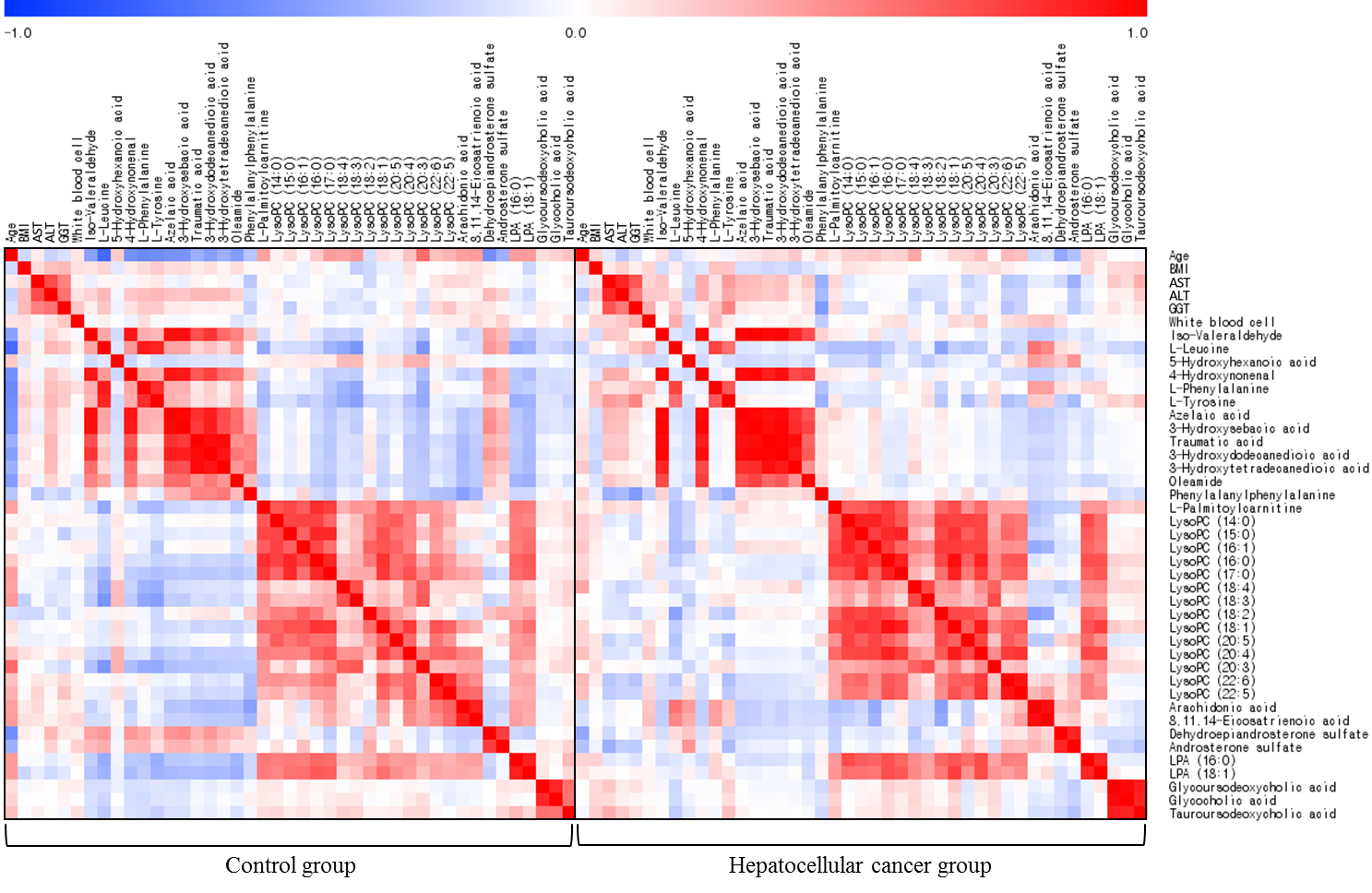
