.11;255.03;270.054;314.176;298.086 | 2367467.79 |
| p-Hydroxybenzaldehyde | Phenols | C1=CC(=CC=C1C=O)O | C7H6O2 | 121.0301 | 76.1491 | 0.527003531261998 | [M-H] | 121.029;122.033;120.022;92.027;93.035 | 77230303.3 |
| Salicylic acid | Phenols | C1=CC=C(C(=C1)C(=O)O)O | C7H6O3 | 137.0249 | 156.022 | 0.575668990529016 | [M-H]- | 93.035;137.025;138.019;94.038;108.022 | 82709744 |
| P-Anisic acid | Phenols | O=C(O)C1=CC=C(OC)C=C1 | C8H8O3 | 151.0405 | 58.9744 | 3.21405050458384 | [M-H]- | 151.041;108.022;109.031;136.016;152.045 | 7721441.72 |
| Vanillin | Phenols | COC1=C(C=CC(=C1)C=O)O | C8H8O3 | 151.0405 | 92.5753 | 3.17519860676397 | [M-H] | 136.018;151.041;137.022;108.022;92.027 | 9795824.98 |
| Methyl vanillate | Phenols | COC1=C(C=CC(=C1)C(=O)OC)O | C9H10O4 | 181.051 | 50.2893 | 0.167979227317567 | [M-H] | 166.028;181.052;92.92;136.91;136.018 | 2318581.15 |
| 3,4-Dihydroxyphenylethanol | Phenols | C1=CC(=C(C=C1CCO)O)O | C8H10O3 | 153.0564 | 115.229 | 2.32129242404724 | [M-H] | 109.066;80.027;153.055;81.034;107.051 | 1423129.41 |
| Ethyl 3,4-dihydroxybenzoate | Phenols | CCOC(=O)C1=CC(=C(C=C1)O)O | C9H10O4 | 181.0509 | 163.804 | 0.278104788150846 | [M-H] | 181.052;108.022;153.019;109.031;92.921 | 2211491.84 |
| Ethylparaben | Phenols | CCOC(=O)c1ccc(O)cc1 | C9H10O3 | 165.0563 | 23.1433 | 1.532338021216 | [M-H]- | 165.056;123.046;121.066;137.062;95.051 | 4254560.26 |
| isoimperatorin | phenylpropanoids | O=C1OC=2C=C3OC=CC3=C(OCC=C(C)C)C2C=C1 | C16H14O4 | 269.0831 | 449.695 | 0.3350164513211 | [M-H]- | 269.081;226.064;225.056;254.06;122.002 | 1474991.64 |
| Honokiol | phenylpropanoids | C=CCC1=CC(=C(C=C1)O)C2=CC(=C(C=C2)O)CC=C | C18H18O2 | 265.124 | 522.509 | 0.180349445259273 | [M-H] | 265.124;247.112;266.128;245.099;96.961 | 157936839 |
| columbianetin | phenylpropanoids | O=C1OC2=C(C=C1)C=CC=3OC(CC32)C(O)(C)C | C14H14O4 | 245.0826 | 400.211 | 2.5587839024017 | [M-H]- | 245.081;190.028;246.084;162.033;160.843 | 3713429.79 |
| Cinnamic acid | phenylpropanoids | OC(=O)\C=C/C1=CC=CC=C1 | C9H8O2 | 147.0457 | 120.169 | 1.94918270916707 | [M-H]- | 147.046;41.003;58.959;102.949;148.048 | 36144432.2 |
| (4S,5Z,6S)-4-(2-methoxy-2-oxoethyl)-5-[2-[(E)-3-phenylprop-2-enoyl]oxyethylidene]-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylic acid | phenylpropanoids | O=C1OC=2C=C3OC(CC3=CC2C=C1)C(OC(=O)C(=CC)C)(C)C | C19H20O5 | 327.1252 | 533.057 | 0.727286761895961 | [M-H]- | 327.128;299.128;328.125;281.119;295.101 | 174843472 |
| isoferulic acid | phenylpropanoids | O=C(O)C=CC1=CC=C(OC)C(O)=C1 | C10H10O4 | 193.0508 | 286.989 | 1.010188706542 | [M-H]- | 134.038;193.051;158.846;146.864;193.816 | 1994597.98 |
| Ethyl caffeate | phenylpropanoids | CCOC(=O)C=CC1=CC(=C(C=C1)O)O | C11H12O4 | 207.0667 | 226.992 | 1.62444980820737 | [M-H] | 207.066;134.038;135.046;179.036;161.025 | 29619597 |
| Haematoxylin | phenylpropanoids | OC1=CC=C2C(OCC3(O)CC4=CC(O)=C(O)C=C4C23)=C1O | C16H14O6 | 301.0731 | 264.65 | 0.37493444344221 | [M-H]- | 301.076;164.012;183.141;286.05;151.005 | 2095190.22 |
| 3-(4-Hydroxyphenyl)-1-propanol | phenylpropanoids | OC1=CC=C(C=C1)CCCO | C9H12O2 | 151.077 | 382.791 | 0.1879602940318 | [M-H]- | 151.075;71.014;118.9;59.014;122.038 | 2501598.11 |
| 3,4,5-trimethoxycinnamic acid | phenylpropanoids | O=C(O)C=CC1=CC(OC)=C(OC)C(OC)=C1 | C12H14O5 | 237.0774 | 25.0836 | 1.78049662948529 | [M-H]- | 237.078;193.087;57.035;59.014;123.046 | 1817197.92 |
| Sinapoyl aldehyde | phenylpropanoids | COC1=CC(C=CC=O)=CC(OC)=C1O | C11H12O4 | 207.0667 | 142.116 | 1.68989093550371 | [M-H]- | 192.044;177.02;127.87;125.873;162.983 | 2759181.09 |
| 14-hydroxy-14-(hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0¹,¹⁰.0⁴,⁹]hexadecane-5-carboxylic acid | terpenoids | O=C(O)C1(C)CCCC2(C)C1CCC34CC(CCC32)C(O)(CO)C4 | C20H32O4 | 335.2237 | 299.513 | 0.892141859701098 | [M-H]- | 335.225;336.229;235.17;81.036;317.215 | 11072877.3 |
| 5-[(Z)-5-hydroxy-3-methylpent-3-enyl]-1,4a-dimethyl-6-methylidene-3,4,5,7,8,8a-hexahydro-2H-naphthalene-1-carboxylic acid | terpenoids | O=C(O)C1(C)CCCC2(C)C(C(=C)CCC12)CCC(=CCO)C | C20H32O3 | 319.2283 | 477.708 | 2.23573200626796 | [M-H]- | 319.232;320.233;261.127;275.172;256.291 | 5252861.21 |
| Asiatic Acid | terpenoids | O=C(O)C12CCC(C)C(C)C2C3=CCC4C5(C)CC(O)C(O)C(C)(CO)C5CCC4(C)C3(C)CC1 | C30H48O5 | 487.345 | 457.946 | 0.07767648582763 | [M-H]- | 487.34;488.348;54.15;162.841;469.332 | 5422358.31 |
| beta-Elemonic acid | terpenoids | CC(=CCCC(C1CCC2(C1(CCC3=C2CCC4C3(CCC(=O)C4(C)C)C)C)C)C(=O)O)C | C30H46O3 | 453.3398 | 750.265 | 1.87118259342724 | [M-H] | 453.344;454.342;50.372;100.934;407.34 | 94539742.8 |
| Curcumenol | terpenoids | OC12OC3(CC1=C(C)C)C(C(=C2)C)CCC3C | C15H22O2 | 233.1552 | 542.441 | 0.912748874152902 | [M-H]- | 233.156;234.16;143.934;189.094;127.289 | 10041818.2 |
| Isokobusone | terpenoids | CC1(C)CC2C1CCC(=C)C(O)CCC2=O | C14H22O2 | 221.1549 | 401.444 | 0.231335121643502 | [M-H]- | 221.155;222.157;59.014;220.148;164.085 | 9013999.83 |
| Oleanolic acid | terpenoids | CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)C)C(=O)O)C | C30H48O3 | 455.3546 | 740.229 | 0.799445318525346 | [M-H]- | 455.356;50.596;456.362;100.933;101.934 | 58446228 |
| Sumaresinolic acid | terpenoids | CC1(CCC2(CCC3(C(=CCC4C3(CC(C5C4(CCC(C5(C)C)O)C)O)C)C2C1)C)C(=O)O)C | C30H48O4 | 471.3508 | 630.614 | 1.75675414298949 | [M-H]- | 471.352;52.373;472.349;277.215;172.87 | 3350462.45 |
| Cholic acid | terpenoids | CC(CCC(=O)O)C1CCC2C1(C(CC3C2C(CC4C3(CCC(C4)O)C)O)O)C | C24H40O5 | 407.2808 | 40.5758 | 2.88244865439248 | [M-H]- | 407.277;408.285;343.266;363.292;289.218 | 119428846 |
| Enoxolone | terpenoids | CC1(C2CCC3(C(C2(CCC1O)C)C(=O)C=C4C3(CCC5(C4CC(CC5)(C)C(=O)O)C)C)C)C | C30H46O4 | 469.3333 | 584.815 | 1.4934823682617 | [M-H]- | 469.332;470.334;52.149;407.336;351.267 | 7605805.34 |
| Hyodeoxycholic acid | terpenoids | CC(CCC(=O)O)C1CCC2C1(CCC3C2CC(C4C3(CCC(C4)O)C)O)C | C24H40O4 | 391.2868 | 780.796 | 2.00778956980286 | [M-H] | 391.283;392.289;345.283;327.271;347.295 | 28813190.4 |
| Abscisic acid | terpenoids | CC1=CC(=O)CC(C1(C=CC(=CC(=O)O)C)O)(C)C | C15H20O4 | 263.1299 | 255.548 | 0.339662958759335 | [M-H] | 263.13;219.14;264.131;217.867;162.838 | 5211458.84 |
| Medicagenic acid | terpenoids | CC1(C)CCC2(CCC3(C)C(=CCC4C5(C)CC(O)C(O)C(C)(C5CCC34C)C(O)=O)C2C1)C(O)=O | C30H46O6 | 501.3246 | 431.918 | 1.28258959333528 | [M-H]- | 501.326;55.704;502.329;152.997;162.841 | 1480670.26 |
| Azuleno(5,6-c)furan-1(3H)-one, 4,4a,5,6,7,7a,8,9-octahydro-3,4,8-trihydroxy-6,6,8-trimethyl- | terpenoids | O=C1OC(O)C2=C1CC(O)(C)C3CC(C)(C)CC3C2O | C15H22O5 | 281.1399 | 255.548 | 0.494433569453489 | [M-H]- | 281.142;59.014;263.13;237.147;109.03 | 1225129.98 |
| Ginsenoside-Rg1 | terpenoids | CC(C)=CCCC(C)(OC1OC(CO)C(O)C(O)C1O)C1CCC2(C)C1C(O)CC1C3(C)CCC(O)C(C)(C)C3C(CC21C)OC1OC(CO)C(O)C(O)C1O | C42H72O14 | 845.4906 | 204.896 | 1.62093548306832 | [M+HCOO]- | 799.489;845.487;845.517;799.516;637.432 | 2840733.87 |
| Atractylenolide III | terpenoids | CC1=C2CC3C(=C)CCCC3(C)CC2(O)OC1=O | C15H20O3 | 247.1347 | 319.785 | 1.0464897187855 | [M-H]- | 247.135;147.046;177.094;187.115;162.841 | 2152741.45 |
| 2,4,6-trihydroxy-5-[1-(4-hydroxy-1,1,4,7-tetramethyl-1a,2,3,4a,5,6,7a,7b-octahydrocyclopropa[h]azulen-7-yl)-3-methylbutyl]benzene-1,3-dicarbaldehyde | terpenoids | CC(C)CC(C1=C(O)C(C=O)=C(O)C(C=O)=C1O)C2(C)CCC3C2C4C(CCC3(C)O)C4(C)C | C28H40O6 | 471.2771 | 676.33 | 0.231174729119088 | [M-H]- | 175.04;471.278;160.016;134.038;295.229 | 100284809 |
| (E)-5-(2,3-dimethyl-4,5,6,7-tetrahydro-1H-tricyclo[2.2.1.02,6]heptan-3-yl)-2-methylpent-2-enoic acid | terpenoids | O=C(O)C(=CCCC1(C)C2CC3C(C2)C31C)C | C15H22O2 | 233.1553 | 433.692 | 1.47291980941623 | [M-H]- | 233.156;99.946;143.936;62.683;54.521 | 2206675.8 |
| 3,12-dihydroxy-4,6a,6b,11,12,14b-hexamethyl-1,2,3,4a,5,6,7,8,9,10,11,12a,14,14a-tetradecahydropicene-4,8a-dicarboxylic acid | terpenoids | O=C(O)C12CCC(C)C(O)(C)C2C3=CCC4C5(C)CCC(O)C(C(=O)O)(C)C5CCC4(C)C3(C)CC1 | C30H46O6 | 501.3249 | 483.034 | 1.700458041809 | [M-H]- | 501.326;439.319;423.287;55.704;502.327 | 4634118.69 |
| 7-hydroxy-1,4a-dimethyl-9-oxo-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthrene-1-carboxylic acid | terpenoids | O=C(O)C1(C)CCCC2(C)C3C(=CC(O)(CC3)C(C)C)C(=O)CC12 | C20H30O4 | 333.2083 | 444.971 | 0.787793723999655 | [M-H]- | 333.208;334.208;265.161;78.958;234.164 | 6371120.87 |
| Ingenol | terpenoids | CC1CC2C(C2(C)C)C3C=C(C(C4(C1(C3=O)C=C(C4O)C)O)O)CO | C20H28O5 | 347.1871 | 353.573 | 0.423675839421798 | [M-H] | 347.186;303.201;259.208;348.19;304.2 | 5700163.07 |
| 4-AMINOBENZOATE |  | C1=CC(=CC=C1C(=O)O)N | C7H7NO2 | 136.0408 | 54.6264 | 1.18269531457685 | [M-H]- | 136.041;137.025;93.035;91.913;94.03 | 2327684.57 |
| 13-HODE |  | CCCCCC(O)C=CC=CCCCCCCCC(O)=O | C18H32O3 | 295.2291 | 632.464 | 0.186001411797472 | [M-H]- | 295.228;296.23;125.097;251.239;151.112 | 283662262 |
| Di-n-butyl phthalate |  | CCCCOC(=O)C1=CC=CC=C1C(=O)OCCCC | C16H22O4 | 277.1452 | 277.392 | 0.86208678147699 | [M-H]- | 277.144;233.156;278.149;234.16;241.793 | 6451976.27 |
| Vanillic acid |  | COc1cc(ccc1O)C(=O)O | C8H8O4 | 167.0356 | 60.1844 | 2.2106575547645 | [M-H]- | 152.013;167.036;123.082;167.835;108.022 | 4267664.97 |
| FA 18:1+1O |  | O=C(O)CCCCCCCC=CCC(O)CCCCCC | C18H34O3 | 297.2443 | 591.127 | 1.07199185651527 | [M-H]- | 297.243;298.248;183.138;279.233;171.104 | 219023770 |
| FA 18:1+3O |  | O=C(O)CCCCCCCC(O)C=CC(O)C(O)CCCCC | C18H34O5 | 329.2348 | 399.4265 | 2.38681734386868 | [M-H]- | 329.234;171.104;311.222;330.241;201.115 | 48384835.9 |
| Zingerone |  | COC1=C(O)C=CC(CCC(C)=O)=C1 | C11H14O3 | 193.0878 | 258.045 | 0.815018961572912 | [M-H]- | 193.087;108.022;158.847;193.817;146.864 | 2852248.79 |
| Hexadecanedioic acid |  | OC(=O)CCCCCCCCCCCCCCC(O)=O | C16H30O4 | 285.2076 | 360.273 | 1.23863021228951 | [M-H]- | 285.21;286.213;267.199;265.181;155.146 | 6174626 |
| gamma-mangostin |  | O=C1C2=C(O)C(=C(O)C=C2OC3=CC(O)=C(O)C(=C13)CC=C(C)C)CC=C(C)C | C23H24O6 | 395.1541 | 628.8815 | 0.143416647351036 | [M-H]- | 395.149;116.929;100.934;99.926;84.939 | 20850818.4 |
| Benzyl alcohol + Hex-Pen |  | OCC3(O)(COC(OCC2OC(OCC1=CC=CC=C1)C(O)C(O)C2(O))C3(O)) | C18H26O10 | 401.1434 | 672.848 | 1.43671404535657 | [M-H]- | 401.139;100.934;99.926;305.047;402.144 | 9378250.27 |
