

**Supplementary Figure 1** Reasonable analysis of the flora in the tested samples by rarefaction curves. A: Rarefaction curve, with the horizontal axis representing sequence number and the vertical axis representing the number of operational taxonomic units (OTUs); B: Simpson curve, with the horizontal axis representing sequencing depth and the vertical axis representing the Simpson index. Each sample is represented by a unique color.

**Supplementary Table 1 Composition of TCCL**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Herb** | **Latin name** | **Family** | **Part used** | **Chinese name** | **Voucher numbers** |
| *Codonopsis pilosula* (Franch.) Nannf. | Radix Codonopsis | *Campanulaceae* | Root | Dang Shen | 170,815 |
| *Salvia miltiorrhiza* Bge. | Radix et Rhizoma Salviae Miltiorrhizae | *Lamiaceae* | Root and rhizome | Dan Shen | 170,405 |
| *Poria cocos* (Schw.) Wolf | Sclerotium Poriae Cocos | *Polyporaceae* | Sclerotium | Fu Ling | 170,207 |
| *Citrus reticulata* Blanco | Pericarpium Citri Reticulatae | *Rutaceae* | Peel | Chen Pi | 170,809 |
| *Ostrea rivularis* Gould | Concha Ostreae | *Ostreidae* | Shell | Mu Li | 170,701 |
| *Fritillaria ussuriensis* Maxim. | Bulbus Fritillariae Ussuriensis | *Liliaceae* | Bulb | Ping Bei Mu | 170,516 |
| *Hordeurn vulgare* L. | Fructus Hordei Germinatus | *Poaceae* | Fruit | Mai Ya | 170,704 |
| *Ziziphus jujuba* Mill. | Semen Ziziphi Spinosae | *Rhamnaceae* | Seed | Suan Zao Ren | 170,711 |

**Supplementary Table 2 The detailed information of 808 active substances determined**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **ID** | **Adducts** | **Formula** | **Score** | **Fragmentation Score** | **Mass Error (ppm)** | **Metabolites** | **Fragment Ions** | **theoretical m/z** | **m/z** | **Retention time (min)** | **Ion mode** | **CHB-1** | **CHB-2** | **CHB-3** | CHB-1（峰面积的比值%） | CHB-2（峰面积的比值%） | CHB-3（峰面积的比值%） | M均值（峰面积的比值%） | **InChIKey** | **SMILES** | **HMDB** | **METLIN** | **LipidMaps** | **KEGG** | **PubChem** | **CAS** | 中文名 | 中文大类 | 中文子类 | 英文大类 | 英文子类 | 货号 | 纯度 | **Level** |
| compound00001 | 1.03\_167.0946n | M+H-H2O, M+H | C9H13NO2 | 58.1 | 93.2 | 0.07 | p-Synephrine | 91.0546, 119.0492, 135.0677, 150.0912 | 150.0913 | 150.0914 | 1.03 | POS | 6327444.133 | 6223468.422 | 6373995.419 | 0.846537752 | 0.847426236 | 0.836531044 | 0.843498344 | YRCWQPVGYLYSOX-UHFFFAOYSA-N | CNCC(O)C1=CC=C(O)C=C1 | HMDB0004826 | 24111 |  | C04548 | 7172 | 94-07-5 | 对辛弗林 | 生物碱 |  | Alkaloids |  | HY-113236 | HPLC≥98% | level1 |
| compound00002 | 1.21\_180.0659m/z | M-H | C9H11NO3 | 54.3 | 80.7 | -3.87 | L-Tyrosine | 71.0127, 72.0080, 89.0234, 93.0335, 101.0233, 109.0284, 119.0492, 136.0393, 163.0391, 180.0659 | 180.0666 | 180.0659 | 1.21 | NEG | 9708.494555 | 9104.38335 | 9443.743975 | 0.001298883 | 0.00123971 | 0.001239409 | 0.001259334 | OUYCCCASQSFEME-QMMMGPOBSA-N | N[C@@H](CC1=CC=C(O)C=C1)C(O)=O | HMDB0000158 | 34 |  | C00082 | 6057 | 60-18-4 | L-酪氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0473 | HPLC≥98% | level1 |
| compound00003 | 1.50\_182.0454m/z | M-H | C8H9NO4 | 59 | 78.2 | -2.89 | 4-Pyridoxic acid | 108.0444, 109.0285, 112.0506, 112.9845, 138.0551, 139.0395, 181.0712, 182.0452 | 182.0459 | 182.0454 | 1.5 | NEG | 30768.38726 | 31510.77323 | 32026.59556 | 0.004116449 | 0.004290703 | 0.00420321 | 0.004203454 | HXACOUQIXZGNBF-UHFFFAOYSA-N | CC1=NC=C(CO)C(C(O)=O)=C1O | HMDB0000017 | 239 |  | C00847 | 6723 | 82-82-6 | 4-吡哆酸 | 吡啶及其衍生物 |  | Pyridines and derivatives |  | HY-113493 | HPLC≥98% | level1 |
| compound00004 | 5.01\_717.1456m/z | M-H | C36H30O16 | 65.3 | 97.2 | -0.7 | Salvianolic acid E | 109.0283, 185.0237, 277.0504, 279.0295, 293.0449, 295.0608, 321.0402, 339.0509, 519.093, 717.1455 | 717.1461 | 717.1456 | 5.01 | NEG | 25547664.53 | 26272084.29 | 24825407.35 | 3.417977629 | 3.577370685 | 3.258117173 | 3.417821829 | SOXUSBQFIOBYJU-UHFFFAOYSA-N | O=C(C=Cc1ccc(O)c(O)c1C(=Cc1ccc(O)c(O)c1)C(=O)OC(Cc1ccc(O)c(O)c1)C(=O)O)OC(Cc1ccc(O)c(O)c1)C(=O)O |  |  |  |  |  | 142998-46-7 | 丹酚酸 E | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | DD0165 | HPLC≥98% | level1 |
| compound00005 | 3.71\_298.0969m/z | M+H | C11H15N5O3S | 57.1 | 67.2 | 0.23 | 5'-Methylthioadenosine | 136.0616, 298.0964 | 298.0968 | 298.0969 | 3.71 | POS | 135957.6798 | 147619.2451 | 149136.0386 | 0.018189542 | 0.020100756 | 0.019572798 | 0.019287699 | WUUGFSXJNOTRMR-IOSLPCCCSA-N | CSC[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=C1N=CN=C2N | HMDB0001173 | 3425 |  | C00170 | 439176 | 2457-80-9 | 5'-甲硫腺苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives |  | HY-16938 | HPLC≥98% | level1 |
| compound00006 | 5.65\_494.1211n | M-H, 2M-H | C26H22O10 | 61.7 | 74.9 | -0.47 | Salvianolic acid A | 109.0284, 135.0441, 159.0442, 185.0236, 197.0449, 295.0608, 313.0715, 493.1137 | 493.114 | 493.1138 | 5.65 | NEG | 24423688 | 23710965.25 | 23610892.97 | 3.267602762 | 3.228632759 | 3.098722804 | 3.198319442 | YMGFTDKNIWPMGF-UCPJVGPRSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=C(C(=C(C=C2)O)O)C=CC3=CC(=C(C=C3)O)O)O)O |  | 68360 |  | C10492 | 5281793 | 96574-01-5 | 丹酚酸 A | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N0318 | HPLC≥98% | level1 |
| compound00007 | 4.75\_521.1298m/z | M-H | C24H26O13 | 61.6 | 93.1 | -0.56 | Salviaflaside | 72.9919, 135.0441, 161.0235, 179.0342, 197.0448, 323.0771, 341.0919, 359.0775, 521.1257 | 521.1301 | 521.1298 | 4.75 | NEG | 929414.9482 | 904732.354 | 937699.0255 | 0.12434481 | 0.123193994 | 0.12306478 | 0.123534528 | DSMWJDJWYGMEBO-PRFRQLEPSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=CC(=C(C=C2)O)OC3C(C(C(C(O3)CO)O)O)O)O)O | HMDB0033705 | 89485 |  |  | 6438919 | 178895-25-5 | 异迷迭香酸苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DY0550-0020 | HPLC≥98% | level1 |
| compound00008 | 4.36\_314.1387m/z | M+H | C18H19NO4 | 65.1 | 83.2 | 0.17 | Laetanine | 86.0968, 237.0907, 265.0856, 282.0873, 297.1116, 313.1603, 313.197, 314.1383 | 314.1387 | 314.1387 | 4.36 | POS | 46155.16511 | 47748.31007 | 47797.3179 | 0.006175019 | 0.006501707 | 0.006272979 | 0.006316569 | URQAEFLEDPPPFX-UHFFFAOYSA-N | COc1cc2c(cc1O)-c1c(OC)c(O)cc3c1C(C2)NCC3 |  |  |  |  |  | 72361-67-2 | 四氢二甲氧基二苯并喹啉二醇 | 生物碱 |  | Alkaloids |  | HY-N4307 | HPLC≥98% | level1 |