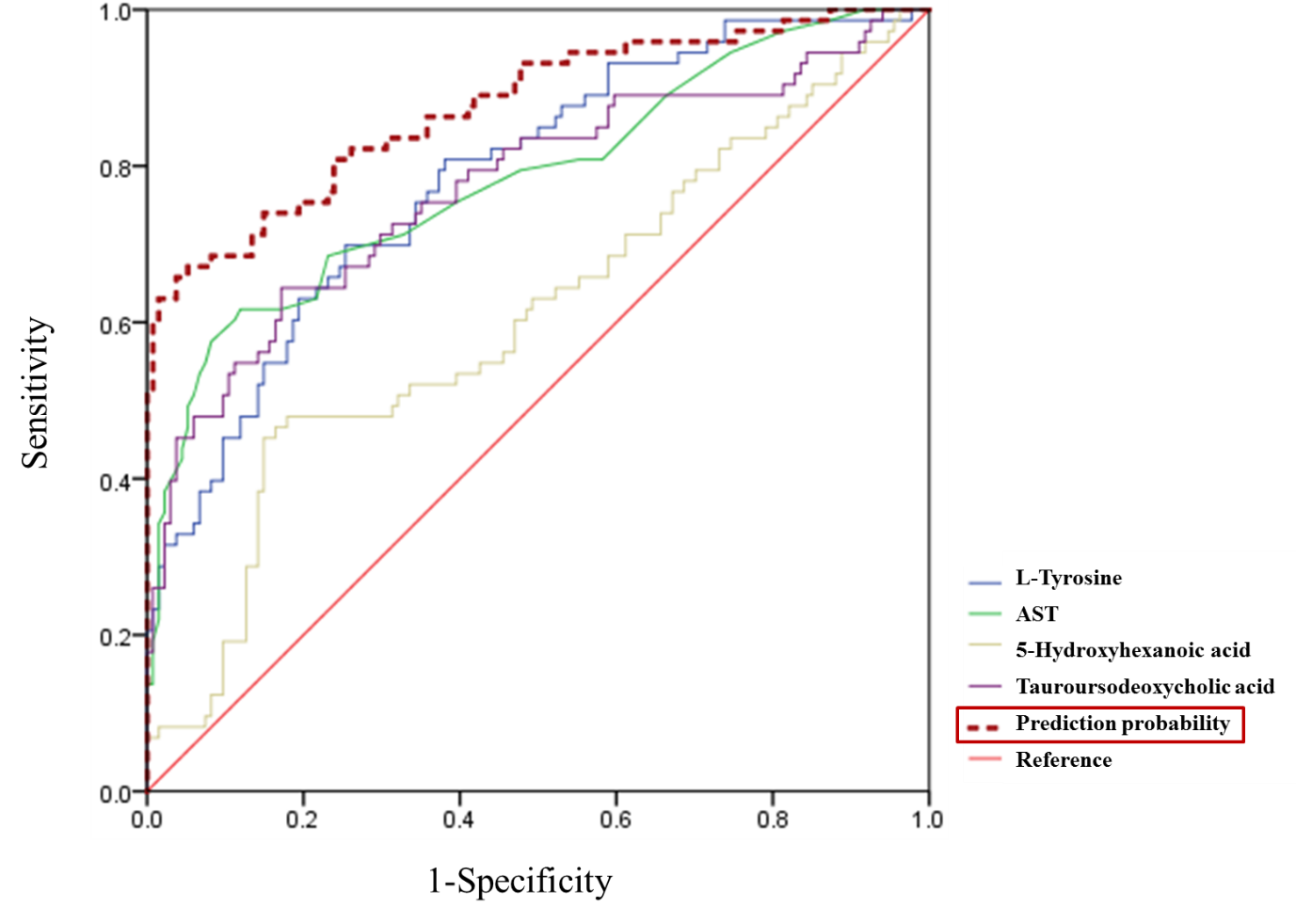