| 9-Hydroxy-10,12,15-octadecatrienoic acid |  | O=C(O)CCCCCCCC(O)C=CC=CCC=CCC | C18H30O3 | 293.2131 | 516.853 | 0.267532984456844 | [M-H]- | 293.211;275.204;171.104;235.17;121.103 | 1808387340 |

**Table S3** 249 compounds identified by GC-MS.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Class** | **Unique Mass** | **R.T. (minutes)** | **Similarity** | **Area** | **Area%** | **CAS** |
| picolinic acid | Alkaloids | 226 | 11.2593 | 284 | 51743 | 0.032436 | 98-98-6 |
| Tyramine | Alkaloids | 73 | 18.226 | 158 | 15658 | 0.009816 | 51-67-2 |
| Pipecolinic acid | Alkaloids | 258 | 11.818 | 208 | 5849.1 | 0.003667 | 535-75-1 |
| DL-Anabasine 2 | Alkaloids | 77 | 15.7167 | 243 | 3859.1 | 0.002419 | 13078-04-1 |
| N-Ethylglycine 1 | Amino acid Derivatives | 174 | 12.3567 | 478 | 609388 | 0.382008 | 627-01-0 |
| N-Ethylglycine 2 | Amino acid Derivatives | 58 | 9.36733 | 346 | 120443.3 | 0.075502 | 627-01-0 |
| alanine 1 | Amino acids | 116 | 8.05 | 823 | 1433015 | 0.898316 | 56-41-7 |
| N-Methyl-L-glutamic acid 2 | Amino acids | 71 | 14.222 | 306 | 275186 | 0.172506 | 6753-62-4 |
| DL-Norleucine | Amino acids | 141 | 9.422 | 167 | 251696 | 0.157781 | 327-57-1 |
| proline | Amino acids | 142 | 10.8367 | 891 | 240730 | 0.150907 | 147-85-3 |
| citrulline 2 | Amino acids | 84 | 16.41 | 309 | 187313 | 0.117421 | 372-75-8 |
| valine | Amino acids | 144 | 9.66733 | 610 | 179100 | 0.112273 | 72-18-4 |
| oxoproline | Amino acids | 156 | 13.81 | 771 | 164245 | 0.10296 | 98-79-3 |
| glutamine 3 | Amino acids | 99 | 13.9753 | 346 | 133677 | 0.083798 | 56-85-9 |
| DL-Threonine | Amino acids | 341 | 10.8633 | 187 | 115912 | 0.072662 | 72-19-5 |
| N-Acetyl-beta-alanine 2 | Amino acids | 73 | 12.0927 | 425 | 77602 | 0.048646 | 3025-95-4 |
| sarcosine | Amino acids | 51 | 8.59267 | 296 | 69932 | 0.043838 | 107-97-1 |
| Cysteine | Amino acids | 73 | 14.2527 | 199 | 56617 | 0.035492 | 52-90-4 |
| serine 2 | Amino acids | 116 | 10.1967 | 377 | 54266 | 0.034018 | 56-45-1 |
| Isoleucine | Amino acids | 158 | 10.7553 | 442 | 47088.6 | 0.029518 | 73-32-5 |
| threonine 2 | Amino acids | 130 | 10.762 | 293 | 45917 | 0.028784 | 72-19-5 |
| L-ornithine | Amino acids | 71 | 16.5073 | 196 | 38834 | 0.024344 | 70-26-8 |
| trans-4-hydroxy-L-proline 2 | Amino acids | 140 | 13.8007 | 456 | 32799 | 0.020561 | 51-35-4 |
| L-glutamic acid | Amino acids | 131 | 13.8753 | 261 | 27155 | 0.017023 | 56-86-0 |
| N-Methyl-DL-alanine | Amino acids | 281 | 9.102 | 239 | 11945 | 0.007488 | 600-21-5 |
| arginine | Amino acids | 71 | 18.158 | 213 | 11213 | 0.007029 | 74-79-3 |
| Allantoic acid 2 | Amino Acids | 57 | 17.846 | 273 | 9814.8 | 0.006153 | 99-16-1 |
| thymidine 3 | Amino acids | 225 | 22.6473 | 292 | 8984.6 | 0.005632 | 50-89-5 |
| L-Allothreonine | Amino acids | 71 | 12.142 | 37 | 6177.5 | 0.003872 | 28954-12-3 |
| thymidine 2 | Amino acids | 148 | 14.942 | 452 | 5095.6 | 0.003194 | 50-89-5 |
| L-cystine | Amino acids | 51 | 21.77 | 89 | 4025.5 | 0.002523 | 923-32-0 |
| Carbobenzyloxy-L-leucine | Amino Acids and Derivatives | 67 | 19.6887 | 257 | 24472 | 0.015341 | 2018-66-8 |
| Carnitine | Amino acids and derivatives | 146 | 9.77267 | 232 | 8437.1 | 0.005289 | 541-15-1 |
| 1-Methylhydantoin 1 | Azolines | 71 | 11.226 | 248 | 1136996 | 0.71275 | 616-04-6 |
| phenylacetaldehyde 1 | Benzene and substituted derivatives | 77 | 19.9807 | 294 | 846188 | 0.530451 | 122-78-1 |
| N-cyclohexylformamide 1 | Benzene and substituted derivatives | 71 | 10.5873 | 373 | 614336 | 0.385109 | 766-93-8 |
| Phenylpyruvic acid | Benzene and substituted derivatives | 77 | 14.6313 | 187 | 57309 | 0.035925 | 156-06-9 |
| Phenylacetic acid | Benzene and substituted derivatives | 90 | 11.0367 | 207 | 57139 | 0.035819 | 103-82-2 |
| phthalic acid | Benzene and substituted derivatives | 221 | 15.7807 | 355 | 27269 | 0.017094 | 88-99-3 |
| N-cyclohexylformamide | Benzene and substituted derivatives | 156 | 9.78867 | 151 | 13978 | 0.008762 | 766-93-8 |
| Phenylacetamide | Benzene and substituted derivatives | 86 | 13.21 | 247 | 7650.9 | 0.004796 | 103-81-1 |
| glycerol | Carbohydrates | 73 | 10.4607 | 944 | 1626022 | 1.019306 | 56-81-5 |
| D-Arabitol | Carbohydrates | 73 | 16.0033 | 936 | 1073678 | 0.673058 | 488-82-4 |
| L-Threose 2 | Carbohydrates | 350 | 12.8713 | 494 | 56452 | 0.035388 | 95-44-3 |
| Lyxose 1 | Carbohydrates | 73 | 15.2273 | 456 | 50053 | 0.031377 | 1114-34-7 |
| 3,6-Anhydro-D-galactose 4 | Carbohydrates | 85 | 16.7727 | 310 | 5258 | 0.003296 | 14122-18-0 |
| Gentiobiose 2 | Carbohydrates | 329 | 25.7847 | 405 | 2539.7 | 0.001592 | 554-91-6 |
| 3-Hydroxypropionic acid 1 | Carboxylic acids | 147 | 8.60733 | 488 | 13298119 | 8.336206 | 503-66-2 |
| lactic acid | Carboxylic acids | 117 | 7.42467 | 933 | 1165210 | 0.730436 | 50-21-5 |
| Cumic Acid | Carboxylic acids | 73 | 13.9993 | 553 | 518923 | 0.325298 | 536-66-3 |
| 4-Acetylbutyric acid 2 | Carboxylic acids | 116 | 11.234 | 374 | 148186 | 0.092894 | 6/1/3128 |
| maleic acid | Carboxylic acids | 341 | 10.8073 | 230 | 90277 | 0.056592 | 110-16-7 |
| 3-Hexenedioic acid | Carboxylic acids | 71 | 13.67 | 336 | 78872.6 | 0.049443 | 4436-74-2 |
| 4-Acetamidobutyric acid 2 | Carboxylic acids | 174 | 13.57 | 365 | 71554 | 0.044855 | 3025-96-5 |
| L-Malic acid | Carboxylic acids | 71 | 13.3167 | 478 | 67995 | 0.042624 | 97-67-6 |
| 4-Methyl-2-oxopentanoic acid | Carboxylic acids | 70 | 9.72333 | 195 | 43107 | 0.027023 | 816-66-0 |
| palmitoleic acid | Carboxylic acids | 117 | 19.2607 | 603 | 18943.8 | 0.011875 | 373-49-9 |
| Allylmalonic acid | Carboxylic acids | 221 | 11.3167 | 372 | 16390 | 0.010274 | 2583-25-7 |
| 4-Acetamidobutyric acid 1 | Carboxylic acids | 91 | 13.3673 | 212 | 16374 | 0.010264 | 3025-96-5 |
| 3-Aminoisobutyric acid 1 | Carboxylic acids and derivatives | 73 | 12.9753 | 566 | 4291023 | 2.689919 | 144-90-1 |
| beta-Alanine 2 | Carboxylic acids and derivatives | 174 | 12.6113 | 590 | 2390182 | 1.498336 | 107-95-9 |
| 4-aminobutyric acid 3 | Carboxylic acids and derivatives | 140 | 8.83933 | 305 | 969913 | 0.60801 | 56-12-2 |
| 4-aminobutyric acid 2 | Carboxylic acids and derivatives | 73 | 10.8007 | 237 | 869707 | 0.545194 | 56-12-2 |
| Tartronic acid | Carboxylic acids and derivatives | 221 | 11.994 | 543 | 175478 | 0.110002 | 80-69-3 |
| oxalic acid | Carboxylic acids and derivatives | 102 | 8.33267 | 489 | 44238 | 0.027732 | 144-62-7 |
| succinic acid | Carboxylic acids and derivatives | 209 | 11.0727 | 345 | 108999 | 0.068328 | 110-15-6 |
| stearic acid | Fatty acids | 117 | 21.27 | 940 | 32248489 | 20.21565 | 57-11-4 |
| palmitic acid | Fatty acids | 117 | 19.4847 | 956 | 29812756 | 18.68875 | 57-10-3 |
| linolenic acid | Fatty acids | 207 | 21.0753 | 902 | 2741323 | 1.718456 | 463-40-1 |
| oleic acid | Fatty acids | 339 | 21.1353 | 953 | 1599263 | 1.002532 | 112-80-1 |
| linoleic acid | Fatty acids | 220 | 21.0193 | 618 | 844258 | 0.529241 | 60-33-3 |
| cis-gondoic acid | Fatty acids | 117 | 22.7087 | 890 | 817947 | 0.512747 | 5561-99-9 |
| 2,2-Dimethylsuccinic Acid | Fatty acids | 69 | 11.0673 | 297 | 257755 | 0.161579 | 597-43-3 |
| Behenic acid | Fatty acids | 117 | 24.4447 | 906 | 128562 | 0.080592 | 112-85-6 |
| arachidonic acid | Fatty acids | 95 | 22.3687 | 401 | 88085.4 | 0.055218 | 506-32-1 |
| Arachidic acid | Fatty acids | 117 | 22.9087 | 897 | 74779 | 0.046877 | 506-30-9 |
| Myristic Acid | Fatty acids | 117 | 17.502 | 888 | 55974 | 0.035088 | 544-63-8 |
| caprylic acid | Fatty acids | 117 | 10.3967 | 763 | 53145.4 | 0.033315 | 124-07-2 |
| Lignoceric acid | Fatty acids | 117 | 25.8767 | 858 | 46244 | 0.028989 | 557-59-5 |
| Citraconic acid 4 | Fatty acids | 221 | 11.558 | 443 | 22448 | 0.014072 | 498-23-7 |
| heptadecanoic acid | Fatty acids | 117 | 20.3713 | 488 | 18520 | 0.01161 | 506-12-7 |
| lauric acid | Fatty acids | 117 | 15.366 | 731 | 15267 | 0.00957 | 143-07-7 |
| Capric Acid | Fatty acids | 125 | 12.9793 | 263 | 5636.8 | 0.003534 | 334-48-5 |
| 2-keto-isovaleric acid 1 | Fatty acyls | 71 | 8.006 | 203 | 781073 | 0.489632 | 759-05-7 |
| 2-ketobutyric acid 2 | Fatty acyls | 85 | 7.54333 | 362 | 671371 | 0.420863 | 600-18-0 |
| Pelargonic acid | Fatty acyls | 69 | 11.73 | 870 | 454982.6 | 0.285215 | 112-05-0 |
| 2-ketobutyric acid 1 | Fatty acyls | 225 | 7.918 | 360 | 220527 | 0.138242 | 600-18-0 |
| 3-hydroxybutyric acid | Fatty acyls | 281 | 8.94733 | 468 | 173997 | 0.109074 | 306-31-0 |
| Octanal | Fatty acyls | 78 | 8.56467 | 38 | 88442 | 0.055442 | 124-13-0 |
| Itaconic acid | Fatty acyls | 227 | 11.362 | 304 | 54074.4 | 0.033898 | 97-65-4 |
| 2-keto-isovaleric acid 2 | Fatty acyls | 141 | 8.36467 | 245 | 50768 | 0.031825 | 759-05-7 |
| Methylmalonic acid | Fatty acyls | 57 | 9.63267 | 558 | 25796 | 0.016171 | 516-05-2 |
| Octadecanol | Fatty acyls | 71 | 20.57 | 56 | 25509 | 0.015991 | 112-92-5 |
| Linoleic acid methyl ester | Fatty acyls | 67 | 20.0127 | 599 | 24149 | 0.015138 | 112-63-0 |
| 5-Aminovaleric acid 2 | Fatty acyls | 73 | 15.438 | 298 | 19246 | 0.012065 | 660-88-8 |
| 3-Methyl-2-oxobutanoic acid | Fatty acyls | 84 | 8.54067 | 142 | 8725.6 | 0.00547 | 759-05-7 |
| pimelic acid | Fatty acyls | 91 | 14.778 | 206 | 7175.4 | 0.004498 | 111-16-0 |
| 6-hydroxy caproic acid | Fatty acyls | 191 | 12.5967 | 468 | 4391.6 | 0.002753 | 1191-25-9 |
| Dodecanol | Fatty acyls | 89 | 14.3753 | 407 | 3943.4 | 0.002472 | 112-53-8 |
| 5-Aminovaleric acid | Fatty acyls | 72 | 15.9233 | 193 | 3550.7 | 0.002226 | 660-88-8 |
| 4-Hydroxybenzoic acid | Flavonoids | 57 | 15.0847 | 336 | 61151 | 0.038334 | 99-96-7 |
| luteolin | Flavonoids | 83 | 29.2273 | 341 | 25078 | 0.015721 | 491-70-3 |
| Hesperitin 2 | Flavonoids | 117 | 27.214 | 435 | 15609 | 0.009785 | 41001-90-5 |
| Tricetin | Flavonoids | 255 | 29.8487 | 633 | 8686.7 | 0.005445 | 520-31-0 |
| 4-hydroxy-3-methoxybenzoic acid; | Flavonoids | 267 | 16.598 | 435 | 6997.2 | 0.004386 | 121-34-6 |
| 3-Phenylpropionic acid | Flavonoids | 143 | 12.6687 | 184 | 4303.2 | 0.002698 | 501-52-0 |
| hydroxylamine | Homogeneous other non-metal compounds | 141 | 8.186 | 290 | 2114468 | 1.325499 | 7803-49-8 |
| 1-Hexadecanol | Lipids | 71 | 18.5873 | 289 | 27284 | 0.017104 | 36653-82-4 |
| phosphate | Non-metal oxoanionic compounds | 299 | 10.4527 | 836 | 334585 | 0.209742 | 7664-38-2 |
| 2-Deoxyuridine | Nucleic acids | 71 | 10.5127 | 350 | 147408 | 0.092406 | 951-78-0 |