| compound00009 | 4.98\_609.1809m/z | M+H | C28H32O15 | 54.4 | 66.7 | -0.75 | Diosmin | 301.0703, 463.1229 | 609.1814 | 609.1809 | 4.98 | POS | 349081.4526 | 349547.0272 | 360535.6766 | 0.046703001 | 0.047596501 | 0.047317148 | 0.04720555 | GZSOSUNBTXMUFQ-YFAPSIMESA-N | C1(O[C@@H]2O[C@@H]([C@H]([C@@H]([C@H]2O)O)O)CO[C@@H]2O[C@H]([C@@H]([C@H]([C@H]2O)O)O)C)=CC2OC(C3C=C(O)C(OC)=CC=3)=CC(=O)C=2C(O)=C1 |  | 3676 | LMPK12110814 | C10039 | 5281613 | 520-27-4 | 地奥司明 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0178 | HPLC≥98% | level1 |
| compound00010 | 5.18\_719.1609m/z | 2M-H | C18H16O8 | 55.6 | 88.1 | -1.23 | Rosmarinic acid | 161.0235, 179.0341, 197.045, 359.077 | 719.1618 | 719.1609 | 5.18 | NEG | 9731942.655 | 10116347.31 | 10223601.22 | 1.302019691 | 1.37750488 | 1.341758072 | 1.340427548 | DOUMFZQKYFQNTF-WUTVXBCWSA-N | OC(=O)[C@@H](CC1=CC(O)=C(O)C=C1)OC(=O)\C=C\C1=CC(O)=C(O)C=C1 | HMDB0003572 | 3504 |  | C01850 | 5281792 | 20283-92-5 | 迷迭香酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | msmls-lot-230-01 | HPLC≥98% | level1 |
| compound00011 | 1.47\_261.1447m/z | M+H | C11H20N2O5 | 55.8 | 84.1 | 0.79 | Leucyl-Glutamate | 84.0812, 86.0968, 130.0498, 143.1178, 148.0602, 171.1127, 260.1961, 261.1446 | 261.1445 | 261.1447 | 1.47 | POS | 145307.3215 | 145745.4859 | 145295.8685 | 0.019440414 | 0.019845613 | 0.01906881 | 0.019451612 | NFNVDJGXRFEYTK-UHFFFAOYSA-N | CC(C)CC(N)C(=O)NC(CCC(O)=O)C(O)=O | HMDB0028928 |  |  |  | 5259589 |  | 亮氨酰谷氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00012 | 4.30\_376.1383n | M+H, M+Na | C17H20N4O6 | 60.8 | 86.2 | -0.06 | Riboflavin | 243.0875, 377.1447 | 377.1456 | 377.1455 | 4.3 | POS | 49948.76219 | 47514.04213 | 49457.96537 | 0.006682558 | 0.006469808 | 0.006490925 | 0.006547764 | AUNGANRZJHBGPY-SCRDCRAPSA-N | CC1=C(C)C=C2N(C[C@H](O)[C@H](O)[C@H](O)CO)C3=NC(=O)NC(=O)C3=NC2=C1 | HMDB0000244 | 233 |  | C00255 | 493570 | 83-88-5 | 核黄素 | 蝶啶及其衍生物 |  | Pteridines and derivatives |  | HY-B0964 | HPLC≥98% | level1 |
| compound00013 | 4.26\_243.1711m/z | M-H | C12H24N2O3 | 62.7 | 68.4 | -1.37 | Leucyl-Isoleucine | 130.0863, 199.1809, 243.171 | 243.1714 | 243.1711 | 4.26 | NEG | 13807.14604 | 13636.59964 | 13136.82354 | 0.001847234 | 0.001856844 | 0.001724093 | 0.00180939 | AZLASBBHHSLQDB-UHFFFAOYSA-N | CCC(C)C(NC(=O)C(N)CC(C)C)C(O)=O | HMDB0028932 |  |  |  | 435718 |  | 亮氨酰异亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | 332P854 |  | level1 |
| compound00014 | 3.64\_474.1735m/z | M+H | C20H23N7O7 | 50.6 | 52.5 | 0.72 | Levoleucovorin | 259.1187, 284.1139, 327.1197, 345.13, 474.1737 | 474.1732 | 474.1735 | 3.64 | POS | 82300.91185 | 80345.39277 | 80877.07832 | 0.011010896 | 0.010940329 | 0.010614408 | 0.010855211 | VVIAGPKUTFNRDU-STQMWFEESA-N | NC1=NC(=O)C2=C(NC[C@H](CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)N2C=O)N1 | HMDB0001562 |  |  | C03479 | 149436 | 68538-85-2 | 醛氢叶酸钙 | 生物碱 |  | Alkaloids |  | HY-13667 | HPLC≥98% | level1 |
| compound00015 | 3.90\_192.0658m/z | M+H | C10H9NO3 | 54.2 | 66.6 | 1.68 | 5-Hydroxyindoleacetic acid | 146.0599, 150.0912, 161.0595, 174.0548, 192.0644 | 192.0655 | 192.0658 | 3.9 | POS | 35342.78975 | 32087.60605 | 34045.91945 | 0.00472845 | 0.004369248 | 0.004468229 | 0.004521976 | DUUGKQCEGZLZNO-UHFFFAOYSA-N | OC(=O)CC1=CNC2=C1C=C(O)C=C2 | HMDB0000763 | 2975 |  | C05635 | 1826 | 54-16-0 | 5-羟基吲哚乙酸 | 吲哚及其衍生物 |  | Indoles and derivatives |  | HY-W008253 | HPLC≥98% | level1 |
| compound00016 | 9.83\_389.1226m/z | M+H | C20H20O8 | 58.8 | 83.3 | -1.37 | 5-O-Demethylnobiletin | 341.0651, 359.0755, 389.1229 | 389.1231 | 389.1226 | 9.83 | POS | 199665.9185 | 196622.867 | 200272.1027 | 0.026712956 | 0.026773395 | 0.026283959 | 0.026590103 | DOFJNFPSMUCECH-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=C(OC)C(OC)=CC=3)=CC(=O)C=2C(O)=C1OC | HMDB0037571 | 49901 | LMPK12111479 |  | 358832 | 2174-59-6 | 去甲基川陈皮素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N1942 | HPLC≥98% | level1 |
| compound00017 | 8.17\_515.1918m/z | M+FA-H | C26H30O8 | 59.1 | 84.9 | -0.9 | Limonin | 469.1864, 515.1878 | 515.1923 | 515.1918 | 8.17 | NEG | 855016.1928 | 809787.454 | 811600.6688 | 0.11439113 | 0.110265705 | 0.106515476 | 0.11039077 | KBDSLGBFQAGHBE-MSGMIQHVSA-N | CC1(C)O[C@H]2CC(=O)OC[C@@]22[C@H]1CC(=O)[C@]1(C)[C@@H]2CC[C@@]2(C)[C@@H](OC(=O)[C@H]3O[C@@]123)C1=COC=C1 | HMDB0302538 | 44458 |  | C03514 | 179651 | 1180-71-8 | 柠檬苦素 | 萜类 | 三萜类 | Terpenes | Triterpenes | HY-17411 | HPLC≥98% | level1 |
| compound00018 | 4.65\_610.1544n | M+H, M+Na | C27H30O16 | 62.7 | 75.3 | 1.65 | Quercetin 3-o-neohesperidoside | 85.0288, 303.0493, 328.0891 | 611.1607 | 611.1617 | 4.65 | POS | 295385.4426 | 289155.1678 | 296311.5565 | 0.039519105 | 0.039373169 | 0.038888295 | 0.03926019 | FYBMGZSDYDNBFX-GXPPAHCZSA-N | C1(O)=CC2OC(C3C=C(O)C(O)=CC=3)=C(O[C@H]3[C@H](O[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)[C@@H](O)[C@H](O)[C@@H](CO)O3)C(=O)C=2C(O)=C1 |  | 50513 | LMPK12112097 |  | 5491657 |  | 槲皮素-3-O-新橙皮苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DH0164-0010 | HPLC≥98% | level1 |
| compound00019 | 8.10\_342.1101n | M+H, M+Na, M+K, M+H-H2O | C19H18O6 | 54.2 | 63.1 | -0.75 | 6-Demethoxytangeretin | 313.0702, 325.1066, 328.0938, 343.1171 | 343.1176 | 343.1174 | 8.1 | POS | 695456.1135 | 700855.2074 | 736913.939 | 0.093043865 | 0.095432812 | 0.096713497 | 0.095063391 | DDGJUTBQQURRGE-UHFFFAOYSA-N | C12C(=O)C=C(C3C=CC(OC)=CC=3)OC=1C(OC)=C(OC)C=C2OC | HMDB0302157 | 49793 | LMPK12111369 |  | 629964 |  | 6-去甲氧基橘皮素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4126 | HPLC≥98% | level1 |
| compound00020 | 8.71\_402.1310n | M+H, M+Na, M+K | C21H22O8 | 59.7 | 78.5 | -1.16 | Quercetagetin 3,5,6,7,3',4'-hexamethyl ether | 373.0913, 388.1157, 403.1382 | 403.1387 | 403.1383 | 8.71 | POS | 8835252.563 | 8784414.609 | 8935809.338 | 1.182053082 | 1.196140624 | 1.172746673 | 1.183646793 | CHXSDKWBSFDZEU-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=C(OC)C(OC)=CC=3)=C(OC)C(=O)C=2C(OC)=C1OC | HMDB0029308 | 51430 | LMPK12113018 |  | 386331 | 1251-84-9 | 3,5,6,7,3',4'-六甲氧基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DL0096 | HPLC≥98% | level1 |
