Table S4. Information of 113 differential abundant metabolites

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound\_ID | NPPS(mean) | PPS(mean) | log2\_FC(PPS/NPPS) | FDR | Vip value | Name |
| M537T175\_POS | 7115.61  | 131946.38  | 4.21  | 0.26  | 1.31  | Telmisartan |
| M100T56\_POS | 265509.54  | 2046250.90  | 2.95  | 0.06  | 5.41  | 2-piperidone |
| M568T157\_POS | 23169.54  | 156825.50  | 2.76  | 0.25  | 1.34  | 1-Stearoyl-sn-glycerol 3-phosphocholine |
| M146T370\_2\_POS | 1720109.41  | 9931868.08  | 2.53  | 0.07  | 11.72  | Deoxycarnitine |
| M309T38\_NEG | 204053.35  | 755007.76  | 1.89  | 0.27  | 2.83  | Eicosenoic acid |
| M86T261\_POS | 58972.90  | 213212.71  | 1.85  | 0.11  | 1.57  | 1,5-pentanediamine |
| M563T171\_POS | 56047.40  | 177816.53  | 1.67  | 0.08  | 1.38  | Protoporphyrin ix |
| M328T35\_POS | 110626.06  | 304725.86  | 1.46  | 0.23  | 1.68  | Stearoyl ethanolamide |
| M255T46\_NEG | 9114555.78  | 20593210.02  | 1.18  | 0.28  | 12.64  | Palmitic acid |
| M227T114\_NEG | 137167.62  | 274519.61  | 1.00  | 0.08  | 1.48  | Ile-Pro |
| M143T132\_NEG | 71048.27  | 138448.75  | 0.96  | 0.14  | 1.06  | Ammeline |
| M241T101\_NEG | 308555.02  | 452319.28  | 0.55  | 0.06  | 1.55  | His-ser |
| M141T347\_2\_NEG | 12756542.08  | 7481904.17  | -0.77  | 0.12  | 9.12  | Cis,cis-muconic acid |
| M181T348\_NEG | 562441.56  | 310826.20  | -0.86  | 0.10  | 2.02  | 3,4-dihydroxyhydrocinnamic acid |
| M288T38\_POS | 1816931.61  | 988924.97  | -0.88  | 0.21  | 3.61  | C17-sphinganine |
| M295T489\_NEG | 794230.58  | 425212.99  | -0.90  | 0.15  | 2.40  | Propanoic acid, 3-[[[2-[(aminoiminomethyl)amino]-4-thiazolyl]methyl]thio]- |
| M454T191\_POS | 359614.00  | 186858.31  | -0.94  | 0.14  | 1.64  | 1-palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine |
| M229T295\_POS | 423391.32  | 219686.21  | -0.95  | 0.13  | 1.79  | Pro-leu |
| M187T338\_2\_NEG | 301475.69  | 141547.58  | -1.09  | 0.15  | 1.58  | Azelaic acid |
| M309T25\_NEG | 252190.86  | 116275.84  | -1.12  | 0.29  | 1.36  | Mestranol |
| M131T122\_NEG | 319108.19  | 128060.07  | -1.32  | 0.29  | 1.64  | 6-hydroxyhexanoate |
| M365T360\_POS | 106754.94  | 42214.15  | -1.34  | 0.07  | 1.04  | Melibiose |
| M434T376\_POS | 141719.88  | 54624.90  | -1.38  | 0.16  | 1.11  | Fluvastatin |
| M395T33\_2\_POS | 145834.38  | 56086.47  | -1.38  | 0.08  | 1.21  | Fucosterol |
| M399T536\_POS | 742724.47  | 284662.28  | -1.38  | 0.14  | 2.66  | S-adenosyl-l-methionine |
| M337T27\_2\_NEG | 153773.55  | 57570.01  | -1.42  | 0.19  | 1.24  | 18-carboxydinorleukotriene b4 |
| M480T188\_POS | 1532850.03  | 551804.55  | -1.47  | 0.22  | 3.64  | 1-oleoyl-sn-glycero-3-phosphoethanolamine |
| M348T250\_POS | 217115.71  | 77763.80  | -1.48  | 0.07  | 1.48  | 2'-deoxyguanosine 5'-monophosphate |