| Cytosin | Nucleic acids | 68 | 13.778 | 255 | 66062 | 0.041412 | 71-30-7 |
| uracil | Nucleic acids | 341 | 11.39 | 408 | 60139.7 | 0.0377 | 66-22-8 |
| guanine 1 | Nucleic acids | 71 | 20.1873 | 255 | 9382.1 | 0.005881 | 73-40-5 |
| ribitol | Organooxygen compounds | 73 | 16.0607 | 801 | 287984 | 0.180529 | 488-81-3 |
| tartaric acid | Organooxygen compounds | 73 | 15.03 | 424 | 216395 | 0.135652 | 133-37-9 |
| D-alanyl-D-alanine 2 | Peptides | 245 | 14.6887 | 230 | 8469.8 | 0.005309 | 923-16-0 |
| Thymol | Phenols | 73 | 11.1393 | 248 | 220607 | 0.138292 | 89-83-8 |
| resorcinol | Phenols | 240 | 12.0033 | 339 | 166370 | 0.104293 | 108-46-3 |
| guaiacol | Phenols | 57 | 9.93533 | 249 | 40091.3 | 0.025132 | 8021-39-4 |
| salicylic acid | Phenols | 267 | 13.638 | 476 | 11092 | 0.006953 | 69-72-7 |
| hydroquinone | Phenols | 189 | 12.23 | 249 | 3424.6 | 0.002147 | 123-31-9 |
| Chlorogenic Acid 1 | Phenylpropanoids | 73 | 27.862 | 177 | 36804 | 0.023071 | 327-97-9 |
| Cinnamic acid | Phenylpropanoids | 131 | 14.3247 | 275 | 23251 | 0.014575 | 140-10-3 |
| Uric acid | Purines | 67 | 19.9513 | 103 | 8634.8 | 0.005413 | 66-22-8 |
| 3-Hydroxypyridine | Pyridines | 152 | 8.62733 | 588 | 284611 | 0.178414 | 109-00-2 |
| 2-hydroxypyridine | Pyridines and derivatives | 152 | 7.162 | 911 | 2034660 | 1.27547 | 142-08-5 |
| quinolinic acid | Pyridines and derivatives | 79 | 16.158 | 456 | 126973 | 0.079596 | 89-00-9 |
| Pyrrole-2-Carboxylic Acid | Pyrroles | 152 | 11.6633 | 286 | 88149 | 0.055258 | 634-97-9 |
| 20alpha-Hydroxycholesterol 1 | Steroids | 129 | 29.8287 | 386 | 27959 | 0.017527 | 516-72-3 |
| lanosterol | Sterol lipids | 218 | 30.1647 | 552 | 716162 | 0.448941 | 79-63-0 |
| 24,25-dihydrolanosterol | Sterol lipids | 55 | 29.842 | 424 | 75330 | 0.047222 | 79-62-9 |
| Tetrahydrocorticosterone 4 | Sterol lipids | 223 | 26.9687 | 179 | 65495 | 0.041057 | 68-42-8 |
| Tetrahydrocorticosterone 3 | Sterol lipids | 117 | 27.1367 | 378 | 5247.4 | 0.003289 | 68-42-8 |
| squalene | Terpenoids | 69 | 25.7793 | 910 | 8486722 | 5.320081 | 111-02-4 |
| Phytol | Terpenoids | 143 | 20.6193 | 498 | 32430 | 0.020329 | 150-86-7 |
| (-)-Dihydrocarveol | Terpenoids | 123 | 10.714 | 275 | 11258 | 0.007057 | 20549-47-7 |
| 2-Mercaptoethanesulfonic acid | Vitamins and cofactors | 80 | 11.5033 | 192 | 25561 | 0.016023 | 3375-50-6 |
| biotin | Vitamins and cofactors | 55 | 23.3967 | 255 | 23153 | 0.014514 | 58-85-5 |
| 5,6-dihydrouracil 1 |  | 133 | 13.454 | 354 | 769202 | 0.482191 | 504-07-4 |
| Carbobenzyloxy-L-leucine degr1 |  | 102 | 10.2207 | 341 | 716920 | 0.449416 | 2018-66-8 |
| cycloleucine 2 |  | 57 | 9.546 | 384 | 699148 | 0.438276 | 52-52-8 |
| Carvone |  | 71 | 11.4727 | 134 | 558442 | 0.350071 | 6485-40-1 |
| Cholestane-3,5,6-triol, (3beta ,5alpha ,6beta)- |  | 75 | 30.498 | 565 | 367406 | 0.230316 | 1253-84-5 |
| Citraconic acid degr1 |  | 68 | 9.98467 | 344 | 333745 | 0.209215 | 498-23-7 |
| 4-Hydroxy-6-methyl-2-pyrone |  | 71 | 13.5287 | 274 | 320679 | 0.201024 | 675-10-5 |
| 4-HYDROXYPYRIDINE |  | 152 | 8.87267 | 547 | 313459.2 | 0.196499 | 626-64-2 |
| 3-Hydroxynorvaline |  | 57 | 11.6167 | 169 | 311272 | 0.195127 | 2280-42-4 |
| 1-Aminocyclopropanecarboxylic acid |  | 86 | 9.70467 | 453 | 304847 | 0.1911 | 22059-21-8 |
| malonic acid 1 |  | 75 | 9.55267 | 620 | 293676 | 0.184097 | 141-82-2 |
| glycolic acid |  | 173 | 7.662 | 431 | 227241.1 | 0.142451 | 79-14-1 |
| 1,4-Cyclohexanedione 2 |  | 69 | 10.9487 | 384 | 226489 | 0.141979 | 637-88-7 |
| 3-Aminoisobutyric acid 2 |  | 102 | 9.62867 | 610 | 198719 | 0.124571 | 144-90-1 |
| D-erythronolactone 1 |  | 73 | 12.766 | 341 | 185474 | 0.116268 | 15667-21-7 |
| Cyclohexylamine |  | 71 | 11.6113 | 130 | 169123 | 0.106018 | 108-91-8 |
| Maleamate 3 |  | 73 | 13.2673 | 542 | 163002.1 | 0.102181 | 557-24-4 |
| 1,4-Cyclohexanedione 1 |  | 73 | 10.9527 | 330 | 159897 | 0.100235 | 637-88-7 |
| 3-Methyloxindole |  | 263 | 14.0033 | 170 | 158967 | 0.099652 | 1504-06-9 |
| Monoolein |  | 79 | 25.314 | 740 | 155197 | 0.097289 | 111-03-5 |
| Dioctyl phthalate |  | 149 | 23.682 | 919 | 145251 | 0.091054 | 117-81-7 |
| 2-amino-2-methylpropane-1,3-diol 1 |  | 130 | 11.1313 | 284 | 135697 | 0.085065 | 115-69-5 |
| 2-Butyne-1,4-diol |  | 75 | 9.89 | 541 | 132010 | 0.082753 | 110-65-6 |
| hydroxyurea |  | 102 | 9.962 | 463 | 129881 | 0.081419 | 127-07-1 |
| 1,4-Cyclohexanedione 2 |  | 57 | 10.8913 | 169 | 129757 | 0.081341 | 637-88-7 |
| 1,4-Cyclohexanedione 2 |  | 71 | 10.8247 | 371 | 129263 | 0.081031 | 637-88-7 |
| D-erythronolactone 2 |  | 73 | 14.7047 | 303 | 124840 | 0.078259 | 15667-21-7 |
| 6-hydroxy caproic acid trimer |  | 57 | 26.334 | 268 | 117843 | 0.073872 | 1191-25-9 |
| alpha-Santonin 1 |  | 51 | 21.4127 | 343 | 113434 | 0.071108 | 481-06-1 |
| 3-aminopropionitrile 1 |  | 55 | 12.198 | 362 | 110002 | 0.068957 | 151-18-8 |
| cis-1,2-Dihydronaphthalene-1,2-diol |  | 57 | 15.6007 | 516 | 96780 | 0.060669 | 51268-88-3 |
| Tropic Acid |  | 119 | 14.7167 | 387 | 94429 | 0.059195 | 529-64-6 |
| oxamic acid |  | 175 | 10.2713 | 302 | 90711 | 0.056864 | 471-47-6 |
| 2-ketoadipate 3 |  | 96 | 10.122 | 420 | 87514 | 0.05486 | 689-31-6 |
| 4-aminophenol 2 |  | 240 | 14.5913 | 241 | 87109 | 0.054606 | 123-30-8 |
| 4-Methylbenzyl alcohol |  | 71 | 10.2793 | 436 | 80699 | 0.050588 | 589-18-4 |
| 1-Indanone 1 |  | 73 | 12.1887 | 319 | 79208 | 0.049653 | 83-33-0 |
| 2,3-Dihydroxypyridine |  | 240 | 11.0593 | 814 | 77246 | 0.048423 | 16867-04-2 |
| Biuret 3 |  | 57 | 12.434 | 324 | 76685 | 0.048072 | 108-19-0 |
| Biuret |  | 85 | 15.918 | 165 | 76052 | 0.047675 | 108-19-0 |
| androsterone 2 |  | 73 | 24.166 | 427 | 75797 | 0.047515 | 53-41-8 |
| Lactamide 2 |  | 308 | 8.59933 | 372 | 75680.7 | 0.047442 | 2043-43-8 |
| 1,4-Cyclohexanedione 2 |  | 71 | 11.0287 | 403 | 71551 | 0.044853 | 637-88-7 |
| 3-Hydroxynorvaline 2 |  | 160 | 11.682 | 515 | 67218 | 0.042137 | 2280-42-4 |
| Abietic Acid 2 |  | 95 | 22.5793 | 481 | 64109 | 0.040188 | 514-10-3 |
| cis,cis-Farnesol |  | 71 | 16.6127 | 188 | 56124 | 0.035183 | 106-28-5 |
| 5-Hydroxyindole-3-acetic acid 2 |  | 324 | 21.106 | 254 | 53642 | 0.033627 | 54-16-0 |
| 1-Indanol |  | 228 | 11.694 | 208 | 53447 | 0.033504 | 6351-10-6 |
| acetanilide 2 |  | 116 | 10.6767 | 424 | 49200 | 0.030842 | 103-84-4 |
| gentisic acid |  | 73 | 16.726 | 403 | 48686 | 0.03052 | 490-79-9 |
| Fames-C12 |  | 69 | 13.8847 | 253 | 46295 | 0.029021 | 111-82-0 |
| Glucoheptonic acid 1 |  | 221 | 21.474 | 330 | 46179 | 0.028948 | 23351-51-1 |
| Unknown 81 |  | 110 | 8.27 | 193 | 45877 | 0.028759 | 7803-49-8 |
| asparagine 4 |  | 74 | 13.5633 | 319 | 44996 | 0.028207 | 70-47-3 |
| 4-Nitrophenol |  | 99 | 13.93 | 188 | 44897 | 0.028145 | 100-02-7 |
| 11-beta-prostaglandin-F-2-alpha 1 |  | 103 | 25.05 | 522 | 43734 | 0.027416 | 38432-87-0 |
| Maleimide |  | 154 | 7.99133 | 598 | 41503 | 0.026017 | 541-59-3 |
| benzyl alcohol |  | 91 | 8.86333 | 692 | 41243 | 0.025854 | 100-51-6 |
| 1,3-Cyclohexanedione 1 |  | 111 | 11.1807 | 303 | 39687 | 0.024879 | 504-02-9 |
| glutaraldehyde |  | 85 | 8.77 | 197 | 37215 | 0.023329 | 111-30-8 |
| 11-beta-prostaglandin-F-2-alpha 1 |  | 103 | 25.05 | 522 | 37194 | 0.023316 | 38432-87-0 |
| 1-Monopalmitin |  | 73 | 24.018 | 678 | 36623 | 0.022958 | 542-44-9 |
| 1,2-Cyclohexanedione 1 |  | 97 | 11.6273 | 276 | 31052 | 0.019466 | 765-87-7 |
| Salicylaldehyde |  | 85 | 11.878 | 217 | 29776 | 0.018666 | 90-02-8 |
| Citraconic acid 1 |  | 71 | 11.7993 | 165 | 29686 | 0.018609 | 498-23-7 |
| glutathione - H2O |  | 73 | 24.2673 | 363 | 26139 | 0.016386 | 70-18-8 |
| N-Oleoyldopamine 1 |  | 73 | 25.7353 | 271 | 25441 | 0.015948 | 105955-11-1 |
| Lactamide 1 |  | 117 | 8.91 | 321 | 25040 | 0.015697 | 2043-43-8 |
| 9-Fluorenone 2 |  | 79 | 16.9047 | 438 | 24259.7 | 0.015208 | 486-25-9 |
| 1,2-Cyclohexanedione 2 |  | 57 | 13.1767 | 290 | 23345 | 0.014634 | 765-87-7 |
| 1-Aminocyclopropanecarboxylic acid |  | 86 | 9.70467 | 453 | 22512 | 0.014112 | 22059-21-8 |
| 5-Dihydrocortisone 2 |  | 73 | 29.6033 | 440 | 21204 | 0.013292 | 68-54-2 |
| phytosphingosine 1 |  | 57 | 24.0247 | 209 | 20663 | 0.012953 | 554-62-1 |
| Biphenyl |  | 327 | 12.49 | 437 | 20168 | 0.012643 | 92-52-4 |
| 3-hydroxy-L-proline 2 |  | 226 | 13.1047 | 247 | 18526.3 | 0.011614 | 8/2/4298 |
| Benzylamine |  | 174 | 12.802 | 305 | 18113 | 0.011355 | 100-46-9 |
| glutathione 1 |  | 93 | 20.6233 | 246 | 15241 | 0.009554 | 70-18-8 |
| 1,6-di-O-phosphono-D-fructose |  | 57 | 24.922 | 154 | 14797 | 0.009276 | 488-69-7 |
| 9-Fluorenone 1 |  | 117 | 18.502 | 375 | 14705 | 0.009218 | 486-25-9 |
| Dehydroascorbic Acid 1 |  | 73 | 17.402 | 247 | 13873 | 0.008697 | 490-83-5 |
| 1,2,4-Benzenetriol |  | 79 | 14.8367 | 149 | 13144 | 0.00824 | 533-73-3 |
| kyotorphin 4 |  | 69 | 25.5153 | 265 | 12749 | 0.007992 | 70904-56-2 |
| (2R,3S)-2-hydroxy-3-isopropylbutanedioic acid |  | 73 | 14.1927 | 251 | 12565 | 0.007877 | 921-28-8 |
| Menthone |  | 108 | 14.142 | 194 | 12314 | 0.007719 | 14073-97-3 |
| 3-Methylamino-1,2-propanediol 2 |  | 184 | 11.9633 | 215 | 11907 | 0.007464 | 40137-22-2 |
| 1,4-Dihydroxy-2-naphthoic acid |  | 73 | 20.8887 | 83 | 11881 | 0.007448 | 31519-22-9 |
| ADRENOSTERONE 2 |  | 73 | 26.4807 | 428 | 11146 | 0.006987 | 382-45-6 |
| phosphomycin |  | 401 | 11.7713 | 279 | 11033 | 0.006916 | 26016-98-8 |
| butyraldehyde 3 |  | 52 | 10.55 | 259 | 9845.7 | 0.006172 | 123-72-8 |
| 1-Methyladenosine 2 |  | 115 | 22.306 | 335 | 8267.3 | 0.005183 | 15763-06-1 |
| Prostaglandin E2 2 |  | 397 | 25.274 | 533 | 8234.4 | 0.005162 | 363-24-6 |
| MALONAMIDE 4 |  | 327 | 12.926 | 376 | 8042 | 0.005041 | 108-13-4 |
| panthenol 2 |  | 117 | 18.338 | 233 | 7993 | 0.005011 | 16485-10-2 |
| glycocyamine 3 |  | 68 | 17.41 | 299 | 7388.5 | 0.004632 | 352-97-6 |
| Fames-C16 |  | 87 | 18.3247 | 427 | 7368.2 | 0.004619 | 112-39-0 |
| Fluorene |  | 191 | 15.018 | 370 | 6940 | 0.00435 | 86-73-7 |
| creatine degr |  | 119 | 15.3353 | 271 | 6822.7 | 0.004277 | 57-00-1 |
| 4-hydroxybutyrate |  | 217 | 9.878 | 552 | 6619.6 | 0.00415 | 502-85-2 |
| Maleamate 2 |  | 80 | 13.806 | 270 | 5802.5 | 0.003637 | 557-24-4 |
| Phenyl beta-D-glucopyranoside |  | 141 | 21.738 | 187 | 5617 | 0.003521 | 1464-44-4 |
| 8-Aminooctanoic acid |  | 87 | 18.2193 | 156 | 5588.3 | 0.003503 | 1002-57-9 |