**Supplementary Figure S1: Permutation plots for the OPLS-DA model showing R2 (black triangle) and Q2 (blue square) values.**



**Supplementary Figure S2.** **Correlation matrix among the clinical parameters and major metabolites in the control and HCC groups.**

Correlations were obtained using Pearson’s correlation coefficient. Red indicates a positive correlation, and blue indicates a negative correlation.



**Supplementary Figure S3. ROC curves for L-tyrosine, AST, 5-hydroxyhexanoic acid, and tauroursodeoxycholic acid for the incidence of hepatocellular cancer.**

AST was tested by logarithmic transformation.

**Supplementary Table S1. Detailed method for pathway analysis.**

|  |
| --- |
| **Pathway analysis** |
| To identify the most relevant pathways associated with the selected metabolites, a metabolic pathway analysis was performed using MetaboAnalyst 3.0, a web-based analysis module (http://metaboanalyst.ca) based on the Kyoto Encyclopedia of Genes and Genomes (KEGG) database. Through pathway analysis, we mapped 11 correlated metabolic pathways with the identified 55 metabolites. Enrichment analysis was conducted for the 55 metabolites (VIP >1.5) and eleven pathways all had low *q*-values (false discovery rate [FDR] <0.05). These pathways also had high pathway impacts (over 0) obtained from topology analysis (Supplementary Table S5).  We performed two different types of pathway analyses: enrichment and topology analyses. The enrichment analysis was conducted using a hypergeometric test that compares the numbers of significant metabolites within a specific pathway with the expected value. In addition to considering the over-representation of significant metabolites in the examined pathways, another important feature of pathway analysis is the structure. The topology analysis considers the position of significant metabolites in metabolic pathways that are annotated by KEGG. Pathway impact was estimated in the topology analysis. The pathway impact is the cumulative value of the significant metabolites and this value is normalized by summing the importance of each metabolite in a particular pathway. |

**Supplementary Table S2. Levels of liver enzymes according to the mean diagnostic time after inclusion.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Mean diagnostic time after inclusion, y** | | | |  |
|  | **<2** | **2 to 4.4** | **4.5 to 5.4** | **≥5.5** | ***P* for trend** |
| Cases (*n*) | 14 | 27 | 16 | 18 |  |
|  | **Mean (SD)** | | | |  |
| AST (IU/L) | 40.5 (15.0) | 41.9 (20.6) | 30.7 (12.1) | 56.4 (62.6) | 0.282 |
| ALT (IU/L) | 40.0 (21.0) | 44.6 (25.5) | 38.0 (22.2) | 77.8 (147.4) | 0.169 |
| γ-GTP (U/L) | 86.6 (80.5) | 109.6 (184.9) | 50.3 (33.2) | 91.8 (113.7) | 0.723 |

**Supplementary Table S3. CV-ANOVA assessing the reliability of the generated models.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Positive ion mode** | **SS** | **DF** | **MS** | **F** | ***P*-value** | **SD** |
| Total correlation | 208 | 208 | 1 |  |  | 1 |
| Regression | 136.907 | 18 | 7.60596 | 20.3275 | 4.46E-35 | 2.75789 |
| Residual | 71.0926 | 190 | 0.374172 |  |  | 0.611696 |
| **Negative ion mode** | **SS** | **DF** | **MS** | **F** | ***P*-value** | **SD** |
| Total correlation | 208 | 208 | 1 |  |  | 1 |
| Regression | 125.531 | 16 | 7.84572 | 18.2661 | 1.63E-30 | 2.80102 |
| Residual | 82.4685 | 192 | 0.429523 |  |  | 0.65538 |

SS: sum of squares, DF: number of degrees of freedom, MS: mean squares, F: F-statistic, SD: standard deviation.

**Supplementary Table S4. Peak intensities of the seven major metabolites according to the mean diagnostic time after inclusion.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Mean diagnostic time after inclusion, y** | | | |  |
|  | **<2** | **2 to 4.4** | **4.5 to 5.4** | **≥5.5** | ***P* for trend** |
| Cases (*n*) | 14 | 27 | 16 | 18 |  |
|  | **Peak intensities** | | | |  |
| 5-Hydroxyhexanoic acid | 7919178 | 2292689 | 6656661 | 1695598 | 0.053 |
| L-Tyrosine | 31457689 | 33660203 | 31624526 | 32004296 | 0.884 |
| Tauroursodeoxycholic acid | 3095822 | 8464559 | 1193367 | 3687906 | 0.401 |
| Oleamide | 1027701 | 1955029 | 1028931 | 6593994 | 0.009 |
| Androsterone sulfate | 10982045 | 11137551 | 19149379 | 8219642 | 0.919 |
| LysoPC (16:1) | 32688629 | 34039566 | 24389358 | 44300927 | 0.192 |
| LysoPC (20:3) | 21682918 | 34039566 | 20303728 | 30908438 | 0.290 |