| M391T32\_2\_NEG | 146078.93  | 51364.64  | -1.51  | 0.09  | 1.24  | Dodecanoic acid, 12-[[(tricyclo[3.3.1.13,7]dec-1-ylamino)carbonyl]amino]- |
| M216T74\_POS | 117665.33  | 40677.06  | -1.53  | 0.14  | 1.10  | Scopoline |
| M747T38\_1\_POS | 868404.20  | 294335.91  | -1.56  | 0.22  | 2.85  | 1-hexadecyl-2-(9z-octadecenoyl)-sn-glycero-3-phosphocholine |
| M293T421\_POS | 173862.97  | 58672.41  | -1.57  | 0.11  | 1.35  | Ethylenediaminetetraacetic acid |
| M149T101\_2\_NEG | 6576650.90  | 2131687.89  | -1.63  | 0.10  | 8.58  | 3-methylphenylacetic acid |
| M375T84\_NEG | 15664414.60  | 5063543.19  | -1.63  | 0.13  | 12.94  | Lithocholic acid |
| M391T159\_POS | 128727.55  | 41509.20  | -1.63  | 0.13  | 1.16  | .gamma.-muricholic acid |
| M449T172\_NEG | 166833.29  | 53058.11  | -1.65  | 0.11  | 1.34  | Vitamin k1 |
| M277T42\_2\_NEG | 585946.17  | 178986.84  | -1.71  | 0.25  | 2.33  | all cis-(6,9,12)-Linolenic acid |
| M211T83\_POS | 93755.64  | 28558.83  | -1.71  | 0.06  | 1.05  | Jasmonic acid |
| M331T159\_NEG | 177129.34  | 53643.12  | -1.72  | 0.11  | 1.42  | 21-Hydroxypregnenolone |
| M411T27\_2\_NEG | 86097.14  | 25827.95  | -1.74  | 0.06  | 1.00  | Pentanoic acid, 5-[(3ar,4r,5r,6as)-3,3-difluorohexahydro-5-hydroxy-4-[(1e,3s,4s)-3-hydroxy-4-methyl-1-nonen-6-ynyl]-2h-cyclopenta[b]furan-2-ylidene]-, (5z)- |
| M337T36\_1\_NEG | 550067.98  | 159681.13  | -1.78  | 0.22  | 2.47  | 2-(2-hydroxybut-3-en-2-yl)-3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1h-benzo[e][1]benzofuran-4,5-diol |
| M363T178\_NEG | 178004.11  | 51277.63  | -1.80  | 0.06  | 1.45  | 9s,11r,15s-trihydroxy-20a,20b-dihomo-5z,13e-prostadienoic acid |
| M195T447\_NEG | 116063.17  | 33032.95  | -1.81  | 0.07  | 1.19  | Galactonic acid |
| M477T86\_NEG | 137486.74  | 38989.33  | -1.82  | 0.17  | 1.21  | 1,4-bis[(p-hydroxyphenethyl)amino]anthraquinone |
| M457T24\_NEG | 883809.10  | 250440.26  | -1.82  | 0.07  | 3.27  | Andrastin c |
| M482T187\_POS | 1758578.06  | 488328.85  | -1.85  | 0.23  | 4.13  | 1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine |
| M302T208\_POS | 97709.63  | 26683.56  | -1.87  | 0.11  | 1.05  | Dihydrocodeine |
| M434T182\_NEG | 88472.01  | 24117.29  | -1.88  | 0.06  | 1.03  | N-acetyl-s-geranylgeranyl-l-cysteine |
| M189T380\_2\_POS | 268842.21  | 72241.45  | -1.90  | 0.10  | 1.75  | N-acetylglutamine |
| M173T235\_2\_POS | 192414.87  | 51034.12  | -1.91  | 0.09  | 1.49  | L-Isoleucine |
| M195T156\_POS | 137862.73  | 36336.57  | -1.92  | 0.07  | 1.27  | Dodecanedioic acid |
| M329T119\_NEG | 116933.25  | 30701.75  | -1.93  | 0.16  | 1.11  | 11beta-hydroxyprogesterone |
| M403T65\_NEG | 108068.87  | 27927.75  | -1.95  | 0.14  | 1.07  | 1-o-(9z-octadecenyl)-sn-glycero-2,3-cyclic-phosphate |
| M182T38\_NEG | 120629.59  | 31048.78  | -1.96  | 0.24  | 1.17  | 4-pyridoxic acid |