| glutaraldehyde 3 |  | 153 | 10.626 | 203 | 5546.1 | 0.003477 | 111-30-8 |
| pyrophosphate 2 |  | 318 | 9.946 | 207 | 5350.9 | 0.003354 | 14000-31-8 |
| 2-amino-2-methylpropane-1,3-diol 2 |  | 285 | 9.058 | 261 | 5333.7 | 0.003344 | 115-69-5 |
| 2-Aminophenol |  | 50 | 14.0727 | 174 | 5079.3 | 0.003184 | 95-55-6 |
| IS |  | 154 | 19.9887 | 300 | 4731.8 | 0.002966 | 112-63-0 |
| 3,6-Anhydro-D-galactose 1 |  | 77 | 15.6647 | 184 | 4599.4 | 0.002883 | 14122-18-0 |
| indole-3-acetamide 4 |  | 63 | 21.466 | 370 | 3640.1 | 0.002282 | 879-37-8 |
| Benzyl thiocyanate |  | 76 | 11.93 | 238 | 3313.2 | 0.002077 | 3012-37-1 |
| Methyl yellow |  | 161 | 21.546 | 220 | 3234.3 | 0.002027 | 60-11-7 |
| 1-Methyladenosine 2 |  | 115 | 22.306 | 335 | 2066.2 | 0.001295 | 15763-06-1 |

**Table S4** DEMs between HFD and CON groups.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **mode** | **VIP** | **Fold change** | **p-value** | **m/z** | **rt(s)** | **HMDB** | **KEGG** | **SuperClass** | **Class** | **SubClass** |
| Glycine | NEG | 2.020894278 | 1.253471581 | 0.005660092 | 74.02476 | 311.038 | HMDB0000123 | C00037 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Lysine | POS | 3.583597459 | 0.802215455 | 0.004524937 | 147.11288 | 542.0215 | HMDB0000182 | C00047 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| D-glutamine | POS | 4.982343785 | 0.790461521 | 0.035578435 | 147.07656 | 394.965 | HMDB0003423 | C00064 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| L-methionine | POS | 2.131057353 | 0.785933816 | 0.004317333 | 150.05854 | 305.012 | HMDB0000696 | C00073 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| DL-tryptophan | NEG | 3.590080262 | 0.597557425 | 0.000163305 | 203.08263 | 280.7495 | HMDB0030396 | C00078 | Organoheterocyclic compounds | Indoles and derivatives | Indolyl carboxylic acids and derivatives |
| Tyrosine | POS | 1.305518998 | 0.622026205 | 0.000102642 | 182.08129 | 322.54 | HMDB0000158 | C00082 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Myo-inositol | NEG | 1.79424367 | 1.219609711 | 0.026527985 | 179.05612 | 414.4915 | HMDB0000211 | C00137 | Organic oxygen compounds | Organooxygen compounds | Alcohols and polyols |
| Phenol | NEG | 4.188593733 | 0.197120448 | 0.000826226 | 93.03445 | 24.4337 | HMDB0000228 | C00146 | Benzenoids | Phenols | 1-hydroxy-4-unsubstituted benzenoids |
| Malate | NEG | 2.406147197 | 0.703310719 | 0.011977893 | 133.01435 | 438.983 | HMDB0000156 | C00149 | Organic acids and derivatives | Hydroxy acids and derivatives | Beta hydroxy acids and derivatives |
| 1,2-dihexadecanoyl-sn-glycero-3-phosphocholine | POS | 5.691780024 | 0.784314754 | 0.009301394 | 734.56913 | 164.8605 | HMDB0000564 | C00157 | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Propionic acid | NEG | 1.333182936 | 0.825793225 | 0.047665956 | 73.0295 | 414.393 | HMDB0000237 | C00163 | Organic acids and derivatives | Carboxylic acids and derivatives | Carboxylic acids |
| Phenylpyruvate | NEG | 1.385107264 | 0.628126118 | 0.015965366 | 163.01785 | 94.2471 | HMDB0000205 | C00166 | Benzenoids | Benzene and substituted derivatives | Phenylpyruvic acid derivatives |
| D-xylose | NEG | 3.447943191 | 2.311435561 | 0.00372218 | 113.02436 | 244.71 | HMDB0060254 | C00181 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Sarcosine | NEG | 2.109260685 | 0.822888393 | 0.03786235 | 88.04039 | 367.5455 | HMDB0000271 | C00213 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| His-ser | NEG | 3.464682594 | 0.781877034 | 0.00931809 | 241.08305 | 90.8845 | HMDB0000273 | C00214 | Nucleosides, nucleotides, and analogues | Pyrimidine nucleosides | Pyrimidine 2'-deoxyribonucleosides |
| Arachidonic acid (peroxide free) | NEG | 8.842973036 | 0.684171555 | 0.011545033 | 303.233 | 42.8967 | HMDB0001043 | C00219 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Succinic semialdehyde | NEG | 2.976116791 | 2.201821373 | 0.004593457 | 101.02446 | 228.286 | HMDB0001259 | C00232 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| D-gluconate | POS | 2.142522225 | 0.31611675 | 0.030244588 | 219.02646 | 327.3435 | HMDB0000625 | C00257 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Hypoxanthine | POS | 27.50731526 | 0.233988604 | 0.015139046 | 137.04584 | 183.213 | HMDB0000157 | C00262 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| Alpha-d-glucose | NEG | 3.099424659 | 0.58546102 | 0.010553099 | 179.05611 | 325.889 | HMDB0003345 | C00267 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| DL-glutamine | NEG | 4.282820342 | 0.771921153 | 0.030766743 | 145.06189 | 395.472 |  | C00303 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| L-carnitine | POS | 13.81839733 | 0.761381582 | 0.000657809 | 162.11198 | 372.9795 | HMDB0062496 | C00318 | Organic nitrogen compounds | Organonitrogen compounds | Quaternary ammonium salts |
| 2-oxoadipic acid | NEG | 1.228185058 | 0.300268405 | 0.000138188 | 159.02996 | 385.1975 | HMDB0000225 | C00322 | Organic acids and derivatives | Keto acids and derivatives | Medium-chain keto acids and derivatives |
| Indole-3-pyruvic acid | NEG | 2.297930401 | 0.631487473 | 0.001590353 | 202.05106 | 72.731 | HMDB0060484 | C00331 | Organoheterocyclic compounds | Indoles and derivatives | Indolyl carboxylic acids and derivatives |
| Xanthine | NEG | 2.352410998 | 0.269767407 | 0.046611046 | 151.02619 | 252.468 | HMDB0000292 | C00385 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| L-Carnosine | NEG | 1.775913827 | 0.586949931 | 0.019878598 | 225.09949 | 440.1715 | HMDB0000033 | C00386 | Organic acids and derivatives | Peptidomimetics | Hybrid peptides |
| L-pipecolic acid | POS | 3.54601141 | 0.785234557 | 0.000811857 | 130.0863 | 542.4745 | HMDB0000716 | C00408 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Biliverdin | POS | 1.413273124 | 0.380512148 | 1.2437E-05 | 583.25634 | 225.794 | HMDB0001008 | C00500 | Organoheterocyclic compounds | Tetrapyrroles and derivatives | Bilirubins |
| Ile-Pro | NEG | 2.09299159 | 0.816739352 | 0.040758981 | 227.06743 | 107.6775 | HMDB0000012 | C00526 | Nucleosides, nucleotides, and analogues | Pyrimidine nucleosides | Pyrimidine 2'-deoxyribonucleosides |
| Pyruvaldehyde | NEG | 2.027984519 | 0.520660722 | 0.034908911 | 71.01386 | 327.4815 | HMDB0001167 | C00546 | Organic oxygen compounds | Organooxygen compounds | Carbonyl compounds |
| N-(octadecanoyl)sphing-4-enine-1-phosphocholine | POS | 3.084264423 | 0.635285471 | 0.004483786 | 731.60608 | 200.8605 | HMDB0001348 | C00550 | Lipids and lipid-like molecules | Sphingolipids | Phosphosphingolipids |
| Guanidoacetic acid | NEG | 2.683949817 | 1.25493735 | 0.004058659 | 116.03538 | 311.0695 | HMDB0000128 | C00581 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| N-acetyl-l-glutamate | NEG | 1.052491536 | 0.729594575 | 0.004128623 | 188.05651 | 414.269 | HMDB0001138 | C00624 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Betaine | POS | 9.7494883 | 0.831625932 | 0.018337217 | 118.08617 | 293.189 | HMDB0000043 | C00719 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Pro-Trp | POS | 1.834107321 | 0.48231859 | 0.041715622 | 302.30526 | 52.24735 | HMDB0000269 | C00836 | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| Pantothenate | NEG | 1.841536149 | 0.737388708 | 0.004987653 | 218.10352 | 300.4585 | HMDB0000210 | C00864 | Organic oxygen compounds | Organooxygen compounds | Alcohols and polyols |
| Porphobilinogen | NEG | 1.110750017 | 0.708952766 | 0.000732682 | 225.06504 | 280.914 | HMDB0000245 | C00931 | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| .gamma.-hydroxybutyric acid | NEG | 1.512588493 | 1.380959695 | 0.013270765 | 103.04011 | 302.6665 | HMDB0000710 | C00989 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 3-hydroxybutyric acid | NEG | 12.90587711 | 1.741948892 | 0.002561008 | 103.04008 | 264.2515 | HMDB0000357 | C01089 | Organic acids and derivatives | Hydroxy acids and derivatives | Beta hydroxy acids and derivatives |
| 7-keto-8-aminopelargonic acid | POS | 5.283150173 | 0.832449215 | 0.01601052 | 188.13939 | 526.0045 |  | C01092 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 5.alpha.-cholest-7-en-3.beta.-ol | POS | 4.736484075 | 2.243957765 | 0.002461749 | 369.35148 | 24.9114 | HMDB0001170 | C01189 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Cholestane steroids |
| Anserine | POS | 2.123085405 | 0.449284524 | 0.049631901 | 241.12956 | 432.931 | HMDB0000194 | C01262 | Organic acids and derivatives | Peptidomimetics | Hybrid peptides |
| Maleic acid | NEG | 1.377005942 | 0.602309856 | 0.002145144 | 115.00372 | 402.198 | HMDB0000176 | C01384 | Organic acids and derivatives | Carboxylic acids and derivatives | Dicarboxylic acids and derivatives |
| Linoleic acid | NEG | 13.52197992 | 1.215674544 | 0.039781431 | 279.23299 | 44.70725 | HMDB0000673 | C01595 | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| Gibberellic acid | NEG | 1.276865528 | 1.599400574 | 0.000507832 | 239.16534 | 94.15715 | HMDB0003559 | C01699 | Lipids and lipid-like molecules | Prenol lipids | Diterpenoids |
| Kynurenic acid | NEG | 1.560988142 | 0.600768569 | 0.015081962 | 188.03532 | 211.11 | HMDB0000715 | C01717 | Organoheterocyclic compounds | Quinolines and derivatives | Quinoline carboxylic acids |
| Lanosterol | NEG | 1.861382755 | 1.986439916 | 0.002236131 | 425.3638 | 92.5127 | HMDB0001251 | C01724 | Lipids and lipid-like molecules | Prenol lipids | Triterpenoids |
| Lumichrome | NEG | 1.890886854 | 14.1186757 | 0.008385744 | 259.08278 | 26.45675 |  | C01727 | Organoheterocyclic compounds | Pteridines and derivatives | Alloxazines and isoalloxazines |
| Xanthosine | NEG | 3.193863296 | 0.471962211 | 0.010681834 | 283.06868 | 337.223 | HMDB0000299 | C01762 | Nucleosides, nucleotides, and analogues | Purine nucleosides |  |
| L-pyroglutamic acid | NEG | 8.642548471 | 0.68928692 | 0.002898347 | 128.03533 | 326.871 | HMDB0000267 | C01879 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| L-(+)-erythrulose | NEG | 1.604959205 | 0.597325471 | 0.037707546 | 101.02444 | 328.139 |  | C02045 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Vitamin k1 | NEG | 1.007391429 | 1.125236325 | 0.039904219 | 449.36377 | 55.4988 | HMDB0003555 | C02059 | Lipids and lipid-like molecules | Prenol lipids | Quinone and hydroquinone lipids |