**Supplementary Table S5. Metabolic pathway analysis of all subjects.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Metabolic pathway** | **Hit(s)** | ***P*** | **FDR** | **Impact** |
| Tyrosine metabolism | L-Tyrosine | 2.64E-19 | 1.85E-18 | 0.04724 |
| Phenylalanine metabolism | L-Tyrosine | 7.92E-19 | 4.16E-18 | 0.11906 |
|  | L-Phenylalanine |  |  |  |
| Phenylalanine, tyrosine and tryptophan biosynthesis | L-Tyrosine | 1.83E-16 | 6.39E-16 | 0.008 |
|  | L-Phenylalanine |  |  |  |
|  | L-Tryptophan |  |  |  |
| Valine, leucine and isoleucine degradation | L-Leucine | 7.29E-12 | 1.70E-11 | 0.02232 |
| Valine, leucine and isoleucine biosynthesis | L-Leucine | 7.29E-12 | 1.70E-11 | 0.01325 |
| Tryptophan metabolism | L-Tryptophan | 1.44E-08 | 2.76E-08 | 0.10853 |
| Glycerophospholipid metabolism | LysoPC (18:1) | 3.11E-06 | 5.45E-06 | 0.10429 |
| Linoleic acid metabolism | Linoleic acid | 2.57E-05 | 4.15E-05 | 0.65625 |
|  | Gamma-linoleic acid |  |  |  |
| Arachidonic acid metabolism | Arachidonic acid | 6.30E-05 | 9.45E-05 | 0.2255 |
|  | 15(S)-HETE |  |  |  |
| Primary bile acid biosynthesis | Glycocholic acid | 0.001403 | 0.001841 | 0.00846 |
| Fatty acid metabolism | Palmitic acid | 0.002902 | 0.003585 | 0.02959 |
|  | L-Palmitoylcarnitine |  |  |  |

*Hit,* the matched metabolites uploaded in MetaboAnalyst. *FDR,* the *P-*value adjusted using the false discovery rate. *Impact,* the pathway impact value calculated from pathway topology analysis.

**Supplementary Table S6. Area under the ROC curve (AUC) for the risk factors of HCC incidence.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **AUC±SE** | ***P*-value** | **Cut-off value** | **Sensitivity** | **Specificity** |
| L-Tyrosine | 0.785±0.033 | <0.001 | 26356320.19 | 0.699 | 0.701 |
| AST | 0.784±0.035 | <0.001 | 26.50 | 0.685 | 0.769 |
| 5-Hydroxyhexanoic acid | 0.608±0.042 | 0.010 | 996837.90 | 0.548 | 0.552 |
| Tauroursodeoxycholic acid | 0.773±0.037 | <0.001 | 314191.00 | 0.699 | 0.701 |
| Prediction probability | 0.875±0.027 | <0.001 |  |  |  |

AST was tested by logarithmic transformation.