| compound00021 | 4.96\_784.2205n | M+H, M+Na | C38H40O18 | 56.2 | 68.7 | -1.26 | 6-Feruloylspinosin | 285.0753, 297.0753, 323.0908, 327.0857, 339.1072, 351.0856, 381.0963, 393.0960, 429.1173, 785.2261 | 785.2287 | 785.2278 | 4.96 | POS | 1097938.273 | 1093113.134 | 1154735.67 | 0.146891253 | 0.148845095 | 0.151548938 | 0.149095095 | WZAXZHIVHPRTIU-IHIXZLSHSA-N | COC1C(=C(C2=C(C=1)OC(=CC2=O)C1=CC=C(C=C1)O)O)[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)COC(/C=C/C1=CC=C(C(=C1)OC)O)=O)O)O)CO |  |  | LMPK12110993 |  | 21597353 |  | 6-阿魏酰斯皮诺素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N2160 | HPLC≥98% | level1 |
| compound00022 | 4.22\_593.1512m/z | M+FA-H | C26H28O13 | 70.1 | 59.4 | 0.02 | Puerarin 6''-O-Xyloside | 353.0666, 383.0771, 593.1509 | 593.1512 | 593.1512 | 4.22 | NEG | 1009247.89 | 1005466.464 | 1001488.828 | 0.135025521 | 0.136910578 | 0.131436633 | 0.134457577 | YCFQXQCEEPCZMO-KATYHMCLSA-N | C1(O)=C([C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]3[C@H](O)[C@@H](O)[C@H](O)CO3)O2)C2OC=C(C3C=CC(O)=CC=3)C(=O)C=2C=C1 |  |  | LMPK12050009 |  | 100990912 |  | 葛根素 6″-O-木糖苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N2135 | HPLC≥98% | level1 |
| compound00023 | 5.31\_701.1489m/z | M+H-H2O | C36H30O16 | 59.2 | 86.9 | -1.69 | Salvianolic acid Y | 181.0492, 249.0542, 267.0649, 277.0498, 295.0595, 296.0632, 323.0548, 341.0648, 521.1100, 701.1470 | 701.1501 | 701.1489 | 5.31 | POS | 1767002.306 | 1793711.945 | 1765207.502 | 0.236404167 | 0.244242994 | 0.231668016 | 0.237438392 | SNKFFCBZYFGCQN-DUMGGQTMSA-N | O=C(/C=C/c1ccc(O)c2c1[C@H](C(=O)O[C@@H](Cc1ccc(O)c(O)c1)C(=O)O)[C@H](c1ccc(O)c(O)c1)O2)O[C@@H](Cc1ccc(O)c(O)c1)C(=O)O |  |  |  |  |  | 1638738-76-7 | 丹酚酸 Y | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | ST55350205 | HPLC≥95% | level1 |
| compound00024 | 5.06\_677.1696m/z | M+FA-H | C30H32O15 | 63.6 | 78.6 | -4.38 | 4-O-galloylalbiflorin | 286.0479, 301.0716, 308.0305, 323.0537, 609.1821, 631.1644, 677.1704 | 677.1725 | 677.1696 | 5.06 | NEG | 1088604.408 | 1179351.977 | 1106430.803 | 0.145642491 | 0.160587913 | 0.145209347 | 0.150479917 | UXHIYEMICNYJGK-NJVRKBDPSA-N | CC12C[C@H]([C@@H]3CC1(C3(C(=O)O2)COC(=O)C4=CC=CC=C4)O[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)CO)O)O)O)OC(=O)C6=CC(=C(C(=C6)O)O)O |  |  |  |  |  | 1201580-97-3 | 4-O-没食子酰白芍苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | DM0224 | HPLC≥95% | level1 |
| compound00025 | 3.72\_371.0982m/z | M+FA-H | C15H18O8 | 51.7 | 52.3 | -0.42 | 4-O-beta-Glucopyranosyl-cis-coumaric acid | 85.0284, 119.0491, 163.0392, 191.0188, 207.976, 209.0295, 302.1718, 325.0926, 371.1042 | 371.0984 | 371.0982 | 3.72 | NEG | 8450.491083 | 8856.065743 | 9065.432353 | 0.001130577 | 0.001205897 | 0.001189759 | 0.001175411 | LJFYQZQUAULRDF-LSSWKVNRSA-N | C1=CC(=CC=C1C=CC(=O)O)OC2C(C(C(C(O2)CO)O)O)O |  |  |  | C06739 | 10604651 |  | 香豆酸-4-葡萄糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DX0066 | HPLC≥98% | level1 |
| compound00026 | 4.87\_580.1794n | M+H, M+K, M+Na, M+H-H2O | C27H32O14 | 58.2 | 82.4 | 0.36 | Naringin | 85.0288, 129.0546, 153.0180, 195.0287, 273.0753, 315.0858, 383.1119, 401.1230, 419.1328, 435.1278 | 581.1865 | 581.1867 | 4.87 | POS | 4973568.293 | 4831083.649 | 4659863.934 | 0.665405056 | 0.65783045 | 0.611566308 | 0.644933938 | DFPMSGMNTNDNHN-CSBXLKJISA-N | CC1O[C@@H](OC2[C@H](Oc3cc(O)c4c(c3)OC(c3ccc(O)cc3)CC4=O)OC(CO)[C@@H](O)[C@H]2O)C(O)[C@@H](O)[C@H]1O |  |  |  |  |  | 10236-47-2 | 柚皮苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0153 | HPLC≥98% | level1 |
| compound00027 | 5.43\_209.0807m/z | M+H | C11H12O4 | 59.1 | 86.6 | -0.75 | Sinapaldehyde | 121.0648, 131.0490, 145.0282, 149.0595, 153.0544, 177.0544, 181.0852, 191.0699, 208.1324, 209.0802 | 209.0808 | 209.0807 | 5.43 | POS | 22543.74932 | 22728.8069 | 22224.38005 | 0.003016089 | 0.003094896 | 0.002916755 | 0.003009247 | CDICDSOGTRCHMG-ONEGZZNKSA-N | COC1=CC(=CC(=C1O)OC)C=CC=O |  | 44806 |  | C05610 | 5280802 | 4206-58-0 | 芥子醛 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1312 | HPLC≥98% | level1 |
| compound00028 | 0.78\_207.0503m/z | M+FA-H | C6H10O5 | 54.2 | 72.6 | -4.46 | 3-Hydroxy-2-methylglutaric acid | 59.0127, 73.0283, 161.0446 | 207.0512 | 207.0503 | 0.78 | NEG | 355080.4368 | 373256.2746 | 371886.4917 | 0.047505594 | 0.0508249 | 0.048806843 | 0.049045779 | JJSWRLIXMHKPEW-IUYQGCFVSA-N | C[C@@H]([C@H](O)CC(O)=O)C(O)=O | HMDB0029169 |  |  |  |  | 1189155-79-0 | 3-羟基-2-甲基戊二酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  |  |  | level1 |
| compound00029 | 1.07\_139.0270n | M+H-H2O, M+H | C6H5NO3 | 52.6 | 64.6 | 0.35 | 3-Hydroxypicolinic acid | 112.0395, 122.0237, 140.0341 | 140.0342 | 140.0343 | 1.07 | POS | 64171.60825 | 65975.86761 | 65982.79674 | 0.008585408 | 0.008983685 | 0.008659664 | 0.008742919 | BRARRAHGNDUELT-UHFFFAOYSA-N | OC(=O)C1=C(O)C=CC=N1 | HMDB0013188 | 64950 |  | C18620 | 13401 | 874-24-8 | 3-羟基吡啶甲酸 | 吡啶及其衍生物 | 氨基酸类 | Pyridines and derivatives |  | HY-Y0030 | HPLC≥98% | level1 |
| compound00030 | 4.88\_217.1074m/z | M-H | C10H18O5 | 53.8 | 68.1 | -3.31 | 3-Hydroxysebacic acid | 155.1069, 171.1018, 217.1075 | 217.1081 | 217.1074 | 4.88 | NEG | 50817.07518 | 52418.53871 | 51731.86483 | 0.006798728 | 0.007137635 | 0.006789354 | 0.006908572 | OQYZCCKCJQWHIE-MRVPVSSYSA-N | O[C@H](CCCCCCC(O)=O)CC(O)=O | HMDB0000350 |  |  |  | 124350389 | 446881-43-2 | 3-羟基癸二酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | H953770 | HPLC≥98% | level1 |
| compound00031 | 9.76\_402.1310n | M+H, M+Na | C21H22O8 | 58.2 | 82.1 | -1.13 | 3-Methoxytangeretin | 355.081, 373.0916, 388.1145, 403.1385 | 403.1387 | 403.1383 | 9.76 | POS | 476723.5178 | 474660.8676 | 489432.6569 | 0.063780011 | 0.064632781 | 0.064233747 | 0.064215513 | OBIOZWXPDBWYHB-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=CC(OC)=CC=3)=C(OC)C(=O)C=2C(OC)=C1OC |  | 51727 | LMPK12113315 |  | 11741814 |  | 3,5,6,7,8,4‘-六甲氧基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DL0335 | HPLC≥98% | level1 |