| Gly-Leu | POS | 1.250167746 | 2.222055387 | 0.034777073 | 189.11295 | 27.1392 | HMDB0000759 | C02155 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| D-pyroglutamic acid | POS | 4.330407583 | 0.798786776 | 0.04324013 | 130.04999 | 394.965 |  | C02237 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| D-Glucuronolactone | NEG | 4.53182588 | 2.376241103 | 0.002869296 | 175.02479 | 244.6765 | HMDB0006355 | C02670 | Organoheterocyclic compounds | Lactones | Gamma butyrolactones |
| N6-methyl-l-lysine | POS | 1.476284333 | 0.882525963 | 0.025858572 | 161.12844 | 546.5295 | HMDB0002038 | C02728 | Organic acids and derivatives | Carboxylic acids and derivatives | "Amino acids, peptides, and analogues" |
| N-acetyltryptophan | NEG | 1.145598651 | 0.692749888 | 0.021749106 | 245.09322 | 217.772 |  | C03137 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 2-hydroxyisocaproic acid | NEG | 6.701562278 | 1.3429213 | 0.037365829 | 131.07141 | 144.0565 | HMDB0000624 | C03264 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 4-nitroquinoline-1-oxide | POS | 2.339388052 | 0.815621806 | 0.033033396 | 191.03999 | 395.145 |  | C03474 | Organoheterocyclic compounds | Quinolines and derivatives | Nitroquinolines and derivatives |
| Hydroxyphenyllactic acid | NEG | 1.546609906 | 0.654728501 | 0.004726522 | 181.05065 | 213.39 | HMDB0000755 | C03672 | Phenylpropanoids and polyketides | Phenylpropanoic acids |  |
| 3-hydroxy-3-methylglutaric acid | NEG | 1.747664574 | 1.33697112 | 0.037937642 | 161.04556 | 419.249 | HMDB0000355 | C03761 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 1-methylhistamine | POS | 2.141040174 | 1.249289735 | 0.010797653 | 126.10264 | 348.9355 | HMDB0000898 | C05127 | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| Melibiose | NEG | 1.045785733 | 0.224775928 | 0.033777751 | 221.06687 | 340.114 | HMDB0000048 | C05402 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acyl glycosides |
| 7.alpha.-hydroxy-4-cholesten-3-one | POS | 1.039185605 | 2.244112824 | 0.000642372 | 383.33093 | 30.21935 | HMDB0001993 | C05455 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Cholestane steroids |
| 11beta-hydroxyprogesterone | NEG | 1.35211569 | 2.783724511 | 0.000788515 | 329.23361 | 183.417 | HMDB0004031 | C05498 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Pregnane steroids |
| 1,4-butynediol | NEG | 1.669042622 | 0.5766971 | 0.036858509 | 85.02946 | 327.512 | HMDB0012136 | C05771 | Organic oxygen compounds | Organooxygen compounds | Alcohols and polyols |
| Cysteine-s-sulfate | NEG | 1.115159383 | 0.628594384 | 0.042650785 | 199.9694 | 332.734 | HMDB0000731 | C05824 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Dl-a-hydroxybutyric acid | NEG | 6.788153322 | 1.468158912 | 0.015523094 | 103.04007 | 213.07 | HMDB0000008 | C05984 | Organic acids and derivatives | Hydroxy acids and derivatives | Alpha hydroxy acids and derivatives |
| Adipic acid | NEG | 1.332405673 | 0.77284814 | 0.034891513 | 127.05133 | 396.0105 | HMDB0000448 | C06104 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 4-hydroxyquinoline | NEG | 1.08882174 | 0.601031892 | 0.011341421 | 144.04552 | 214.316 |  | C06343 | Organoheterocyclic compounds | Quinolines and derivatives | Quinolones and derivatives |
| Myristic acid | NEG | 5.006607204 | 0.685429311 | 0.017703584 | 227.20167 | 47.3207 | HMDB0000806 | C06424 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Prostaglandin e3 | NEG | 2.031323383 | 0.134705734 | 0.022739597 | 331.19168 | 95.12045 | HMDB0002664 | C06439 | Lipids and lipid-like molecules | Fatty Acyls | Eicosanoids |
| Solanidine | POS | 1.992795977 | 0.821745262 | 0.033642867 | 398.32656 | 196.55 | HMDB0003236 | C06543 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Steroidal alkaloids |
| Cycloheximide | POS | 2.492234613 | 0.697130931 | 0.00019083 | 246.17016 | 261.6035 |  | C06685 | Organoheterocyclic compounds | Pyridines and derivatives | Hydropyridines |
| Fenfluramine | POS | 6.071285053 | 0.131686244 | 0.018712062 | 159.02757 | 182.3175 |  | C06996 | Benzenoids | Benzene and substituted derivatives | Phenethylamines |
| Pamidronic acid | POS | 1.140318921 | 0.624029716 | 0.001450246 | 257.99299 | 321.2545 | HMDB0014427 | C07395 | Organic acids and derivatives | Organic phosphonic acids and derivatives | Bisphosphonates |
| Pentazocine | POS | 1.022029597 | 0.592079883 | 1.53989E-05 | 286.20156 | 231.185 | HMDB0014790 | C07421 | Alkaloids and derivatives | 6,7-benzomorphans | 2,6-dimethyl-3-benzazocines |
| Dapsone | POS | 1.003876928 | 0.742572342 | 0.005440613 | 249.06101 | 279.479 | HMDB0014395 | C07666 | Benzenoids | Benzene and substituted derivatives | Benzenesulfonyl compounds |
| Tazobactam | POS | 1.536892594 | 0.439189392 | 0.016605372 | 323.03914 | 336.5405 |  | C07771 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Metipranolol | POS | 1.880947947 | 0.519291057 | 7.62497E-06 | 310.20134 | 223.7725 | HMDB0015345 | C07915 |  |  |  |
| Indole-3-carboxaldehyde | POS | 1.059467498 | 0.618700086 | 0.001056799 | 146.06004 | 279.3565 | HMDB0029737 | C08493 | Organoheterocyclic compounds | Indoles and derivatives | Indoles |
| Pristimerin | NEG | 2.394091076 | 2.160632363 | 1.45508E-05 | 463.30975 | 40.49765 |  | C08633 | Lipids and lipid-like molecules | Prenol lipids | Triterpenoids |
| Melamine | POS | 1.12458329 | 0.774107704 | 0.04238908 | 127.09776 | 472.909 | HMDB0041922 | C08737 | Organoheterocyclic compounds | Triazines | 1,3,5-triazines |
| Nepodin | NEG | 4.337703632 | 2.370244138 | 0.00284939 | 215.07329 | 263.4525 |  | C09954 | Benzenoids | Naphthalenes | Naphthols and derivatives |
| Chrysosplenetin | POS | 1.278724989 | 0.832359914 | 0.022056001 | 375.09863 | 329.237 |  | C10030 | Phenylpropanoids and polyketides | Flavonoids | O-methylated flavonoids |
| Swainsonine | POS | 1.711905626 | 1.570192958 | 0.024215674 | 174.12394 | 333.569 |  | C10173 |  |  |  |
| Trichloroacetic acid | NEG | 2.529925362 | 1.26371485 | 0.035722098 | 160.89684 | 31.6763 | HMDB0042048 | C11150 | Organic acids and derivatives | Carboxylic acids and derivatives | Alpha-halocarboxylic acids and derivatives |
| Tetrabenazine | POS | 1.321520182 | 1.394260716 | 0.02417497 | 318.19136 | 396.893 | HMDB0015592 | C11168 |  |  |  |
| Perillic acid | NEG | 2.666751786 | 0.556620616 | 0.000289838 | 165.09207 | 65.4721 | HMDB0004586 | C11924 | Lipids and lipid-like molecules | Prenol lipids | Monoterpenoids |
| 3-amino-2,3-dihydrobenzoic acid | POS | 2.781606016 | 0.829971031 | 0.023096805 | 140.06817 | 293.189 |  | C12110 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Paxilline | NEG | 1.635380631 | 0.372859154 | 0.013371266 | 434.23693 | 35.5653 | HMDB0030323 | C13782 |  |  |  |
| (-)-catechin | POS | 1.67689668 | 0.630204908 | 0.032180653 | 165.05049 | 247.385 |  | C14079 | Phenylpropanoids and polyketides | Flavonoids | Flavans |
| 7-methyluric acid | POS | 1.574918822 | 0.471188375 | 0.021584232 | 183.06256 | 299.996 | HMDB0011107 | C16355 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| 5-hydroxyvalproic acid | NEG | 1.442244711 | 0.515002028 | 0.000375195 | 159.10265 | 93.6574 | HMDB0013898 | C16650 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Shikonin | NEG | 1.065159033 | 0.637209027 | 0.000536435 | 218.02252 | 322.886 | HMDB0030579 | C17412 | Benzenoids | Naphthalenes | Naphthoquinones |
| Bisdemethoxycurcumin | NEG | 1.349971962 | 0.597213995 | 0.030820195 | 307.08433 | 328.785 | HMDB0002114 | C17743 | Phenylpropanoids and polyketides | Diarylheptanoids | Linear diarylheptanoids |
| Nootkatone | POS | 3.949896846 | 0.625083069 | 0.004420707 | 219.17426 | 28.9515 |  | C17914 | Lipids and lipid-like molecules | Prenol lipids | Sesquiterpenoids |
| 16-hydroxyhexadecanoic acid | NEG | 2.787440366 | 1.538160115 | 0.02893184 | 271.22796 | 54.8142 | HMDB0006294 | C18218 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Azaconazole | POS | 1.184165794 | 1.486751515 | 0.004023321 | 232.98547 | 24.3465 |  | C18701 | Benzenoids | Benzene and substituted derivatives | Halobenzenes |
| Propanoic acid, 2-(4-chloro-2-methylphenoxy)- | NEG | 1.967127395 | 0.545854981 | 0.040807611 | 213.01719 | 210.485 |  | C18742 | Benzenoids | Benzene and substituted derivatives | 2-phenoxypropionic acids |
| 1-(3-pyridyl)-1-butanone-4-carboxylic acid | NEG | 1.35691909 | 0.211612829 | 0.042316589 | 178.05091 | 217.317 | HMDB0000992 | C19569 | Organic acids and derivatives | Keto acids and derivatives | Gamma-keto acids and derivatives |
| D-turanose | NEG | 1.578055707 | 0.509426027 | 0.029288132 | 161.04554 | 327.521 | HMDB0011740 | C19636 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acyl glycosides |
| Sulfobacin b | NEG | 20.22277975 | 0.020220969 | 0.000491432 | 574.45094 | 32.9733 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty amides |
| N-palmitoyl-d-erythro-dihydroceramide-1-phosphate | NEG | 9.792340407 | 0.027619937 | 6.12932E-13 | 618.47707 | 35.0466 | HMDB0010698 |  | Lipids and lipid-like molecules | Sphingolipids | Phosphosphingolipids |
| Ethcathinone | POS | 10.69070392 | 0.28683522 | 3.03777E-07 | 160.13322 | 404.104 |  |  | Organic oxygen compounds | Organooxygen compounds | Carbonyl compounds |
| Minoxidil | NEG | 1.998249168 | 0.289570515 | 0.019443574 | 207.99416 | 86.6394 | HMDB0014494 |  | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| 4-bromoamphetamine | POS | 1.132538528 | 0.309444859 | 0.02203589 | 197.00472 | 235.611 |  |  | Benzenoids | Benzene and substituted derivatives | Phenethylamines |
| N-(4-morpholin-4-ylphenyl)-2-nitrobenzenesulfonamide | POS | 1.002812362 | 0.434926923 | 0.018007816 | 177.0872 | 350.588 |  |  | Organoheterocyclic compounds | Oxazinanes | Morpholines |
| D-saccharic acid 1,4-lactone | NEG | 1.732843395 | 0.446398307 | 0.030526607 | 383.06516 | 326.885 | HMDB0041862 |  | Organoheterocyclic compounds | Lactones | Gamma butyrolactones |
| Alitame | POS | 1.058858489 | 0.446437109 | 0.017596687 | 159.07651 | 227.233 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Trans-3'-hydroxycotinine o-.beta.-d-glucuronide | NEG | 9.866366696 | 0.477746929 | 0.022847044 | 367.10521 | 328.142 |  |  | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Urushiol ii | NEG | 1.125974594 | 0.491762292 | 0.000979434 | 347.29561 | 183.351 |  |  | Benzenoids | Phenols | Benzenediols |