**Supplementary Table S7. List of unidentified peaks with VIP values >1.5.**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **List of unidentified peaks** |  | **Observed mass (M+H)** |  | **Normalized peak intensities** | | | |  | **VIP** |
|  |  | **Control** | | **HCC** | |  |
| 1 |  | 100.0754*†* |  | 17,203,479 | ±568,850 | 11,775,370 | ±660,630 |  | 9.4773 |
| 2 |  | 100.0754*†* |  | 53,749,033 | ±1,546,057 | 34,191,407 | ±2,211,825 |  | 6.7567 |
| 3 |  | 100.0755*†* |  | 374,859,942 | ±7,204,392 | 311,099,966 | ±10,985,945 |  | 3.4623 |
| 4 |  | 100.0756*†* |  | 63,491 | ±7,778 | 983,916 | ±228,620 |  | 4.2576 |
| 5 |  | 100.0756*†* |  | 3,788,471 | ±194,191 | 3,852,503 | ±310,395 |  | 2.7944 |
| 6 |  | 100.0756*†* |  | 4,040,208 | ±131,314 | 2,756,594 | ±156,160 |  | 1.7093 |
| 7 |  | 100.0760*†* |  | 30,783,899 | ±1,198,836 | 21,249,064 | ±1,169,993 |  | 7.2749 |
| 8 |  | 101.0788*†* |  | 34,281 | ±5,960 | 707,279 | ±224,883 |  | 2.2422 |
| 9 |  | 105.0909*†* |  | 6,858,542 | ±387,869 | 3,552,791 | ±368,485 |  | 1.8699 |
| 10 |  | 122.0573*†* |  | 34,071,292 | ±1,165,417 | 21,977,310 | ±1,348,694 |  | 1.9119 |
| 11 |  | 145.1220*†* |  | 133,297,241 | ±2,410,890 | 98,990,432 | ±4,565,633 |  | 2.8711 |
| 12 |  | 149.0118*†* |  | 136,198,345 | ±2,290,225 | 112,824,177 | ±4,351,170 |  | 3.1896 |
| 13 |  | 149.0119*†* |  | 56,946,168 | ±1,626,400 | 36,111,046 | ±2,116,962 |  | 3.6394 |
| 14 |  | 149.0119*†* |  | 79,703,111 | ±1,390,478 | 63,175,379 | ±2,229,433 |  | 2.6943 |
| 15 |  | 149.0119*†* |  | 44,525,529 | ±2,339,038 | 25,877,605 | ±1,796,047 |  | 3.5097 |
| 16 |  | 149.0120*†* |  | 5,176,223 | ±163,739 | 4,479,058 | ±247,891 |  | 2.7288 |
| 17 |  | 149.0120*†* |  | 41,629,281 | ±1,082,018 | 29,892,302 | ±1,732,810 |  | 2.7373 |
| 18 |  | 159.1376*†* |  | 13,915,225 | ±578,491 | 10,684,993 | ±721,312 |  | 3.3309 |
| 19 |  | 163.9760*†* |  | 4,271,841 | ±252,204 | 4,038,232 | ±310,408 |  | 2.0456 |
| 20 |  | 163.9764*†* |  | 12,998,144 | ±214,949 | 13,649,003 | ±526,232 |  | 3.0559 |
| 21 |  | 163.9764*†* |  | 60,456,619 | ±11,716,153 | 107,824,040 | ±17,421,549 |  | 2.5710 |
| 22 |  | 164.9842*†* |  | 33,236,168 | ±6,721,510 | 53,836,205 | ±9,476,952 |  | 1.6443 |
| 23 |  | 168.5829*†* |  | 9,972,534 | ±1,857,600 | 15,642,016 | ±2,669,653 |  | 1.5851 |
| 24 |  | 184.0729*†* |  | 16,497,467 | ±3,294,312 | 22,026,259 | ±3,751,353 |  | 4.3022 |
| 25 |  | 187.0963*†* |  | 6,365,553 | ±1,155,608 | 10,599,632 | ±1,896,849 |  | 1.8709 |
| 26 |  | 188.0702*†* |  | 2,057,759 | ±365,164 | 4,106,384 | ±803,255 |  | 1.5936 |
| 27 |  | 188.0703*†* |  | 52,458,566 | ±10,300,553 | 69,481,113 | ±10,413,058 |  | 3.2712 |