| compound00032 | 3.95\_772.2054n | M-H, M+FA-H | C33H40O21 | 54.6 | 69 | -1.01 | Kaempferol 3-sophoroside-7-glucoside | 85.0284, 191.019, 299.0195, 385.0775, 462.0801, 609.1458, 771.1992 | 771.1989 | 771.1982 | 3.95 | NEG | 169902.268 | 177257.3353 | 173487.3734 | 0.022730929 | 0.024136463 | 0.022768698 | 0.02321203 | MBFNAZBJKVFNKZ-JGPRCQAHSA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=CC2OC(C3C=CC(O)=CC=3)=C(O[C@H]3[C@H](O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)[C@@H](O)[C@H](O)[C@@H](CO)O3)C(=O)C=2C(O)=C1 |  | 50173 | LMPK12111757 |  | 12960460 |  | 山柰酚-3-O-槐二糖-7-O-葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DS0115-0005 | HPLC≥98% | level1 |
| compound00033 | 1.22\_205.1184m/z | M+H | C8H16N2O4 | 61 | 74.9 | 0.51 | Serylvaline | 118.0864, 149.0234, 158.1172, 159.1127, 187.0087, 187.1076, 204.0863, 204.1378, 205.0698, 205.1180 | 205.1183 | 205.1184 | 1.22 | POS | 18625.83163 | 19187.74256 | 18912.55638 | 0.002491918 | 0.002612723 | 0.002482107 | 0.002528916 | ILVGMCVCQBJPSH-WDSKDSINSA-N | CC(C)[C@H](NC(=O)[C@@H](N)CO)C(O)=O | HMDB0029052 | 23827 |  |  | 7020158 | 51782-06-0 | 丝氨酰缬氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | 332P1402 |  | level1 |
| compound00034 | 1.79\_269.1133m/z | M+H | C12H16N2O5 | 50.6 | 55.5 | 0.55 | Seryltyrosine | 136.0757, 165.0545, 182.0812, 210.0747, 223.1075, 251.1021, 252.0868, 268.1022, 269.0647, 269.1188 | 269.1132 | 269.1133 | 1.79 | POS | 12848.68519 | 13872.28442 | 13371.23251 | 0.001719003 | 0.001888937 | 0.001754857 | 0.001787599 | MALNXHYEPCSPPU-UWVGGRQHSA-N | N[C@@H](CO)C(=O)N[C@@H](CC1=CC=C(O)C=C1)C(O)=O | HMDB0029051 | 23778 |  |  | 7021865 | 21435-27-8 | 丝氨酰酪氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00035 | 3.61\_253.1184m/z | M+H | C12H16N2O4 | 58.3 | 76.3 | 0.44 | Serylphenylalanine | 60.045, 120.0808, 166.0861, 197.1169, 207.1127, 234.1337, 235.1085, 236.055, 253.1193 | 253.1183 | 253.1184 | 3.61 | POS | 33586.89346 | 35003.06739 | 35919.87145 | 0.004493532 | 0.004766236 | 0.004714168 | 0.004657979 | PPQRSMGDOHLTBE-UWVGGRQHSA-N | N[C@@H](CO)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)=O | HMDB0029046 | 23895 |  |  | 7009597 | 16875-28-8 | 丝氨酰苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00036 | 4.80\_253.1797m/z | M+H | C15H24O3 | 51.6 | 53.1 | -0.29 | 4,10-Epizedoarondiol | 217.1586, 223.1683, 235.1326, 235.1688, 252.1585, 253.0489, 253.1000, 253.1405, 253.1521, 253.1800 | 253.1798 | 253.1797 | 4.8 | POS | 34326.75151 | 34915.69896 | 35872.34366 | 0.004592516 | 0.004754339 | 0.004707931 | 0.004684929 | TXIKNNOOLCGADE-OSRDXIQISA-N | CC(=C1C[C@H]2[C@@H](CC[C@@]2(C)O)[C@@](CC1=O)(C)O)C |  |  |  |  |  | 98644-24-7 | 蓬莪二醇 | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | DE0191 | HPLC≥98% | level1 |
| compound00037 | 5.33\_538.1107n | M+H-H2O, M+H | C27H22O12 | 54.8 | 50.9 | -0.79 | Lithospermic acid | 249.0542, 267.0644, 277.0491, 281.0440, 295.0595, 323.0544, 341.0648, 502.3154, 520.3261, 521.1074 | 521.1078 | 521.1074 | 5.33 | POS | 28554321.76 | 28692993.73 | 28222006.1 | 3.820233073 | 3.907016797 | 3.703890996 | 3.810380289 | UJZQBMQZMKFSRV-UJVFRBSWSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=C3C(C(OC3=C(C=C2)O)C4=CC(=C(C=C4)O)O)C(=O)O)O)O |  |  |  | C08745 | 5281302 |  | 紫草酸 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0823 | HPLC≥98% | level1 |
| compound00038 | 0.73\_174.1116n | M+H-H2O, M+H | C6H14N4O2 | 55.9 | 78.7 | -0.17 | L-Arginine | 70.0656, 95.0606, 110.0714, 112.087, 116.0707, 156.0767 | 175.119 | 175.1189 | 0.73 | POS | 14358951.34 | 14489106.23 | 14680224.09 | 1.921059139 | 1.972926978 | 1.926650771 | 1.940212296 | ODKSFYDXXFIFQN-BYPYZUCNSA-N | N[C@@H](CCCNC(N)=N)C(O)=O | HMDB0000517 | 13 |  | C00062 | 6322 | 74-79-3 | L-精氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0455 | HPLC≥98% | level1 |
| compound00039 | 8.79\_343.1172m/z | M+H | C19H18O6 | 57 | 78.8 | -1.36 | Scutellarein tetramethyl ether | 238.1304, 282.0882, 299.0908, 313.0702, 343.1172 | 343.1176 | 343.1172 | 8.79 | POS | 152353.975 | 152453.4552 | 150102.618 | 0.020383173 | 0.020759012 | 0.019699653 | 0.020280613 | URSUMOWUGDXZHU-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC(OC)=CC=3)=CC(=O)C=2C(OC)=C1OC | HMDB0030575 | 49592 | LMPK12111167 | C14472 | 96118 | 1168-42-9 | 4',5,6,7-四甲氧基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4314 | HPLC≥98% | level1 |
| compound00040 | 5.39\_146.0599m/z | M+H | C9H7NO | 61.9 | 87.5 | -1.16 | 4-formyl Indole | 99.0443, 118.0652, 146.0599 | 146.06 | 146.0599 | 5.39 | POS | 9771.860956 | 10069.08031 | 10192.87535 | 0.00130736 | 0.001371069 | 0.001337726 | 0.001338718 | JFDDFGLNZWNJTK-UHFFFAOYSA-N | C1=CC(=C2C=CNC2=C1)C=O |  | 96392 |  |  |  |  | 4-甲酰吲哚 | 吲哚及其衍生物 |  | Indoles and derivatives |  | S32109 |  | level1 |
| compound00041 | 0.79\_148.0603m/z | M+H | C5H9NO4 | 57.3 | 83.8 | -0.61 | L-Glutamic acid | 84.0448, 102.0552, 130.0498, 130.0973, 147.0961, 148.0603 | 148.0604 | 148.0603 | 0.79 | POS | 509794.7607 | 513707.1679 | 521555.801 | 0.068204555 | 0.069949569 | 0.068449629 | 0.068867917 | WHUUTDBJXJRKMK-VKHMYHEASA-N | N[C@@H](CCC(O)=O)C(O)=O | HMDB0000148 | 19 |  | C00025 | 33032 | 56-86-0 | L-谷氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-14608 | HPLC≥98% | level1 |
| compound00042 | 0.78\_147.0763m/z | M+H | C5H10N2O3 | 57.6 | 82.2 | -0.65 | L-Glutamine | 84.0448, 87.0443, 102.0552, 130.0498, 146.1066 | 147.0764 | 147.0763 | 0.78 | POS | 178576.8784 | 183241.3144 | 182751.7525 | 0.02389149 | 0.024951279 | 0.023984566 | 0.024275778 | ZDXPYRJPNDTMRX-VKHMYHEASA-N | N[C@@H](CCC(N)=O)C(O)=O | HMDB0000641 | 18 |  | C00064 | 5961 | 56-85-9 | L-谷氨酰胺 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0390 | HPLC≥98% | level1 |
| compound00043 | 0.66\_156.0768m/z | M+H | C6H9N3O2 | 55.3 | 70.5 | 0.3 | L-Histidine | 95.0607, 110.009, 110.0714, 128.0192, 156.0766 | 156.0768 | 156.0768 | 0.66 | POS | 53919.40244 | 56990.12679 | 56730.77023 | 0.007213783 | 0.007760131 | 0.007445416 | 0.00747311 | HNDVDQJCIGZPNO-YFKPBYRVSA-N | N[C@@H](CC1=CN=CN1)C(O)=O | HMDB0000177 | 21 |  | C00135 | 6274 | 71-00-1 | L-组氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0832 | HPLC≥98% | level1 |