| Docosatrienoic acid | POS | 1.512498221 | 0.50537415 | 0.005482035 | 335.29451 | 31.7893 | HMDB0002823 |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| 4-methylcyclohexaneacetic acid | NEG | 1.852004831 | 0.537949398 | 0.006000864 | 155.10776 | 51.8572 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Carboxylic acids |
| Fingolimod | POS | 3.155689288 | 0.542906833 | 0.018186968 | 290.26895 | 72.50885 |  |  | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| 4-hexylresorcinol | NEG | 1.03291786 | 0.565936523 | 0.001897802 | 193.12341 | 52.4136 | HMDB0032567 |  | Benzenoids | Phenols | Benzenediols |
| 1-myristoyl-2-palmitoyl-sn-glycero-3-phosphocholine | POS | 2.496233031 | 0.601568768 | 2.31341E-09 | 706.53747 | 167.042 | HMDB0007869 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 2,4,6-tri-tert-butylaniline | POS | 1.031252657 | 0.619738246 | 0.030420263 | 246.24266 | 48.0954 |  |  | Benzenoids | Benzene and substituted derivatives | Phenylpropanes |
| 1-(3,5-dihydroxyphenyl)-2-[(1,1-dimethylethyl)amino]ethanone | NEG | 1.133289151 | 0.622767142 | 0.028424278 | 222.11361 | 167.601 |  |  | Organic oxygen compounds | Organooxygen compounds | Carbonyl compounds |
| Dodeca-2(e),4(e)-dienoic acid | NEG | 1.372866507 | 0.658152148 | 0.009440781 | 195.13904 | 34.81115 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| (2-aminoethoxy)[2-[docosa-4.7.10.13.16.19-hexaenoyloxy]-3-[hexadec-1-en-1-yloxy]propoxy]phosphinic acid | NEG | 3.398175579 | 0.669663843 | 0.000257528 | 746.51302 | 153.8135 | HMDB0005780 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Ile-Asn | POS | 1.498020223 | 0.676422073 | 0.004341014 | 246.12398 | 258.8855 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 1-heptadecanoyl-sn-glycero-3-phosphocholine | POS | 3.379876411 | 0.685008602 | 0.025657067 | 510.35558 | 215.281 | HMDB0012108 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-oleoyl-2-myristoyl-sn-glycero-3-phosphocholine | POS | 5.034865312 | 0.686037322 | 0.000417687 | 732.55336 | 163.8885 | HMDB0008097 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Ethyl 2,4-dihydroxy-6-methylbenzoate | POS | 1.527857364 | 0.687284509 | 0.028671947 | 169.05769 | 395.201 |  |  | Benzenoids | Benzene and substituted derivatives | Benzoic acids and derivatives |
| 1-stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine | POS | 10.92077567 | 0.69477271 | 7.50095E-05 | 834.59966 | 149.481 | HMDB0008057 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pi 40:6 | NEG | 1.620398883 | 0.716583106 | 0.00054025 | 909.54918 | 219.78 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine | POS | 13.56932476 | 0.722130696 | 2.02711E-05 | 568.33973 | 212.742 |  |  |  |  |  |
| 3,5-dihydroxybenzoic acid | NEG | 1.07504077 | 0.72956452 | 0.035072157 | 307.06463 | 26.4389 | HMDB0013677 |  | Benzenoids | Benzene and substituted derivatives | Benzoic acids and derivatives |
| L-leucyl-l-proline | POS | 2.469069586 | 0.734980219 | 0.001434469 | 229.15484 | 387.986 | HMDB0011175 |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 1-(1z-octadecenyl)-2-(5z,8z,11z,14z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine | NEG | 2.130530581 | 0.738787199 | 0.004383469 | 750.54385 | 153.7435 | HMDB0005779 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 1-myristoyl-sn-glycero-3-phosphocholine | POS | 5.405433933 | 0.742467554 | 0.001297035 | 468.3083 | 221.7175 | HMDB0010379 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Isobutyryl-l-carnitine | POS | 1.169826514 | 0.747999469 | 0.024547985 | 232.15435 | 277.098 | HMDB0000736 |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty acid esters |
| 2-amino-4,6-dihydroxypyrimidine | NEG | 1.37053828 | 0.756101489 | 0.016101614 | 126.01969 | 294.621 |  |  | Organoheterocyclic compounds | Diazines | Pyrimidines and pyrimidine derivatives |
| (2-aminoethoxy)[3-[hexadec-1-en-1-yloxy]-2-[icosa-5.8.11.14-tetraenoyloxy]propoxy]phosphinic acid | NEG | 1.937573504 | 0.768570633 | 0.008323766 | 722.51316 | 155.156 | HMDB0011352 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 5-methyl-7-methoxyisoflavone | POS | 1.450945513 | 0.771834613 | 0.010081082 | 267.1106 | 322.5795 |  |  | Phenylpropanoids and polyketides | Isoflavonoids | O-methylated isoflavonoids |
| Pe 34:0 | NEG | 1.265452137 | 0.776182344 | 0.012473062 | 718.53882 | 165.806 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 2',2'-difluoro-2'-deoxyuridine | NEG | 1.310373324 | 0.797134115 | 0.019833193 | 263.04412 | 107.737 |  |  | Nucleosides, nucleotides, and analogues | Pyrimidine nucleosides | Pyrimidine 2'-deoxyribonucleosides |
| 1-hexadecyl-2-(5z,8z,11z,14z-eicosatetraenoyl)-sn-glycero-3-phosphocholine | POS | 2.008349958 | 0.803306492 | 0.00928072 | 768.59017 | 153.747 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-o-hexadecyl-2-o-(5z,8z,11z,14z,17z-eicosapentaenoyl)-sn-glyceryl-3-phosphorylcholine | POS | 1.97545153 | 0.819660672 | 0.015660226 | 766.57413 | 148.388 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| N-acetyl-dl-serine | NEG | 1.844605022 | 0.822405916 | 0.015231247 | 146.04588 | 327.525 |  |  |  |  |  |
| Pc 38:6 | NEG | 3.154824561 | 0.859034443 | 0.000981578 | 864.57577 | 153.8235 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-stearoyl-2-arachidonyl-sn-glycero-3-phosphocholine | POS | 7.394117089 | 0.866692946 | 0.027919761 | 810.59995 | 151.188 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine | POS | 8.59403661 | 0.889198169 | 0.003110684 | 806.56909 | 153.2585 | HMDB0007991 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-hexadecanoyl-2-octadecadienoyl-sn-glycero-3-phosphocholine | POS | 16.29063622 | 1.100029888 | 0.033872787 | 758.56916 | 161.593 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 2-arachidonoyl-1-stearoyl-sn-glycero-3-phosphoethanolamine | NEG | 2.262616553 | 1.155449805 | 0.03611219 | 766.53886 | 156.8625 | HMDB0009003 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Pe 36:2 | NEG | 3.468913789 | 1.180071771 | 0.038524643 | 742.5391 | 162.408 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 1,2-dilinoleoylglycerol | POS | 3.234590483 | 1.2918924 | 0.000177257 | 599.50347 | 222.35 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| 1-arachidoyl-2-hydroxy-sn-glycero-3-phosphocholine | POS | 3.059721599 | 1.316985741 | 0.004967824 | 552.4024 | 211.2925 | HMDB0010390 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 7-methoxy-2-propylquinolin-4-ol | NEG | 4.049265638 | 1.339081948 | 0.00870577 | 201.05767 | 263.4855 |  |  | Organoheterocyclic compounds | Quinolines and derivatives | Quinolones and derivatives |
| Pi 36:4 | NEG | 4.594709047 | 1.353307279 | 0.000614147 | 857.51818 | 222.854 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 4'-o-.beta.-d-glucosyl-5-o-methylvisamminol | POS | 3.610255441 | 1.360967117 | 0.000413164 | 453.16728 | 34.22385 |  |  | Organoheterocyclic compounds | Benzopyrans | 1-benzopyrans |
| S4:18(p3:16/f1:2) | NEG | 1.125015215 | 1.439130042 | 0.023111077 | 695.3117 | 28.9938 |  |  |  |  |  |
| Lpe 18:2 | POS | 4.246922721 | 1.442557321 | 0.034846015 | 478.29282 | 223.481 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Angeloylgomisin h | POS | 1.569141833 | 1.471187597 | 0.01605675 | 523.24563 | 31.6216 |  |  | Phenylpropanoids and polyketides | Tannins | Hydrolyzable tannins |
| Pc 36:2 | NEG | 4.480087661 | 1.49723163 | 0.002052957 | 844.60637 | 124.816 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 2-linoleoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine | POS | 3.15626632 | 1.500067083 | 1.6697E-06 | 575.50358 | 225.252 | HMDB0008928 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Pi 34:2 | NEG | 3.063119211 | 1.552683028 | 7.11361E-06 | 833.5185 | 225.316 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 1-palmitoyl-2-linoleoyl-rac-glycerol | POS | 1.682125169 | 1.556841405 | 0.006362586 | 337.27383 | 223.0485 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| Drofenine | POS | 2.574982437 | 1.569838337 | 0.008269396 | 318.2403 | 33.1795 |  |  |  |  |  |
| Met-Met-Arg | POS | 6.784132091 | 1.634768489 | 0.024878956 | 437.19328 | 34.1354 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 1.alpha.-methyl-5.alpha.-androstan-3.alpha.,17.beta.-diol glucuronide | NEG | 1.482672955 | 1.645232457 | 0.000118565 | 481.29895 | 27.0478 |  |  |  |  |  |
| 4-(1-piperazinyl)-1h-indole | POS | 2.038753691 | 1.650906982 | 0.004450533 | 202.11883 | 289.463 |  |  | Organoheterocyclic compounds | Diazinanes | Piperazines |
| 1h-imidazole, 2-[(1-methylpropyl)dithio]- | POS | 1.281730098 | 1.808699718 | 0.012727816 | 132.98723 | 142.949 |  |  | Organoheterocyclic compounds | Azoles | Imidazoles |
| Pe 34:2 | NEG | 2.214010313 | 1.841269324 | 0.012424464 | 714.50783 | 167.8075 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Pi 36:3 | NEG | 4.493858112 | 1.842757828 | 2.28612E-06 | 859.53146 | 223.9225 |  |  |  |  |  |
| 1-palmitoyl-2-oleoyl-3-linoleoyl-rac-glycerol | POS | 1.074252814 | 2.013984091 | 0.003521502 | 601.51935 | 165.357 |  |  | Lipids and lipid-like molecules | Glycerolipids | Triradylcglycerols |
| N-palmitoyl-d-sphingosine | NEG | 2.312051665 | 2.205087769 | 1.20417E-06 | 536.50455 | 32.2434 | HMDB0004949 |  | Lipids and lipid-like molecules | Sphingolipids | Ceramides |
| N-[1,3-dihydroxyoctadec-4-en-2-yl]tetracos-15-enamide | NEG | 3.3824879 | 2.262474506 | 0.000120717 | 646.61415 | 31.584 |  |  | Lipids and lipid-like molecules | Sphingolipids | Ceramides |
| Fahfa 36:1 | NEG | 1.650018766 | 2.282656959 | 0.000371926 | 563.50393 | 45.0079 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Fa 18:2+1o | NEG | 7.127819602 | 2.561070768 | 0.000714502 | 295.2279 | 52.6503 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| Propanoic acid, 3-[[[2-[(aminoiminomethyl)amino]-4-thiazolyl]methyl]thio]- | NEG | 5.182481167 | 3.020761426 | 0.02621025 | 187.00708 | 45.1952 |  |  | Organoheterocyclic compounds | Azoles | Thiazoles |

Note: The red font represents the up-regulated differential metabolites, and the blue font represents the down-regulated differential metabolites.