| 28 |  | 189.0429*†* |  | 3,338,387 | ±692,026 | 5,842,669 | ±1,026,503 |  | 2.7148 |
| 29 |  | 201.1118*†* |  | 3,247,924 | ±438,778 | 917,265 | ±332,762 |  | 2.5130 |
| 30 |  | 211.0937*†* |  | 37,541,010 | ±358,613 | 39,039,244 | ±255,621 |  | 1.7119 |
| 31 |  | 215.1275*†* |  | 40,345,828 | ±664,511 | 40,346,712 | ±996,759 |  | 2.6623 |
| 32 |  | 217.1433*†* |  | 1,497,213 | ±133,520 | 349,588 | ±53,967 |  | 1.7595 |
| 33 |  | 231.1230*‡* |  | 21,364,998 | ±983,789 | 12,117,416 | ±1,465,854 |  | 1.5248 |
| 34 |  | 233.1381*†* |  | 1,776,337 | ±334,656 | 4,128,601 | ±632,202 |  | 2.9400 |
| 35 |  | 241.1042*†* |  | 1,097,374 | ±129,418 | 414,472 | ±102,186 |  | 2.5303 |
| 36 |  | 245.1385*‡* |  | 1,872,943 | ±690,592 | 1,317,903 | ±693,309 |  | 1.7457 |
| 37 |  | 255.1201*†* |  | 3,629,031 | ±104,099 | 4,427,303 | ±179,418 |  | 2.9059 |
| 38 |  | 256.2354*‡* |  | 83,415,450 | ±1,519,941 | 68,432,925 | ±2,325,892 |  | 2.1448 |
| 39 |  | 257.1742*†* |  | 7,029,196 | ±132,260 | 8,448,979 | ±328,302 |  | 1.7735 |
| 40 |  | 257.1745*†* |  | 280,740 | ±60,862 | 847,751 | ±306,856 |  | 2.9426 |
| 41 |  | 262.0857*†* |  | 1,470,337 | ±159,901 | 631,588 | ±122,467 |  | 1.5336 |
| 42 |  | 269.1356*†* |  | 8,015,637 | ±670,236 | 2,392,490 | ±444,135 |  | 3.4624 |
| 43 |  | 273.1700*‡* |  | 27,058,510 | ±602,753 | 21,736,109 | ±902,854 |  | 1.7599 |
| 44 |  | 280.2353*‡* |  | 3,746,321 | ±281,165 | 2,942,424 | ±259,793 |  | 1.9657 |
| 45 |  | 282.2515*‡* |  | 4,157,394 | ±471,261 | 24,345,518 | ±5,798,547 |  | 2.6199 |
| 46 |  | 297.1670*†* |  | 6,166,486 | ±190,835 | 4,598,178 | ±195,626 |  | 3.1856 |
| 47 |  | 304.2355*‡* |  | 427,693 | ±66,317 | 5,333,525 | ±1,929,371 |  | 1.9856 |
| 48 |  | 304.2606*†* |  | 38,671,311 | ±758,897 | 45,781,998 | ±530,815 |  | 1.5919 |
| 49 |  | 312.3619*†* |  | 74,264,728 | ±836,604 | 82,972,517 | ±567,544 |  | 2.2269 |
| 50 |  | 314.1575*†* |  | 67,157,445 | ±1,156,921 | 73,223,785 | ±780,392 |  | 1.5367 |
| 51 |  | 317.2083*†* |  | 80,891,564 | ±1,029,837 | 89,589,376 | ±663,323 |  | 2.0012 |
| 52 |  | 319.2238*†* |  | 60,840,461 | ±604,189 | 66,124,333 | ±296,307 |  | 2.2332 |
| 53 |  | 325.1978*†* |  | 79,316,307 | ±1,196,267 | 85,412,864 | ±564,563 |  | 1.5001 |
| 54 |  | 327.2314*†* |  | 2,540,670 | ±266,534 | 1,234,723 | ±183,641 |  | 3.0162 |
| 55 |  | 328.2353*‡* |  | 86,599 | ±16,969 | 1,467,996 | ±562,118 |  | 2.0370 |
| 56 |  | 339.2323*‡* |  | 417,805 | ±65,851 | 4,764,811 | ±1,088,275 |  | 3.7453 |
| 57 |  | 340.2355*‡* |  | 82,775 | ±21,529 | 1,661,412 | ±495,514 |  | 1.8606 |
| 58 |  | 341.2079*†* |  | 1,262,213 | ±143,545 | 618,307 | ±105,304 |  | 1.9090 |
| 59 |  | 342.3360*†* |  | 2,357,745 | ±79,511 | 1,691,435 | ±82,772 |  | 2.0913 |