| compound00044 | 1.41\_132.1021m/z | M+H | C6H13NO2 | 58.9 | 82.7 | 1.52 | L-Isoleucine | 69.0704, 86.0968 | 132.1019 | 132.1021 | 1.41 | POS | 2436821.233 | 2386179.231 | 2434236.728 | 0.326018077 | 0.324917031 | 0.31947224 | 0.323469116 | AGPKZVBTJJNPAG-WHFBIAKZSA-N | C([C@@H](N)[C@@H](C)CC)(=O)O | HMDB0000172 | 23 | LMFA01100047 | C00407 | 6306 | 73-32-5 | L-异亮氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0771 | HPLC≥98% | level1 |
| compound00045 | 0.64\_146.1056n | M+H-H2O, M+H | C6H14N2O2 | 56.6 | 84.9 | 0.49 | L-Lysine | 84.0812, 88.9529, 101.02, 129.0198 | 147.1128 | 147.1129 | 0.64 | POS | 100347.046 | 98200.17584 | 101309.1502 | 0.013425257 | 0.013371548 | 0.013295938 | 0.013364248 | KDXKERNSBIXSRK-YFKPBYRVSA-N | NCCCC[C@H](N)C(O)=O | HMDB0000182 | 25 |  | C00047 | 5962 | 56-87-1 | L-赖氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N0469 | HPLC≥98% | level1 |
| compound00046 | 3.91\_305.0666m/z | M-H | C15H14O7 | 61.8 | 91.9 | -0.34 | Epigallocatechin | 125.0234, 137.0235, 139.039, 165.0185, 167.0342, 179.0343, 219.0655, 305.0665 | 305.0667 | 305.0666 | 3.91 | NEG | 18443.40397 | 19452.38165 | 18772.95264 | 0.002467511 | 0.002648757 | 0.002463786 | 0.002526685 | XMOCLSLCDHWDHP-IUODEOHRSA-N | C1(O)C=C2O[C@H](C3=CC(O)=C(O)C(O)=C3)[C@H](O)CC2=C(O)C=1 | HMDB0038361 | 44010 | LMPK12020004 | C12136 | 72277 | 970-74-1 | 表没食子儿茶素 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | HY-N0225 | HPLC≥98% | level1 |
| compound00047 | 4.36\_290.0789n | M-H, M+FA-H | C15H14O6 | 61.4 | 91.3 | -0.4 | Epicatechin | 109.0284, 125.0234, 203.0706, 245.0816, 289.0716 | 289.0718 | 289.0716 | 4.36 | NEG | 59671.66396 | 59854.40813 | 59809.65451 | 0.007983368 | 0.008150149 | 0.007849493 | 0.007994337 | PFTAWBLQPZVEMU-UKRRQHHQSA-N | C1(O)C=C2O[C@H](C3=CC=C(O)C(O)=C3)[C@H](O)CC2=C(O)C=1 | HMDB0001871 | 3420 | LMPK12020003 | C09727 | 72276 | 490-46-0 | L-表儿茶素 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | HY-N0001 | HPLC≥98% | level1 |
| compound00048 | 0.75\_116.0708m/z | M+H | C5H9NO2 | 58.7 | 92.6 | 1.67 | L-Proline | 70.0657, 116.0707 | 116.0706 | 116.0708 | 0.75 | POS | 4420001.684 | 4596050.714 | 4582946.93 | 0.591344342 | 0.625826901 | 0.601471625 | 0.606214289 | ONIBWKKTOPOVIA-BYPYZUCNSA-N | OC(=O)[C@@H]1CCCN1 | HMDB0000162 | 29 |  | C00148 | 145742 | 147-85-3 | L-脯氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-Y0252 | HPLC≥98% | level1 |
| compound00049 | 5.92\_201.1126m/z | M-H | C10H18O4 | 60.9 | 85.3 | -3.17 | Sebacic acid | 139.1118, 183.1019, 201.1124 | 201.1132 | 201.1126 | 5.92 | NEG | 51733.58828 | 52124.05938 | 52143.26112 | 0.006921347 | 0.007097537 | 0.006843346 | 0.006954077 | CXMXRPHRNRROMY-UHFFFAOYSA-N | C(CCCCCCCCC(=O)O)(=O)O | HMDB0000792 | 4240 | LMFA01170006 | C08277 | 5192 | 111-20-6 | 癸二酸 | 脂肪酰类 | 脂肪酸及其衍生物 | Fatty Acyls | Fatty acid and derivatives | HY-W014787 | HPLC≥98% | level1 |
| compound00050 | 10.37\_279.0660m/z | M-H2O-H | C17H14O5 | 56.2 | 67.2 | -0.99 | 7,4'-Di-O-methylapigenin | 251.071, 279.0658 | 279.0663 | 279.066 | 10.37 | NEG | 24340.09187 | 27175.48893 | 24744.84315 | 0.003256419 | 0.003700384 | 0.003247544 | 0.003401449 | LZERJKGWTQYMBB-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC(OC)=CC=3)=CC(=O)C=2C(O)=C1 | HMDB0132454 | 49456 | LMPK12111029 | C10019 | 5281601 | 5128-44-9 | 芹菜素二甲醚 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N2144 | HPLC≥98% | level1 |
| compound00051 | 4.78\_463.0883m/z | M-H | C21H20O12 | 58.3 | 58.5 | 0.21 | 7-[(beta-D-Glucopyranosyl)oxy]-3',4',5,8-tetrahydroxyflavone | 300.027, 301.0346, 342.068, 462.1073, 463.0875 | 463.0882 | 463.0883 | 4.78 | NEG | 28035.66944 | 27202.85314 | 26678.37808 | 0.003750843 | 0.00370411 | 0.003501303 | 0.003652086 | BIPHTXZNUUXTIC-GHNMMOQISA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=C(O)C2OC(C3C=C(O)C(O)=CC=3)=CC(=O)C=2C(O)=C1 |  |  | LMPK12111371 |  | 44217932 |  | 海波拉亭 7-O-β-D-吡喃葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DH0323-0005 | HPLC≥98% | level1 |
| compound00052 | 4.83\_593.1511m/z | M-H | C27H30O15 | 68.3 | 58 | -0.23 | Lonicerin | 284.0323, 285.04, 593.1506 | 593.1512 | 593.1511 | 4.83 | NEG | 329779.2738 | 319821.3456 | 337974.7554 | 0.044120596 | 0.043548867 | 0.044356225 | 0.044008563 | SHPPXMGVUDNKLV-KMFFXDMSSA-N | C1(O[C@H]2[C@H](O[C@H]3[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O3)[C@@H](O)[C@H](O)[C@@H](CO)O2)=CC2OC(C3C=C(O)C(O)=CC=3)=CC(=O)C=2C(O)=C1 | HMDB0005799 | 49089 | LMPK12110659 | C12630 | 5282152 | 25694-72-8 | 忍冬苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4136 | HPLC≥98% | level1 |
| compound00053 | 5.40\_447.0915m/z | M+H | C21H18O11 | 58.9 | 84.8 | -1.46 | Baicalin | 271.0596, 447.0927 | 447.0922 | 447.0915 | 5.4 | POS | 403451.8836 | 405042.8667 | 387495.9841 | 0.053977126 | 0.05515316 | 0.050855452 | 0.05332858 | IKIIZLYTISPENI-ZFORQUDYSA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](C(=O)O)O2)=CC2OC(C3C=CC=CC=3)=CC(=O)C=2C(O)=C1O |  | 49507 | LMPK12111081 | C10025 | 64982 | 21967-41-9 | 黄芩苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0197 | HPLC≥98% | level1 |
| compound00054 | 0.71\_225.0610m/z | M+FA-H | C6H12O6 | 56.1 | 62.9 | -3.55 | myo-Inositol | 113.0235, 119.0341, 129.0185, 143.0340, 161.0445, 179.0554, 206.0379, 224.0490, 225.0072, 225.0609 | 225.0618 | 225.061 | 0.71 | NEG | 835774.94 | 881767.1526 | 915293.2698 | 0.111816876 | 0.120066909 | 0.120124221 | 0.117336002 | CDAISMWEOUEBRE-GPIVLXJGSA-N | O[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@H](O)[C@@H]1O | HMDB0000211 | 5221 |  | C00137 |  | 87-89-8 | 肌醇 | 其他 |  | Others |  | HY-B1411 | HPLC≥98% | level1 |
| compound00055 | 1.34\_292.1402m/z | M-H | C12H23NO7 | 53.1 | 63.9 | 0.13 | N-(1-Deoxy-1-fructosyl)leucine | 85.0285, 101.0233, 129.0182, 130.0862, 172.097, 202.1077 | 292.1402 | 292.1402 | 1.34 | NEG | 62719.43404 | 66139.36665 | 65230.77293 | 0.008391124 | 0.009005948 | 0.008560967 | 0.00865268 | KGTRBDVOUPALMB-PPNLDZOPSA-N | CC(C)C[C@H](NCC1(O)O[C@H](CO)[C@@H](O)[C@@H]1O)C(O)=O | HMDB0037840 |  |  |  | 131752244 | 34393-18-5 | N-(1-脱氧-1-果糖基)亮氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids |  |  | level1 |