**Table S5** DEMs between PVSO and HFD groups.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | mode | **VIP** | **Fold change** | **p-value** | **m/z** | **rt(s)** | **HMDB** | **KEGG** | **SuperClass** | **Class** | **SubClass** |
| Pyruvate | NEG | 29.93832313 | 0.385982267 | 0.001684692 | 87.00873 | 144.36 | HMDB0000243 | C00022 | Organic acids and derivatives | Keto acids and derivatives | Alpha-keto acids and derivatives |
| DL-Glutamic acid | NEG | 4.876326863 | 0.686565885 | 0.006912093 | 146.04593 | 422.402 | HMDB0060475 | C00025 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Glycine | NEG | 2.533862362 | 0.731142263 | 0.005161274 | 74.02476 | 311.038 | HMDB0000123 | C00037 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Lysine | POS | 2.125296933 | 0.837436295 | 0.009197467 | 147.11288 | 542.0215 | HMDB0000182 | C00047 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Uracil | NEG | 5.308762143 | 0.819337101 | 0.039573377 | 111.02 | 77.9762 | HMDB0000300 | C00106 | Organoheterocyclic compounds | Diazines | Pyrimidines and pyrimidine derivatives |
| Choline | POS | 19.25550731 | 0.782909188 | 0.000562434 | 104.10695 | 278.863 | HMDB0000097 | C00114 | Organic nitrogen compounds | Organonitrogen compounds | Quaternary ammonium salts |
| DL-asparagine | NEG | 1.540650927 | 0.785853808 | 0.029395853 | 131.04624 | 405.979 | HMDB0000168 | C00152 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 1,2-dihexadecanoyl-sn-glycero-3-phosphocholine | POS | 4.407106976 | 0.836806442 | 0.007686516 | 734.56913 | 164.8605 | HMDB0000564 | C00157 | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Glycolate | NEG | 3.014391186 | 1.262060466 | 0.031590491 | 75.00875 | 111.89 | HMDB0000115 | C00160 | Organic acids and derivatives | Hydroxy acids and derivatives | Alpha hydroxy acids and derivatives |
| S-methyl-5'-thioadenosine | POS | 1.44142883 | 1.904342726 | 0.008398076 | 298.09676 | 84.89085 | HMDB0001173 | C00170 | Nucleosides, nucleotides, and analogues | 5'-deoxyribonucleosides | 5'-deoxy-5'-thionucleosides |
| Pyridoxal | NEG | 1.418714099 | 3.665654378 | 1.8454E-05 | 166.03767 | 277.1505 | HMDB0001545 | C00250 | Organoheterocyclic compounds | Pyridines and derivatives | Pyridine carboxaldehydes |
| D-arabinose | NEG | 1.192400011 | 2.457842817 | 0.048230581 | 131.03492 | 328.179 | HMDB0029942 | C00259 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Hypoxanthine | POS | 38.47646998 | 6.40423621 | 1.78934E-07 | 137.04584 | 183.213 | HMDB0000157 | C00262 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| Inosine | NEG | 10.67336477 | 20.98375213 | 0.015384007 | 267.07365 | 238.137 | HMDB0000195 | C00294 | Nucleosides, nucleotides, and analogues | Purine nucleosides |  |
| Indole-3-pyruvic acid | NEG | 1.939464021 | 1.307334469 | 0.039437698 | 202.05106 | 72.731 | HMDB0060484 | C00331 | Organoheterocyclic compounds | Indoles and derivatives | Indolyl carboxylic acids and derivatives |
| L-dihydroorotate | NEG | 1.704162065 | 0.520209806 | 0.022013909 | 315.08115 | 422.1255 | HMDB0003349 | C00337 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Uric acid | NEG | 1.203685881 | 1.498229249 | 0.048212544 | 167.02107 | 351.759 | HMDB0000289 | C00366 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| Xanthine | NEG | 2.516208864 | 2.687757523 | 0.005233914 | 151.02619 | 252.468 | HMDB0000292 | C00385 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| Quercetin | NEG | 1.439235626 | 0.531136576 | 3.21663E-06 | 179.02112 | 311.505 | HMDB0005794 | C00389 | Phenylpropanoids and polyketides | Flavonoids | Flavones |
| D-aspartic acid | NEG | 2.741085883 | 0.54952148 | 0.003664453 | 132.03032 | 431.468 | HMDB0006483 | C00402 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| L-pipecolic acid | POS | 1.205195088 | 0.888559571 | 0.00327058 | 130.0863 | 542.4745 | HMDB0000716 | C00408 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Mevalonic acid | NEG | 1.114095207 | 0.658937954 | 0.038631751 | 147.06629 | 211.254 | HMDB0059629 | C00418 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Cytidine | NEG | 2.934729966 | 0.67797183 | 0.002622039 | 242.07994 | 406.179 | HMDB0000089 | C00475 | Nucleosides, nucleotides, and analogues | Pyrimidine nucleosides |  |
| Ile-Pro | NEG | 2.152146439 | 0.773346706 | 0.037487645 | 227.06743 | 107.6775 | HMDB0000012 | C00526 | Nucleosides, nucleotides, and analogues | Pyrimidine nucleosides | Pyrimidine 2'-deoxyribonucleosides |
| Guanidoacetic acid | NEG | 3.328665071 | 0.729863521 | 0.004953239 | 116.03538 | 311.0695 | HMDB0000128 | C00581 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Glycerophosphocholine | POS | 16.25813053 | 0.598265868 | 0.002938255 | 258.11005 | 405.453 | HMDB0000086 | C00670 | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pterine | NEG | 2.347172301 | 0.762763678 | 0.000684629 | 119.03498 | 303.67 | HMDB0000802 | C00715 | Organoheterocyclic compounds | Pteridines and derivatives | Pterins and derivatives |
| D-proline | NEG | 2.184056427 | 0.800940444 | 0.003654637 | 114.05614 | 332.7405 | HMDB0003411 | C00763 | Organic acids and derivatives | Carboxylic acids and derivatives | "Amino acids, peptides, and analogues" |
| Serotonin | POS | 3.098198836 | 0.655449612 | 0.00115546 | 160.07568 | 248.5485 | HMDB0000259 | C00780 | Organoheterocyclic compounds | Indoles and derivatives | Tryptamines and derivatives |
| DL-arginine | POS | 9.15500792 | 0.815042045 | 0.013999489 | 175.11892 | 536.4035 |  | C00792 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| .gamma.-hydroxybutyric acid | NEG | 1.422342121 | 0.747771462 | 0.020918695 | 103.04011 | 302.6665 | HMDB0000710 | C00989 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Piperidine | POS | 4.342010347 | 0.638377355 | 0.006287609 | 86.0966 | 295.596 | HMDB0034301 | C01746 |  |  |  |
| Glycocholic acid | NEG | 1.399440366 | 0.734312508 | 0.003222322 | 464.31476 | 211.874 | HMDB0000138 | C01921 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Bile acids, alcohols and derivatives |
| L-(+)-erythrulose | NEG | 2.826486378 | 2.243433153 | 0.00625568 | 101.02444 | 328.139 |  | C02045 | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| Vitamin k1 | NEG | 2.091137748 | 1.281996288 | 0.005806958 | 449.36377 | 55.4988 | HMDB0003555 | C02059 | Lipids and lipid-like molecules | Prenol lipids | Quinone and hydroquinone lipids |
| Pseudouridine | NEG | 2.527650935 | 0.83683838 | 0.018114851 | 243.06234 | 264.61 | HMDB0000767 | C02067 | Nucleosides, nucleotides, and analogues | Nucleoside and nucleotide analogues |  |
| 4-nitrocatechol | NEG | 3.189926474 | 0.766525486 | 0.003378847 | 154.02578 | 160.8905 | HMDB0002916 | C02235 | Benzenoids | Phenols | Nitrophenols |
| L-homocitrulline | NEG | 1.30822051 | 0.61213243 | 0.00200259 | 188.08294 | 281.1605 | HMDB0000679 | C02427 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| .beta.-cyano-l-alanine | NEG | 1.383861891 | 0.814079978 | 0.001326071 | 96.02024 | 312.9485 | HMDB0060245 | C02512 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| N-methyl-l-alanine | NEG | 1.609309324 | 0.69559232 | 0.007481129 | 102.0561 | 422.402 | HMDB0094692 | C02721 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| N6-methyl-l-lysine | POS | 1.16596786 | 0.837300189 | 0.012532848 | 161.12844 | 546.5295 | HMDB0002038 | C02728 | Organic acids and derivatives | Carboxylic acids and derivatives | "Amino acids, peptides, and analogues" |
| L-palmitoylcarnitine | POS | 3.537545242 | 0.750772262 | 0.0014216 | 400.34223 | 194.773 | HMDB0000222 | C02990 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acid esters |
| Ng,ng-dimethyl-l-arginine | POS | 6.506432386 | 0.779096463 | 0.004700613 | 116.07067 | 331.895 | HMDB0001539 | C03626 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Acadesine (drug) | POS | 1.14571597 | 0.710124113 | 0.024815776 | 242.07893 | 429.5535 | HMDB0062179 | C04663 |  |  |  |
| Prostaglandin a1 | NEG | 2.494095029 | 0.65799924 | 0.013958442 | 335.22294 | 82.68475 | HMDB0002656 | C04685 | Lipids and lipid-like molecules | Fatty Acyls | Eicosanoids |
| Melibiose | NEG | 1.986882783 | 7.694331143 | 0.007214033 | 221.06687 | 340.114 | HMDB0000048 | C05402 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acyl glycosides |
| Taurochenodeoxycholate | NEG | 2.070863421 | 0.668738781 | 0.048437942 | 498.2896 | 179.42 | HMDB0000951 | C05465 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Bile acids, alcohols and derivatives |
| L-threonine | NEG | 1.452036861 | 0.843069622 | 0.029041293 | 118.05101 | 377.2225 | HMDB0004041 | C05519 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| DL-Vanillylmandelic acid | NEG | 15.52721583 | 0.758511802 | 0.00174075 | 197.03188 | 160.894 | HMDB0133489 | C05584 | Benzenoids | Phenols | Methoxyphenols |
| Trans-3,5-dimethoxy-4-hydroxycinnamaldehyde | NEG | 1.543669828 | 0.461410884 | 0.036556005 | 207.06635 | 52.9846 |  | C05610 | Benzenoids | Phenols | Methoxyphenols |
| 4-hydroxy-l-glutamic acid | POS | 1.306681177 | 0.557581663 | 0.002732233 | 146.02722 | 255.651 |  | C05947 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Terephthalic acid | NEG | 3.088420111 | 0.764544159 | 0.002052619 | 165.00521 | 160.896 | HMDB0002428 | C06337 | Benzenoids | Benzene and substituted derivatives | Benzoic acids and derivatives |
| Prostaglandin f1.alpha. | NEG | 1.079053244 | 1.863628973 | 0.040930691 | 355.26419 | 41.08745 | HMDB0002685 | C06475 | Lipids and lipid-like molecules | Fatty Acyls | Eicosanoids |
| Solanidine | POS | 1.694706532 | 0.783692574 | 0.008577714 | 398.32656 | 196.55 | HMDB0003236 | C06543 | Lipids and lipid-like molecules | Steroids and steroid derivatives | Steroidal alkaloids |
| 4-methylbenzyl alcohol | POS | 4.58622165 | 1.147705266 | 0.015285127 | 105.0701 | 34.8777 | HMDB0041609 | C06757 | Benzenoids | Benzene and substituted derivatives | Benzyl alcohols |
| Fenfluramine | POS | 8.611942947 | 11.87461497 | 2.66533E-06 | 159.02757 | 182.3175 |  | C06996 | Benzenoids | Benzene and substituted derivatives | Phenethylamines |
| Glutethimide | POS | 3.504942325 | 0.820552375 | 0.021447235 | 190.09765 | 254.948 | HMDB0015505 | C07489 | Organoheterocyclic compounds | Piperidines | Phenylpiperidines |
| Topiramate | POS | 1.642517687 | 0.562045318 | 0.005591452 | 362.0836 | 405.46 | HMDB0005034 | C07502 | Organoheterocyclic compounds | Dioxolopyrans |  |
| 4-hydroxycyclophosphamide | POS | 2.822844509 | 0.718425991 | 0.002283109 | 221.01854 | 405.4705 | HMDB0013856 | C07643 | Organic nitrogen compounds | Organonitrogen compounds | Nitrogen mustard compounds |
| Ellipticine | POS | 1.025384355 | 0.527919689 | 0.003724566 | 247.14007 | 371.004 |  | C09154 | Organoheterocyclic compounds | Indoles and derivatives | Carbazoles |
| Stachydrine | POS | 1.073956789 | 0.697693452 | 0.000376439 | 144.10192 | 377.648 | HMDB0004827 | C10172 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 2-aminobenzimidazole | NEG | 1.756891233 | 1.406071891 | 0.049140505 | 132.04557 | 28.3292 |  | C10901 |  |  |  |
| Tetrabenazine | POS | 1.091626583 | 0.679399687 | 0.033661939 | 318.19136 | 396.893 | HMDB0015592 | C11168 |  |  |  |
| 2-arachidonoylglycerol | POS | 1.205703708 | 0.623251838 | 0.004488604 | 361.27398 | 270.539 | HMDB0004666 | C13856 |  |  |  |