| M332T180\_POS | 455819.17  | 112798.78  | -2.01  | 0.21  | 2.33  | 1h-indazole-3-carboxamide, n-[(1s)-1-(aminocarbonyl)-2-methylpropyl]-1-(5-fluoropentyl)- |
| M347T95\_NEG | 205135.39  | 50470.06  | -2.02  | 0.23  | 1.56  | Anacardic acid |
| M389T114\_NEG | 13504749.64  | 3143242.24  | -2.10  | 0.12  | 13.09  | Cholic acid |
| M473T27\_NEG | 208768.32  | 48385.54  | -2.11  | 0.06  | 1.62  | Amastatin |
| M391T119\_2\_POS | 7014043.55  | 1582530.62  | -2.15  | 0.26  | 9.15  | 12-ketodeoxycholic acid |
| M432T162\_NEG | 232824.04  | 52128.49  | -2.16  | 0.10  | 1.70  | Lithocholylglycine |
| M193T382\_NEG | 226637.87  | 50559.19  | -2.16  | 0.09  | 1.69  | 2-keto-d-gluconic acid |
| M299T390\_POS | 76810.37  | 17002.76  | -2.18  | 0.05  | 1.01  | Olomoucine |
| M341T388\_NEG | 115722.45  | 24817.74  | -2.22  | 0.06  | 1.23  | D-Maltose |
| M309T119\_POS | 958132.85  | 205457.71  | -2.22  | 0.13  | 3.49  | 4.alpha.-hydroxystanozolol |
| M337T116\_POS | 664396.11  | 138671.70  | -2.26  | 0.23  | 2.88  | Prostaglandin b1 |
| M563T159\_NEG | 100500.06  | 20773.25  | -2.27  | 0.23  | 1.12  | L-homoarginine |
| M365T413\_POS | 302332.02  | 61219.92  | -2.30  | 0.11  | 1.98  | Cellobiose |
| M195T413\_NEG | 141137.60  | 28213.36  | -2.32  | 0.04  | 1.38  | D-gluconate |
| M439T23\_NEG | 268508.77  | 52932.53  | -2.34  | 0.06  | 1.89  | 5-hydroxy-l-tryptophan |
| M771T136\_POS | 3657008.00  | 720298.29  | -2.34  | 0.11  | 6.65  | 1-hexadecyl-2-(8z,11z,14z-eicosatrienoyl)-sn-glycero-3-phosphocholine |
| M275T156\_POS | 210337.21  | 40443.33  | -2.38  | 0.07  | 1.65  | 9-oxo-10e,12z,15z-octadecatrienoic acid |
| M506T174\_2\_POS | 2015781.49  | 377947.51  | -2.42  | 0.07  | 5.15  | 1-stearoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| M464T243\_2\_NEG | 883369.96  | 164757.28  | -2.42  | 0.13  | 3.35  | Glycocholic acid |
| M373T175\_POS | 157537.45  | 29187.27  | -2.43  | 0.10  | 1.46  | .beta.-muricholic acid |
| M448T200\_2\_NEG | 2058155.94  | 350879.03  | -2.55  | 0.13  | 5.09  | Glycodeoxycholic acid |
| M373T117\_POS | 3561457.58  | 596517.80  | -2.58  | 0.19  | 6.91  | Ursocholic acid |
| M410T157\_2\_POS | 4092987.72  | 634807.58  | -2.69  | 0.09  | 7.59  | Ursodeoxycholic acid |
| M329T37\_1\_NEG | 250349.50  | 38589.38  | -2.70  | 0.12  | 1.82  | Quercetin 3,7-dimethyl ether |
| M215T156\_POS | 202604.31  | 31063.07  | -2.71  | 0.04  | 1.71  | 5alpha-androstan-17beta-ol-3-one |
| M229T89\_NEG | 316513.12  | 47735.49  | -2.73  | 0.06  | 2.10  | D-ribulose 5-phosphate |
| M417T47\_POS | 161216.08  | 23859.28  | -2.76  | 0.08  | 1.52  | 3r-[[(4-fluorophenyl)sulfonyl]amino]-1,2,3,4-tetrahydro-9h-carbazole-9-propanoic acid |
| M347T33\_NEG | 357515.82  | 52287.20  | -2.77  | 0.04  | 2.27  | Camptothecin |
| M193T414\_NEG | 79465.05  | 10418.95  | -2.93  | 0.09  | 1.08  | D-galacturonic acid |
| M302T206\_POS | 223577.77  | 28854.86  | -2.95  | 0.06  | 1.80  | Dobutamine |