| compound00056 | 2.24\_107.0495m/z | M+H | C7H6O | 54 | 56.5 | 3.52 | Benzaldehyde | 53.0392, 79.0547, 80.05, 91.0546, 95.0496, 105.0703, 107.0494 | 107.0491 | 107.0495 | 2.24 | POS | 10139.79189 | 10213.0941 | 9939.188777 | 0.001356585 | 0.001390679 | 0.001304431 | 0.001350565 | HUMNYLRZRPPJDN-UHFFFAOYSA-N | O=CC1=CC=CC=C1 | HMDB0006115 | 58358 |  | C00261 | 240 | 100-52-7 | 苯甲醛 | 其他 |  | Others |  | RMT10550 | HPLC≥98% | level1 |
| compound00057 | 2.16\_327.1319n | M+H-H2O, M+H, M+Na | C15H21NO7 | 55.9 | 78.2 | 0.2 | N-(1-Deoxy-1-fructosyl)phenylalanine | 120.0809, 132.0808, 166.0862, 178.0861, 246.1118, 264.1225, 292.1174, 309.2023, 310.089, 310.1276 | 328.1391 | 328.1391 | 2.16 | POS | 360358.0324 | 362253.707 | 368036.1564 | 0.048211675 | 0.049326722 | 0.04830152 | 0.048613306 | FAVRCIXPIVJIPN-VJDSNFAGSA-N | OC[C@H]1OC(O)(CN[C@@H](CC2=CC=CC=C2)C(O)=O)[C@@H](O)[C@@H]1O | HMDB0037846 |  |  |  | 101039148 | 87251-83-0 | N-(1-脱氧-1-果糖基)苯丙氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids |  |  | level1 |
| compound00058 | 1.03\_191.0193m/z | M-H | C6H8O7 | 59.9 | 96.4 | -2.26 | Citric acid | 85.0285, 87.0078, 111.0077, 129.0183, 191.019 | 191.0197 | 191.0193 | 1.03 | NEG | 15151527.19 | 14978300.8 | 15443898.3 | 2.027096485 | 2.039538759 | 2.026876319 | 2.031170521 | KRKNYBCHXYNGOX-UHFFFAOYSA-N | OC(=O)CC(O)(CC(O)=O)C(O)=O | HMDB0000094 | 124 |  | C00158 | 311 | 77-92-9 | 柠檬酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | HY-N1428 | HPLC≥98% | level1 |
| compound00059 | 1.12\_343.1269n | M+H-H2O, M+H | C15H21NO8 | 53 | 70 | 0.52 | N-(1-Deoxy-1-fructosyl)tyrosine | 136.0756, 148.0755, 165.0544, 182.0811, 280.1176, 308.1126, 326.1228, 344.0888, 344.1341 | 344.134 | 344.1342 | 1.12 | POS | 246369.081 | 237908.4865 | 242264.7086 | 0.032961291 | 0.032395102 | 0.03179512 | 0.032383838 | QLJKHQIODQKMNW-VJDSNFAGSA-N | OC[C@H]1OC(O)(CN[C@@H](CC2=CC=C(O)C=C2)C(O)=O)[C@@H](O)[C@@H]1O | HMDB0037845 |  |  |  | 131752248 | 34393-22-1 | N-(1-脱氧-1-果糖基)酪氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids |  |  | level1 |
| compound00060 | 9.01\_281.0804m/z | M+H | C17H12O4 | 56.3 | 73.7 | -1.39 | Nortanshinone | 149.0233, 207.0804, 235.0757, 235.112, 253.0855, 263.1069, 281.0812 | 281.0808 | 281.0804 | 9.01 | POS | 20524.39719 | 21282.09467 | 20698.42172 | 0.002745923 | 0.002897903 | 0.002716486 | 0.002786771 | YUFZXVOYNSJPSJ-UHFFFAOYSA-N | CC1=COC2=C1C(=O)C(=O)C3=C2C=CC4=C3CCCC4=O |  |  |  |  |  | 97399-70-7 | 降丹参酮 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | DJ0319 | HPLC≥98% | level1 |
| compound00061 | 4.92\_147.0440m/z | M+H-H2O | C9H8O3 | 59.5 | 66.4 | -0.27 | cis-p-Coumaric acid | 84.0448, 91.0546, 119.0493, 146.06, 147.0439 | 147.0441 | 147.044 | 4.92 | POS | 15924.39752 | 16273.07692 | 15556.91255 | 0.002130497 | 0.002215844 | 0.002041708 | 0.00212935 | NGSWKAQJJWESNS-UTCJRWHESA-N | OC(=O)\C=C/C1=CC=C(O)C=C1 | HMDB0030677 | 87135 |  | C06738 | 1549106 | 4501-31-9 | 顺-对香豆酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | H825070-25mg | HPLC≥98% | level1 |
| compound00062 | 1.12\_188.0559m/z | M-H | C7H11NO5 | 58.6 | 93.5 | -2.85 | N-Acetyl-L-glutamic acid | 59.0128, 100.0757, 102.055, 121.0434, 126.055, 128.0343, 144.0656, 146.0448, 170.045, 188.0557 | 188.0564 | 188.0559 | 1.12 | NEG | 100549.2424 | 98553.13049 | 99974.55728 | 0.013452308 | 0.013419608 | 0.013120785 | 0.0133309 | RFMMMVDNIPUKGG-YFKPBYRVSA-N | CC(=O)N[C@@H](CCC(O)=O)C(O)=O | HMDB0001138 | 3325 |  | C00624 | 70914 | 1188-37-0 | N-乙酰-L-谷氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | S20284-25g | HPLC≥98% | level1 |
| compound00063 | 12.69\_282.2788m/z | M+H | C18H35NO | 69.3 | 87.6 | -1.31 | Oleamide | 69.0704, 81.0701, 83.0858, 95.0857, 97.1012, 135.1166, 247.242, 265.2524, 282.279 | 282.2791 | 282.2788 | 12.69 | POS | 270512.0176 | 275569.4136 | 298700.1823 | 0.036191333 | 0.037523248 | 0.039201781 | 0.037638787 | FATBGEAMYMYZAF-KTKRTIGZSA-N | C(CCCCCCC(=O)N)/C=C\CCCCCCCC | HMDB0002117 | 4115 | LMFA08010004 | C19670 | 5283387 | 301-02-0 | 油酰胺 | 脂肪酰类 | 脂肪酸及其衍生物 | Fatty Acyls | Fatty acid and derivatives | HY-N2327 | HPLC≥98% | level1 |
| compound00064 | 4.70\_206.0816m/z | M-H | C11H13NO3 | 58.1 | 89.3 | -3.11 | N-Acetyl-L-phenylalanine | 58.0288, 70.0288, 147.0442, 161.0447, 164.0708, 206.0816 | 206.0823 | 206.0816 | 4.7 | NEG | 68514.22963 | 70914.25683 | 69435.82262 | 0.0091664 | 0.009656127 | 0.009112843 | 0.00931179 | CBQJSKKFNMDLON-JTQLQIEISA-N | CC(=O)N[C@@H](CC1=CC=CC=C1)C(O)=O | HMDB0000512 | 34536 |  | C03519 | 74839 | 2018-61-3 | N-乙酰-L-苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-Y0068 | HPLC≥98% | level1 |
| compound00065 | 4.45\_172.0971m/z | M-H | C8H15NO3 | 57.1 | 86.7 | -4.75 | N-Acetylleucine | 111.0805, 128.107, 130.0862, 172.0969 | 172.0979 | 172.0971 | 4.45 | NEG | 20591.36282 | 20530.46733 | 20291.55391 | 0.002754883 | 0.002795556 | 0.002663089 | 0.002737843 | WXNXCEHXYPACJF-ZETCQYMHSA-N | CC(C)C[C@H](NC(C)=O)C(O)=O | HMDB0011756 | 43866 |  | C02710 | 70912 | 1188-21-2 | N-乙酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-59291 | HPLC≥98% | level1 |
| compound00066 | 11.07\_579.1773m/z | M+Na | C36H28O6 | 60.9 | 89.1 | -0.88 | Neoprzewaquinone A | 301.0831 | 579.1778 | 579.1773 | 11.07 | POS | 73086.31469 | 77859.6768 | 88661.66085 | 0.009778091 | 0.010601859 | 0.011636066 | 0.010672005 | SXQCYGZVSVUMEL-LSCVHKIXSA-N | C=C1CCCc2c(ccc3c2C(=O)C(=O)c2c(C)coc2-3)/C(C)=C\CCc2c1ccc1c2C(=O)C(=O)c2c(C)coc2-1 |  |  |  |  |  | 630057-39-5 | 甘西鼠尾新酮 A | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-N3201 | HPLC≥98% | level1 |
| compound00067 | 3.53\_468.1721m/z | M+FA-H | C17H29NO11 | 61.4 | 95.5 | -0.27 | Neolinustatin | 89.0234, 101.0234, 113.0230, 153.0184, 161.0449, 175.0003, 323.0983, 337.0532, 422.1665, 468.1751 | 468.1723 | 468.1721 | 3.53 | NEG | 35703.84652 | 37020.66919 | 37185.71551 | 0.004776756 | 0.005040965 | 0.004880299 | 0.00489934 | WOSYVGNDRYBQCQ-BARGLTKPSA-N | CCC(C)(C#N)OC1C(C(C(C(O1)COC2C(C(C(C(O2)CO)O)O)O)O)O)O |  | 66915 |  | C08336 | 119533 | 72229-42-6 | 新亚麻氰苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DX0162 | HPLC≥98% | level1 |