| 3-nitrophenol | NEG | 1.283404358 | 3.352323645 | 0.021724418 | 108.02039 | 236.647 |  | C14418 | Benzenoids | Phenols | Nitrophenols |
| 12s-hydroxy-5z,8z,10e,14z-eicosatetraenoic acid | NEG | 10.33958362 | 0.805856197 | 0.036126148 | 319.22791 | 50.50415 |  | C14777 | Lipids and lipid-like molecules | Fatty Acyls | Eicosanoids |
| Purine | NEG | 2.708920563 | 0.80705797 | 0.027890842 | 119.03502 | 280.613 | HMDB0001366 | C15587 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| 7-methylxanthine | NEG | 2.038043858 | 1.160795983 | 0.045698057 | 165.03395 | 293.9425 | HMDB0001991 | C16353 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| 7-methyluric acid | POS | 2.039986944 | 2.503997721 | 6.24497E-05 | 183.06256 | 299.996 | HMDB0011107 | C16355 | Organoheterocyclic compounds | Imidazopyrimidines | Purines and purine derivatives |
| 2-hydroxylamino-4,6-dinitrotoluene | NEG | 3.680121312 | 1.430503313 | 0.017527186 | 194.01287 | 62.9157 |  | C16393 | Benzenoids | Benzene and substituted derivatives | Toluenes |
| L-homocysteic acid | NEG | 1.053421267 | 0.671480196 | 0.005114387 | 182.0224 | 406.587 | HMDB0002205 | C16511 | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 2-methoxy-5-nitrophenol | NEG | 1.403532204 | 0.72824037 | 0.0010436 | 168.02653 | 422.402 |  | C17385 | Benzenoids | Benzene and substituted derivatives | Nitrobenzenes |
| 16-hydroxyhexadecanoic acid | NEG | 3.088551462 | 0.647585271 | 0.033209476 | 271.22796 | 54.8142 | HMDB0006294 | C18218 | Lipids and lipid-like molecules | Fatty Acyls | Fatty acids and conjugates |
| Pyroquilon | POS | 1.813009431 | 0.336007116 | 0.010019576 | 174.08746 | 421.356 | HMDB0037113 | C18487 | Organoheterocyclic compounds | Quinolines and derivatives | Quinolones and derivatives |
| 4,6-dinitro-o-cresol | NEG | 3.383816837 | 1.206708064 | 0.036644042 | 180.03363 | 93.84325 |  | C18653 | Benzenoids | Phenols | Nitrophenols |
| Barbamate | POS | 1.116639266 | 0.824056365 | 0.002104699 | 214.00436 | 421.5415 |  | C19059 | Benzenoids | Benzene and substituted derivatives | Phenylcarbamic acid esters |
| 2-chloro-2',6'-diethylacetanilide | POS | 4.003722489 | 0.661527738 | 0.010825297 | 226.0839 | 406.579 | HMDB0032855 | C21712 | Benzenoids | Benzene and substituted derivatives | Anilides |
| 1h-imidazole, 2-[(1-methylpropyl)dithio]- | POS | 1.532477853 | 0.376931747 | 0.000504245 | 132.98723 | 142.949 |  |  | Organoheterocyclic compounds | Azoles | Imidazoles |
| Pro-Glu | POS | 1.180218837 | 0.394700296 | 0.027429977 | 245.11334 | 439.014 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Sulfanitran | POS | 1.881971175 | 0.576502231 | 0.002527771 | 336.08751 | 405.454 |  |  | Benzenoids | Benzene and substituted derivatives | Sulfanilides |
| Hexanoylglycine | NEG | 3.310107619 | 0.598851181 | 0.006741868 | 172.09776 | 207.179 | HMDB0000701 |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 3-bromo-n,n-dimethylaniline | POS | 1.051281661 | 0.605475355 | 0.000709666 | 199.99062 | 430.1165 |  |  | Organic nitrogen compounds | Organonitrogen compounds | Amines |
| sn-Glycerol 3-phosphoethanolamine | NEG | 2.252166979 | 0.615352825 | 0.001071105 | 214.04864 | 414.4645 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Benzylphosphonic acid | NEG | 1.548674204 | 0.622943889 | 0.003524838 | 152.99589 | 300.8685 |  |  |  |  |  |
| Thieno[2,3-b]pyridine-5-carbonitrile, 6,7-dihydro-4-hydroxy-3-(2'-hydroxy[1,1'-biphenyl]-4-yl)-6-oxo- | NEG | 1.826173098 | 0.627257091 | 0.008903542 | 359.04489 | 422.16 |  |  | Benzenoids | Benzene and substituted derivatives | Biphenyls and derivatives |
| Diflufenzopyr | NEG | 1.236514219 | 0.63430265 | 0.002774656 | 333.05958 | 459.91 |  |  | Benzenoids | Benzene and substituted derivatives | N-phenylureas |
| Fa 18:2+1o | NEG | 5.431735499 | 0.644008464 | 0.014686579 | 295.2279 | 52.6503 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| 1-palmitoyl-2-linoleoyl-rac-glycerol | POS | 1.392029716 | 0.671808764 | 0.000343626 | 337.27383 | 223.0485 |  |  | Lipids and lipid-like molecules | Fatty Acyls | Lineolic acids and derivatives |
| Lys-Gly | NEG | 1.278471428 | 0.677951615 | 0.021094515 | 202.1085 | 204.5595 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| Pc 38:4 | NEG | 1.375230631 | 0.705098435 | 0.006385639 | 868.60602 | 38.93425 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Lpe 18:2 | POS | 3.654806703 | 0.713628463 | 0.003825137 | 478.29282 | 223.481 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 4-aminophenyl-1-thio-.beta.-d-galactopyranoside | POS | 1.552180182 | 0.727677345 | 0.002312225 | 192.02425 | 421.408 |  |  | Organic oxygen compounds | Organooxygen compounds | Carbohydrates and carbohydrate conjugates |
| 4'-hydroxydiclofenac | NEG | 1.011111798 | 0.729606529 | 0.003954529 | 312.00233 | 386.41 | HMDB0013974 |  | Benzenoids | Benzene and substituted derivatives | Halobenzenes |
| 3,6-dimethyl-4-hydroxycoumarin | NEG | 1.939492101 | 0.730591266 | 0.000727649 | 189.06642 | 280.4985 |  |  | Phenylpropanoids and polyketides | Coumarins and derivatives | Hydroxycoumarins |
| S4:18(p3:16/f1:2) | NEG | 1.029558601 | 0.745939222 | 0.035995748 | 695.3117 | 28.9938 |  |  |  |  |  |
| Asn-Asp | POS | 2.169630038 | 0.747604621 | 0.010349336 | 248.06585 | 406.795 |  |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| 4-(1-piperazinyl)-1h-indole | POS | 1.32107187 | 0.749250498 | 0.026175018 | 202.11883 | 289.463 |  |  | Organoheterocyclic compounds | Diazinanes | Piperazines |
| 1-o-hexadecyl-2-o-(5z,8z,11z,14z,17z-eicosapentaenoyl)-sn-glyceryl-3-phosphorylcholine | POS | 1.754690748 | 0.755016408 | 0.009706634 | 766.57413 | 148.388 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Alanine conjugated cholic acid | POS | 3.164614315 | 0.770991237 | 0.0098031 | 502.29277 | 220.3735 |  |  | Lipids and lipid-like molecules | Steroids and steroid derivatives | Bile acids, alcohols and derivatives |
| 1-myristoyl-sn-glycero-3-phosphocholine | POS | 4.052200888 | 0.775965756 | 0.000239873 | 468.3083 | 221.7175 | HMDB0010379 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pc 36:2 | NEG | 3.500977272 | 0.781952937 | 0.016925171 | 844.60637 | 124.816 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pi 34:2 | NEG | 2.288824411 | 0.783100552 | 0.004050815 | 833.5185 | 225.316 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 1-octadecanoyl-sn-glycero-3-phospho-(1'-myo-inositol) | NEG | 1.193129693 | 0.785180174 | 0.000428322 | 599.3205 | 273.7045 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 1-(1z-octadecenyl)-2-(5z,8z,11z,14z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine | NEG | 1.530903366 | 0.787313075 | 0.024136764 | 750.54385 | 153.7435 | HMDB0005779 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Leukotriene b4 dimethylamide | POS | 1.059266542 | 0.78956436 | 0.023386645 | 386.2902 | 224.7655 | HMDB0005085 |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty amides |
| (2-aminoethoxy)[3-[hexadec-1-en-1-yloxy]-2-[icosa-5.8.11.14-tetraenoyloxy]propoxy]phosphinic acid | NEG | 1.507356884 | 0.790246075 | 0.046010262 | 722.51316 | 155.156 | HMDB0011352 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Pi 36:4 | NEG | 3.927771795 | 0.800628248 | 0.004039967 | 857.51818 | 222.854 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| Pi 36:3 | NEG | 2.86959655 | 0.801553948 | 0.006999843 | 859.53146 | 223.9225 |  |  |  |  |  |
| 3-cysteinylacetaminophen | NEG | 5.357096852 | 0.807561971 | 0.001785885 | 182.032 | 313.018 | HMDB0240217 |  | Organic acids and derivatives | Carboxylic acids and derivatives | Amino acids, peptides, and analogues |
| N-palmitoyl-d-sphingosine | NEG | 1.158306469 | 0.811952316 | 0.011293825 | 536.50455 | 32.2434 | HMDB0004949 |  | Lipids and lipid-like molecules | Sphingolipids | Ceramides |
| 1-stearoyl-2-arachidonyl-sn-glycero-3-phosphocholine | POS | 8.306736857 | 0.831893466 | 0.00242596 | 810.59995 | 151.188 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Linoleoylcarnitine | POS | 1.148780802 | 0.832986517 | 0.018771517 | 424.34227 | 192.4975 | HMDB0006469 |  | Lipids and lipid-like molecules | Fatty Acyls | Fatty acid esters |
| 1-palmitoyl-sn-glycero-3-phosphocholine | POS | 4.887860854 | 0.83745072 | 0.005906442 | 184.0733 | 210.7045 | HMDB0010382 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-oleoyl-sn-glycero-3-phosphoethanolamine | NEG | 1.665512505 | 0.83948688 | 0.047198153 | 478.29401 | 220.623 | HMDB0011506 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 2-linoleoyl-1-palmitoyl-sn-glycero-3-phosphoethanolamine | POS | 1.249874765 | 0.852896538 | 0.023047428 | 575.50358 | 225.252 | HMDB0008928 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| 1-hexadecyl-sn-glycero-3-phosphocholine | POS | 2.400746849 | 0.875624824 | 0.021870243 | 482.36016 | 221.32 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Lpc 16:0 | POS | 12.87010548 | 0.877786825 | 0.013494695 | 496.33965 | 217.288 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pi 38:4 | NEG | 5.300852183 | 0.879984565 | 0.015042938 | 885.54941 | 220.8255 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 1-pentadecanoyl-sn-glycero-3-phosphocholine | POS | 1.409135247 | 0.880107082 | 0.015121159 | 482.32532 | 220.3865 | HMDB0010381 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-behenoyl-2-hydroxy-sn-glycero-3-phosphocholine | POS | 1.145173418 | 1.087754037 | 0.041490879 | 580.43384 | 209.0915 | HMDB0010398 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 1-palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine | POS | 13.97863718 | 1.120560539 | 0.001342303 | 806.56909 | 153.2585 | HMDB0007991 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| Pi 40:6 | NEG | 1.288971182 | 1.188553563 | 0.042981901 | 909.54918 | 219.78 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoinositols |
| 2-docosahexaenoyl-1-stearoyl-sn-glycero-3-phosphoethanolamine | NEG | 3.550557959 | 1.25104103 | 0.000328549 | 790.53887 | 154.408 | HMDB0009012 |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| Pc 38:6 | NEG | 5.989389802 | 1.296635934 | 7.72317E-07 | 864.57577 | 153.8235 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphocholines |
| 5-methylisoxazol-3-amine | POS | 1.068649274 | 1.309013074 | 0.03038649 | 99.0554 | 352.197 |  |  |  |  |  |
| Lauryldimethylamine oxide | POS | 1.752557344 | 1.33137562 | 0.022278524 | 230.24786 | 145.337 |  |  | Organic nitrogen compounds | Organonitrogen compounds | Aminoxides |
| Pe 38:6 | NEG | 3.488130205 | 1.484956364 | 0.019480015 | 762.50761 | 160.41 |  |  | Lipids and lipid-like molecules | Glycerophospholipids | Glycerophosphoethanolamines |
| O,o-dimethyl dithiophosphate | NEG | 1.583056488 | 1.559469311 | 0.015675818 | 156.93679 | 24.30645 | HMDB0061737 |  | Organic acids and derivatives | Organic dithiophosphoric acids and derivatives | Dithiophosphate O-esters |
| N-palmitoyl-d-erythro-dihydroceramide-1-phosphate | NEG | 1.592078922 | 1.822216455 | 0.002731279 | 618.47707 | 35.0466 | HMDB0010698 |  | Lipids and lipid-like molecules | Sphingolipids | Phosphosphingolipids |
| Minoxidil | NEG | 2.719142382 | 3.939036238 | 0.004209576 | 207.99416 | 86.6394 | HMDB0014494 |  | Organic nitrogen compounds | Organonitrogen compounds | Amines |

Note: The red font represents the up-regulated differential metabolites, and the blue font represents the down-regulated differential metabolites.