| M391T149\_2\_NEG | 97025108.96  | 12397972.62  | -2.97  | 0.06  | 37.96  | Deoxycholic acid |
| M321T157\_POS | 412313.50  | 48264.75  | -3.09  | 0.04  | 2.48  | 3.beta.-hydroxy-5-cholenoic acid |
| M221T385\_NEG | 95770.25  | 10768.09  | -3.15  | 0.06  | 1.18  | Palatinose |
| M121T218\_POS | 179889.30  | 19862.80  | -3.18  | 0.26  | 1.57  | Tyramine |
| M486T78\_POS | 121787.34  | 12701.11  | -3.26  | 0.26  | 1.30  | Dibutyryl-cgmp |
| M169T30\_NEG | 867462.54  | 86308.55  | -3.33  | 0.04  | 3.61  | Phloroglucinolcarboxylic acid |
| M209T46\_1\_POS | 83142.22  | 8264.07  | -3.33  | 0.10  | 1.10  | Trans-3,5-dimethoxy-4-hydroxycinnamaldehyde |
| M425T92\_NEG | 1089083.03  | 105265.14  | -3.37  | 0.05  | 4.05  | L-cysteine-glutathione disulfide |
| M417T330\_POS | 94242.05  | 8872.64  | -3.41  | 0.27  | 1.07  | Leu-Glu-Arg |
| M529T388\_NEG | 311003.56  | 26948.72  | -3.53  | 0.12  | 2.05  | Harpagoside |
| M499T33\_1\_NEG | 1172287.99  | 94395.96  | -3.63  | 0.16  | 4.03  | Silydianin |
| M349T32\_NEG | 1071335.21  | 85349.63  | -3.65  | 0.04  | 4.09  | Idarubicin |
| M241T111\_NEG | 617544.97  | 49152.23  | -3.65  | 0.10  | 3.08  | D-glucose 6-phosphate |
| M519T78\_NEG | 93753.02  | 7456.69  | -3.65  | 0.20  | 1.17  | [2-(3,4-dihydroxyphenyl)-5-hydroxy-7-methoxy-4-oxo-3-[(2s,3r,4r,5r,6s)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-8-yl] acetate |
| M455T152\_POS | 234307.35  | 18609.10  | -3.65  | 0.09  | 1.90  | 14z,17z,20z,23z,26z,29z-dotriacontahexaen-1-ol |
| M245T25\_NEG | 639812.82  | 48006.38  | -3.74  | 0.28  | 3.02  | 3-Methoxy-4-Hydroxyphenylglycol Sulfate |
| M441T33\_NEG | 181668.84  | 12266.58  | -3.89  | 0.06  | 1.68  | .alpha.-apooxytetracycline |
| M689T454\_POS | 80714.34  | 5114.56  | -3.98  | 0.08  | 1.13  | Maltotetraose |
| M527T409\_POS | 363072.61  | 22135.41  | -4.04  | 0.04  | 2.38  | Gentianose |
| M449T86\_NEG | 338946.90  | 20366.94  | -4.06  | 0.25  | 2.22  | N-acetyl-p-fluoro-dl-phenylalanine |
| M327T32\_NEG | 370982.45  | 20879.31  | -4.15  | 0.08  | 2.43  | 3-hydroxy-6,2',4'-trimethoxyflavone |
| M314T46\_POS | 1405245.13  | 71421.08  | -4.30  | 0.15  | 4.66  | Feruloyl tyramine |
| M379T149\_NEG | 337491.24  | 16421.75  | -4.36  | 0.16  | 2.27  | Daunorubicin |
| M363T85\_NEG | 2313872.45  | 111455.20  | -4.38  | 0.25  | 5.83  | 1-methyluric acid |
| M273T92\_NEG | 310117.21  | 14149.00  | -4.45  | 0.09  | 2.23  | Phenylbenzimidazolesulfonic acid |
| M465T127\_NEG | 371631.51  | 15903.50  | -4.55  | 0.06  | 2.45  | Agnuside |
| M328T55\_NEG | 279216.99  | 11760.94  | -4.57  | 0.23  | 2.05  | (e)-n-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide |
| M312T55\_POS | 1723442.32  | 62957.48  | -4.77  | 0.16  | 5.17  | Icilin |
| M493T120\_POS | 112027.60  | 2684.01  | -5.38  | 0.23  | 1.30  | 5-glc tricin |