| compound00068 | 5.80\_282.1489m/z | M+H | C18H19NO2 | 58.2 | 90.1 | 0.21 | N-Nornuciferine | 234.1036, 250.0983, 265.1218, 282.148 | 282.1489 | 282.1489 | 5.8 | POS | 119887.0069 | 117544.3379 | 117925.2242 | 0.016039474 | 0.016005569 | 0.015476652 | 0.015840565 | QQKAHDMMPBQDAC-CQSZACIVSA-N | COc1cc2c3c(c1OC)-c1ccccc1C[C@H]3NCC2 |  |  |  |  |  | 4846-19-9 | N-去甲荷叶碱 | 生物碱 |  | Alkaloids |  | HY-N2129 | HPLC≥98% | level1 |
| compound00069 | 4.08\_353.0878m/z | M-H | C16H18O9 | 59 | 71.4 | -0.11 | Chlorogenic acid | 173.0447, 179.0347, 191.0555, 353.081 | 353.0878 | 353.0878 | 4.08 | NEG | 31974.38441 | 32138.91379 | 31513.10136 | 0.004277797 | 0.004376235 | 0.004135818 | 0.004263283 | CWVRJTMFETXNAD-JUHZACGLSA-N | O[C@@H]1C[C@](O)(C[C@@H](OC(=O)\C=C\C2=CC(O)=C(O)C=C2)[C@@H]1O)C(O)=O | HMDB0003164 | 3498 |  | C00852 | 1794427 | 202650-88-2 | 绿原酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N0055 | HPLC≥98% | level1 |
| compound00070 | 10.26\_314.1515n | M+H, M+K | C19H22O4 | 60.8 | 93.3 | -1.06 | Neocryptotanshinone | 251.1429, 279.1377, 297.1483, 315.1585 | 315.1591 | 315.1588 | 10.26 | POS | 1340861.873 | 1344695.684 | 1391516.212 | 0.179391579 | 0.183102143 | 0.182624309 | 0.18170601 | LGZFJHSOBYVDLA-JTQLQIEISA-N | C[C@@H](CO)C1=C(O)c2ccc3c(c2C(=O)C1=O)CCCC3(C)C |  |  |  |  |  | 109664-02-0 | 新隐丹参酮 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-119720 | HPLC≥98% | level1 |
| compound00071 | 3.61\_311.0407m/z | M-H | C13H12O9 | 58.5 | 70.1 | -0.42 | Caftaric acid | 78.9179, 87.0076, 135.0441, 149.0082, 177.0551, 179.0342, 243.0439 | 311.0409 | 311.0407 | 3.61 | NEG | 119368.2942 | 119769.8196 | 120240.8181 | 0.015970077 | 0.016308605 | 0.015780554 | 0.016019745 | SWGKAHCIOQPKFW-JTNORFRNSA-N | O[C@H]([C@@H](OC(=O)\C=C\C1=CC(O)=C(O)C=C1)C(O)=O)C(O)=O | HMDB0013680 | 85252 |  |  | 6440397 | 67879-58-7 | 咖啡酰基酒石酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N0321 | HPLC≥98% | level1 |
| compound00072 | 4.98\_625.1756m/z | M+H | C28H32O16 | 65.9 | 80 | -1.19 | Narcissin | 85.0288, 128.1069, 317.0653, 479.1175 | 625.1763 | 625.1756 | 4.98 | POS | 407921.3677 | 398208.9428 | 412526.3133 | 0.054575091 | 0.054222611 | 0.054140464 | 0.054312722 | UIDGLYUNOUKLBM-GEBJFKNCSA-N | CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)OC)O)O)O)O)O)O |  | 49017 |  |  | 5481663 |  | 水仙苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N0649 | HPLC≥98% | level1 |
| compound00073 | 9.43\_418.1257n | M+H, M+Na | C21H22O9 | 60.7 | 94.5 | -1.54 | Natsudaidain | 361.0911, 389.0859, 404.1093, 419.1335 | 419.1337 | 419.133 | 9.43 | POS | 569518.1611 | 607063.043 | 609218.4145 | 0.076194845 | 0.082661486 | 0.079954578 | 0.079603636 | CCJBNIRSVUKABH-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=C(OC)C(OC)=CC=3)=C(O)C(=O)C=2C(OC)=C1OC | HMDB0030160 | 51756 | LMPK12113344 |  | 3084605 | 35154-55-3 | 柚皮黄素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DN0123 | HPLC≥98% | level1 |
| compound00074 | 4.12\_291.0864m/z | M+H | C15H14O6 | 61.2 | 84.2 | 0.32 | Catechin | 123.0441, 139.0389, 147.0439, 165.0545, 207.065, 291.0865 | 291.0863 | 291.0864 | 4.12 | POS | 49212.76467 | 52758.22669 | 52226.24934 | 0.00658409 | 0.007183889 | 0.006854238 | 0.006874072 | PFTAWBLQPZVEMU-DZGCQCFKSA-N | C1(O)C=C2O[C@H](C3=CC=C(O)C(O)=C3)[C@@H](O)CC2=C(O)C=1 | HMDB0002780 | 3419 | LMPK12020001 | C06562 | 9064 | 154-23-4 | 儿茶素 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | HY-N0898 | HPLC≥98% | level1 |
| compound00075 | 0.98\_217.1296m/z | M+H | C8H16N4O3 | 53.9 | 73 | 0.28 | N-Acetylarginine | 70.0656, 115.0867, 157.0968, 158.0806, 175.1194, 200.1033, 216.1227, 217.1291 | 217.1295 | 217.1296 | 0.98 | POS | 223850.017 | 213358.7441 | 220141.5511 | 0.029948505 | 0.029052256 | 0.02889165 | 0.02929747 | SNEIUMQYRCDYCH-LURJTMIESA-N | CC(=O)N[C@@H](CCCNC(N)=N)C(O)=O | HMDB0004620 |  |  |  | 67427 | 155-84-0 | N-α-乙酰-L-精氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-W014130 | HPLC≥98% | level1 |
| compound00076 | 4.96\_224.0683n | M+H-H2O, M+H | C11H12O5 | 58 | 80.5 | -0.96 | Sinapinic acid | 91.0545, 119.0492, 147.0438, 175.0388, 192.0416, 207.0649 | 207.0652 | 207.065 | 4.96 | POS | 33185.42256 | 33868.91244 | 33634.89058 | 0.00443982 | 0.004611802 | 0.004414285 | 0.004488636 | PCMORTLOPMLEFB-ONEGZZNKSA-N | COC1=CC(\C=C\C(O)=O)=CC(OC)=C1O | HMDB0032616 | 45738 |  | C00482 | 637775 | 7362-37-0 | 芥子酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-W009732 | HPLC≥98% | level1 |
| compound00077 | 5.25\_187.0967m/z | M-H | C9H16O4 | 59.8 | 82.8 | -4.82 | Azelaic acid | 125.0962, 187.0969 | 187.0976 | 187.0967 | 5.25 | NEG | 146389.4163 | 143538.3672 | 146218.1838 | 0.019585186 | 0.019545078 | 0.019189855 | 0.01944004 | BDJRBEYXGGNYIS-UHFFFAOYSA-N | C(CCCCCCCC(=O)O)(=O)O | HMDB0000784 | 5750 | LMFA01170054 | C08261 | 2266 | 123-99-9 | 壬二酸 | 脂肪酰类 | 脂肪酸及其衍生物 | Fatty Acyls | Fatty acid and derivatives | HY-B0704 | HPLC≥98% | level1 |
| compound00078 | 3.21\_247.1289m/z | M+H | C10H18N2O5 | 55.7 | 76.1 | 0.27 | Aspartyl-Leucine | 183.1122, 187.1073, 194.9736, 201.1232, 212.0916, 217.9890, 229.1183, 247.0706, 247.1031, 247.1305 | 247.1288 | 247.1289 | 3.21 | POS | 29581.59295 | 30092.12982 | 30685.01423 | 0.00395767 | 0.004097532 | 0.004027139 | 0.004027447 | ZVDPYSVOZFINEE-UHFFFAOYSA-N | CC(C)CC(NC(=O)C(N)CC(O)=O)C(O)=O | HMDB0028757 |  |  |  | 332962 |  | 天冬氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00079 | 5.52\_279.9975n | M+H, M+K, M+Na | C11H8N2O3S2 | 60.6 | 85.3 | -0.5 | Luciferin | 177.0114, 193.9727, 234.9991, 281.0045 | 281.0049 | 281.0048 | 5.52 | POS | 7313324.864 | 7345918.841 | 7273193.415 | 0.978437021 | 1.000266078 | 0.954542902 | 0.977748667 | BJGNCJDXODQBOB-SSDOTTSWSA-N | C1C(N=C(S1)C2=NC3=C(S2)C=C(C=C3)O)C(=O)O |  | 65823 |  | C02740 | 92934 | 2591-17-5 | 虫荧光素游离酸 | 其他 |  | Others |  | HY-12591A | HPLC≥98% | level1 |
| compound00080 | 4.01\_577.1350m/z | M-H | C30H26O12 | 58.7 | 78.1 | -0.28 | Procyanidin B1 | 125.0234, 137.0237, 161.0235, 245.0808, 287.0559, 289.0718, 407.0768, 425.0880, 451.1038, 577.1348 | 577.1351 | 577.135 | 4.01 | NEG | 51871.59207 | 57219.19019 | 53040.07024 | 0.00693981 | 0.007791321 | 0.006961044 | 0.007230725 | XFZJEEAOWLFHDH-UKWJTHFESA-N | C1(O)=CC2O[C@H](C3C=CC(O)=C(O)C=3)[C@H](O)[C@@H](C3=C(O)C=C(O)C4C[C@H](O)[C@@H](C5C=CC(O)=C(O)C=5)OC=43)C=2C(O)=C1 | HMDB0029754 | 47500 | LMPK12030001 | C10221 | 11250133 | 20315-25-7 | 原花青素 B1 | 黄酮类 | 原花青素类 | Flavonoids | Procyanidins | HY-N0795 | HPLC≥98% | level1 |