| 60 |  | 343.2237*†* |  | 10,916,881 | ±919,960 | 3,303,821 | ±612,463 |  | 2.6543 |
| 61 |  | 343.2255*†* |  | 52,651,423 | ±788,743 | 56,104,239 | ±718,584 |  | 2.1502 |
| 62 |  | 345.2817*‡* |  | 4,297,426 | ±170,101 | 2,725,905 | ±228,840 |  | 2.2046 |
| 63 |  | 359.2186*†* |  | 53,929,166 | ±845,792 | 61,102,380 | ±764,335 |  | 1.5778 |
| 64 |  | 359.2216*‡* |  | 9,121,573 | ±263,900 | 7,371,656 | ±295,973 |  | 1.5022 |
| 65 |  | 367.2238*†* |  | 60,252,248 | ±820,788 | 65,803,649 | ±696,648 |  | 3.0821 |
| 66 |  | 383.2188*†* |  | 39,308,451 | ±456,175 | 41,499,485 | ±418,761 |  | 2.0768 |
| 67 |  | 410.2381*‡* |  | 3,330,518 | ±292,848 | 1,714,208 | ±210,259 |  | 1.9220 |
| 68 |  | 414.2995*†* |  | 6,101,987 | ±132,652 | 7,041,210 | ±181,860 |  | 3.1627 |
| 69 |  | 415.3028*†* |  | 1,837,004 | ±404,881 | 2,870,440 | ±553,680 |  | 1.6065 |
| 70 |  | 427.2683*†* |  | 1,599,937 | ±160,869 | 823,223 | ±110,457 |  | 1.5620 |
| 71 |  | 432.3099*†* |  | 2,262,625 | ±248,007 | 1,077,948 | ±149,934 |  | 3.9561 |
| 72 |  | 433.2352*‡* |  | 40,571 | ±28,558 | 3,883,435 | ±3,787,212 |  | 1.5160 |
| 73 |  | 433.3133*†* |  | 2,187,427 | ±236,994 | 890,879 | ±179,055 |  | 2.0458 |
| 74 |  | 437.0533*‡* |  | 11,298,688 | ±982,762 | 8,373,687 | ±821,276 |  | 1.5695 |
| 75 |  | 443.2635*‡* |  | 6,289,367 | ±336,637 | 7,887,979 | ±1,010,196 |  | 2.0281 |
| 76 |  | 445.2788*†* |  | 554,243 | ±54,127 | 1,309,497 | ±382,071 |  | 2.9129 |
| 77 |  | 446.2823*†* |  | 35,033,681 | ±1,161,279 | 23,595,696 | ±995,188 |  | 1.7736 |
| 78 |  | 448.3048*†* |  | 1,239,575 | ±155,340 | 438,670 | ±78,275 |  | 1.6103 |
| 79 |  | 449.3085*‡* |  | 54,478 | ±54,076 | 7,655,778 | ±7,652,060 |  | 2.3304 |
| 80 |  | 451.3241*†* |  | 1,231,453 | ±154,733 | 437,412 | ±79,677 |  | 1.9437 |
| 81 |  | 464.2819*†* |  | 3,377,533 | ±450,042 | 1,051,928 | ±286,397 |  | 1.9459 |
| 82 |  | 467.2605*†* |  | 1,762,035 | ±136,915 | 1,091,082 | ±90,721 |  | 2.8030 |
| 83 |  | 467.3185*†* |  | 52,164,542 | ±772,593 | 49,910,925 | ±1,250,202 |  | 1.6427 |
| 84 |  | 469.3112*†* |  | 39,023,817 | ±1,053,679 | 30,265,433 | ±1,347,970 |  | 2.1745 |
| 85 |  | 472.3022*†* |  | 7,382,112 | ±748,169 | 2,412,247 | ±655,622 |  | 3.0433 |
| 86 |  | 473.3056*†* |  | 4,536,642 | ±124,798 | 3,492,685 | ±158,756 |  | 1.5358 |
| 87 |  | 482.2924*†* |  | 10,690,197 | ±1,009,001 | 14,627,035 | ±2,236,760 |  | 1.5084 |
| 88 |  | 482.3589*†* |  | 2,523,113 | ±254,605 | 1,232,389 | ±183,629 |  | 2.2880 |
| 89 |  | 488.2968*†* |  | 8,621,148 | ±314,785 | 10,462,976 | ±288,423 |  | 1.7196 |
| 90 |  | 490.2897*†* |  | 866,307 | ±100,114 | 2,160,132 | ±697,150 |  | 2.2164 |
| 91 |  | 495.3265*†* |  | 5,807,033 | ±761,707 | 1,655,870 | ±538,400 |  | 2.8403 |
| 92 |  | 497.3420*†* |  | 7,354,310 | ±173,230 | 7,978,144 | ±213,216 |  | 5.1341 |
| 93 |  | 498.3443*†* |  | 3,558,151 | ±407,078 | 1,351,443 | ±325,984 |  | 1.7976 |
| 94 |  | 511.3581*†* |  | 6,170,205 | ±806,500 | 1,581,190 | ±601,182 |  | 1.8999 |
| 95 |  | 516.3049*†* |  | 3,022,973 | ±422,825 | 923,573 | ±239,138 |  | 2.7721 |
| 96 |  | 518.3204*†* |  | 1,973,807 | ±233,277 | 561,038 | ±140,273 |  | 1.8197 |
| 97 |  | 519.3264*†* |  | 656,364 | ±125,928 | 1,882,444 | ±626,272 |  | 2.1346 |
| 98 |  | 521.3419*†* |  | 510,138 | ±102,857 | 1,046,317 | ±280,605 |  | 3.9686 |
| 99 |  | 522.2849*†* |  | 1,207,937 | ±137,469 | 371,464 | ±89,123 |  | 1.6470 |
| 100 |  | 523.3575*†* |  | 1,412,439 | ±185,750 | 427,337 | ±140,873 |  | 3.2514 |
| 101 |  | 531.3520*†* |  | 1,037,517 | ±168,732 | 211,933 | ±85,276 |  | 1.5945 |
| 102 |  | 532.3360*†* |  | 7,594,126 | ±1,024,939 | 1,901,580 | ±700,771 |  | 2.0721 |
| 103 |  | 542.3198*†* |  | 27,155,222 | ±553,812 | 29,621,993 | ±758,759 |  | 2.2428 |
| 104 |  | 543.3260*†* |  | 5,835,262 | ±736,477 | 1,654,259 | ±594,476 |  | 3.1196 |
| 105 |  | 544.3354*†* |  | 1,268,056 | ±197,855 | 282,363 | ±117,127 |  | 2.4752 |
| 106 |  | 545.3418*†* |  | 1,053,272 | ±163,477 | 208,397 | ±78,496 |  | 2.7729 |
| 107 |  | 547.3580*†* |  | 7,448,073 | ±909,366 | 1,960,273 | ±682,742 |  | 2.5223 |
| 108 |  | 553.3336*†* |  | 258,131 | ±44,233 | 843,100 | ±323,740 |  | 1.9657 |
| 109 |  | 556.3233*‡* |  | 2,360,034 | ±300,871 | 618,887 | ±230,060 |  | 1.8792 |
| 110 |  | 564.3042*†* |  | 3,021,544 | ±384,858 | 911,077 | ±329,027 |  | 2.3664 |
| 111 |  | 569.3415*†* |  | 7,383,765 | ±1,172,396 | 1,491,070 | ±629,629 |  | 2.3398 |
| 112 |  | 570.3394*‡* |  | 2,961,368 | ±376,350 | 775,624 | ±285,772 |  | 3.3541 |
| 113 |  | 571.3425*‡* |  | 2,400,076 | ±164,909 | 1,276,798 | ±104,624 |  | 1.7970 |
| 114 |  | 594.3400*‡* |  | 3,876,468 | ±587,726 | 857,140 | ±343,815 |  | 1.8992 |
| 115 |  | 596.3549*‡* |  | 9,879,787 | ±543,267 | 11,007,832 | ±916,373 |  | 1.7969 |
| 116 |  | 724.5433*†* |  | 987,728 | ±162,108 | 185,925 | ±84,500 |  | 1.6904 |
| 117 |  | 899.6337*†* |  | 1,034,299 | ±189,784 | 141,928 | ±67,097 |  | 2.0515 |
| 118 |  | 991.6690*†* |  | 2,257,960 | ±256,653 | 684,583 | ±213,049 |  | 5.7658 |
| 119 |  | 992.6730*†* |  | 1,684,789 | ±114,164 | 743,418 | ±96,377 |  | 4.0087 |
| 120 |  | 993.6772*†* |  | 1,105,026 | ±188,175 | 215,187 | ±84,872 |  | 1.9486 |

Mean±SE. *†*Metabolites obtained in ESI-positive ion mode (*M/Z* [M+H]). *‡*Metabolites obtained in ESI-negative ion mode (*M/Z* [M-H]). VIP: variable importance in the projection.