| compound00081 | 5.32\_717.1459m/z | M-H | C36H30O16 | 65.6 | 87 | -0.29 | Magnesium Lithospermate B | 109.0284, 185.0238, 277.0503, 279.0297, 293.0451, 295.0606, 321.0402, 339.0509, 519.093, 717.1459 | 717.1461 | 717.1459 | 5.32 | NEG | 235612117.1 | 221330467.2 | 242024525.3 | 31.52213558 | 30.13773541 | 31.76359812 | 31.14115637 | SNKFFCBZYFGCQN-UHFFFAOYSA-N | OC(=O)C(CC1=CC=C(O)C(O)=C1)OC(=O)C=CC1=CC=C(O)C2=C1C(C(O2)C1=CC=C(O)C(O)=C1)C(=O)OC(CC1=CC=C(O)C(O)=C1)C(O)=O | HMDB0242648 |  |  |  | 119177 |  | 丹参酸B镁 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | HY-126415 | HPLC≥98% | level1 |
| compound00082 | 10.51\_484.3186n | M+H-H2O, M+H | C30H44O5 | 61.4 | 93.5 | -0.47 | Poricoic acid B | 267.1740, 283.1692, 289.1950, 307.2046, 325.2157, 353.2466, 407.2557, 431.2932, 449.3040, 467.3152 | 485.3262 | 485.3259 | 10.51 | POS | 125067.9492 | 122852.3196 | 124681.043 | 0.016732624 | 0.016728337 | 0.016363294 | 0.016608085 | NXAZWYWJZDFISF-KXGBKNTBSA-N | C=C(C)[C@@H]1CC=C2C(=CC[C@]3(C)[C@@H]([C@@H](CCC=C(C)C)C(=O)O)[C@H](O)C[C@@]23C)[C@@]1(C)CCC(=O)O |  |  |  |  |  | 137551-39-4 | 茯苓新酸B | 萜类 | 三萜类 | Terpenes | Triterpenes | B25590-10mg | HPLC≥95% | level1 |
| compound00083 | 5.74\_594.1948n | M+H, M+Na, M+K, M+H-H2O | C28H34O14 | 55.9 | 73.1 | -0.1 | Poncirin | 153.0180, 161.0595, 195.0286, 263.0546, 287.0910, 329.1014, 397.1277, 415.1381, 433.1483, 449.1435 | 595.2021 | 595.2021 | 5.74 | POS | 2457338.667 | 2354634.766 | 2392294.271 | 0.328763069 | 0.32062174 | 0.31396766 | 0.32111749 | NLAWPKPYBMEWIR-YZOWQMJMSA-N | COc1ccc(C2CC(=O)c3c(O)cc(O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)cc3O2)cc1 |  |  |  |  |  | 14941-08-3 | 枸橘苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N2258 | HPLC≥98% | level1 |
| compound00084 | 1.29\_267.0968n | M+H, M+Na | C10H13N5O4 | 60.5 | 95.9 | 0.26 | Adenosine | 136.0616, 268.1034 | 268.104 | 268.1041 | 1.29 | POS | 5099271.974 | 4964696.671 | 5075772.333 | 0.682222733 | 0.676024031 | 0.666150641 | 0.674799135 | OIRDTQYFTABQOQ-KQYNXXCUSA-N | NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1 | HMDB0000050 | 86 |  | C00212 | 60961 | 58-61-7 | 腺苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives | Purine nucleosides | HY-B0228 | HPLC≥98% | level1 |
| compound00085 | 0.68\_828.2743n | M-H, M+FA-H | C30H52O26 | 50.8 | 54.7 | -0.46 | Maltopentaose | 89.0234, 101.0234, 383.1194, 827.2676 | 873.2729 | 873.2725 | 0.68 | NEG | 2123660.995 | 2215666.189 | 2496414.27 | 0.284120913 | 0.301698913 | 0.327632497 | 0.304484108 | FJCUPROCOFFUSR-GMMZZHHDSA-N | O=C[C@H](O)[C@@H](O)[C@H](O[C@H]1O[C@H](CO)[C@@H](O[C@H]2O[C@H](CO)[C@@H](O[C@H]3O[C@H](CO)[C@@H](O[C@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O)[C@H](O)CO |  |  |  |  |  | 34620-76-3 | 麦芽五糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N1495 | HPLC≥98% | level1 |
| compound00086 | 9.45\_295.0973m/z | M-H | C18H16O4 | 59.7 | 88.1 | -0.8 | Danshenxinkun A | 237.0915, 265.0866, 267.1022, 295.097 | 295.0976 | 295.0973 | 9.45 | NEG | 734404.4138 | 695742.4247 | 660522.4499 | 0.09825469 | 0.094736623 | 0.086687783 | 0.093226366 | GRGPQNRHXNRJFL-UHFFFAOYSA-N | O=C1C(=O)C(=C(O)C=2C=CC3=C(C=CC=C3C)C12)C(C)CO |  |  |  |  |  | 65907-75-7 | 丹参新醌甲 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-N3680 | HPLC≥98% | level1 |
| compound00087 | 0.64\_130.0864m/z | M+H | C6H11NO2 | 49.7 | 50.2 | 1.13 | D-Pipecolic acid | 60.0563, 72.0813, 84.0118, 84.045, 84.0812, 85.0844, 88.953, 112.0064, 114.1028, 130.0863 | 130.0863 | 130.0864 | 0.64 | POS | 62709.74793 | 61662.84442 | 62748.87217 | 0.008389828 | 0.008396397 | 0.00823524 | 0.008340488 | HXEACLLIILLPRG-RXMQYKEDSA-N | OC(=O)[C@H]1CCCCN1 | HMDB0005960 | 58337 |  |  | 736316 | 1723-00-8 | D-哌啶酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-Y0181 | HPLC≥98% | level1 |
| compound00088 | 0.68\_503.1612m/z | M-H | C18H32O16 | 54.4 | 76 | -1.14 | Manninotriose | 59.0128, 71.0128, 89.0234, 101.0234, 113.0234, 161.0446, 179.0554, 221.0662, 341.1088, 503.1616 | 503.1618 | 503.1612 | 0.68 | NEG | 650700.0874 | 663286.0286 | 743824.2862 | 0.087056034 | 0.090317158 | 0.09762042 | 0.091664537 | FZWBNHMXJMCXLU-YRBKNLIBSA-N | O=C[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO[C@H]1O[C@H](CO[C@H]2O[C@H](CO)[C@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 13382-86-0 | 甘露三糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N0913 | HPLC≥98% | level1 |
| compound00089 | 0.66\_132.0900n | M+H-H2O, M+H | C5H12N2O2 | 53.9 | 65.6 | 0.88 | Ornithine | 70.0656, 115.0867 | 133.0972 | 133.0973 | 0.66 | POS | 26941.52506 | 26436.08697 | 27362.39747 | 0.00360446 | 0.003599702 | 0.003591075 | 0.003598412 | AHLPHDHHMVZTML-BYPYZUCNSA-N | NCCC[C@H](N)C(O)=O | HMDB0000214 | 45121 |  | C00077 | 6262 | 3184-13-2 | 鸟氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-W017018 | HPLC≥98% | level1 |
| compound00090 | 0.90\_244.0928m/z | M+H | C9H13N3O5 | 57.4 | 83 | 0.02 | Cytarabine | 112.0507 | 244.0928 | 244.0928 | 0.9 | POS | 847263.9862 | 837790.6379 | 842547.8766 | 0.113353976 | 0.114078793 | 0.110577026 | 0.112669932 | UHDGCWIWMRVCDJ-CCXZUQQUSA-N | NC1=NC(=O)N(C=C1)[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O | HMDB0015122 | 567 |  | C02961 | 6253 | 147-94-4 | 阿糖胞嘧啶 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-13605 | HPLC≥98% | level1 |
| compound00091 | 0.79\_504.1689n | M+NH4, M+Na, M+H, M+H-H2O | C18H32O16 | 50.6 | 55.9 | -0.35 | Melezitose | 97.0287, 109.0284, 127.0390, 145.0494, 162.0760, 163.0600, 180.0870, 289.0893, 325.1125, 343.1232 | 527.1583 | 527.1581 | 0.79 | POS | 2896843.052 | 2891510.297 | 2888504.454 | 0.387563596 | 0.393726058 | 0.379090898 | 0.386793517 | QWIZNVHXZXRPDR-WSCXOGSTSA-N | OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H]1O | HMDB0011730 | 43984 |  | C08243 | 92817 | 597-12-6 | 松三糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N2340 | HPLC≥98% | level1 |
| compound00092 | 2.00\_293.1379n | M+H, M+Na | C14H19N3O4 | 55.5 | 71.7 | 1.01 | Phenylalanylglutamine | 84.0451, 120.0809, 130.0499, 147.0763, 165.1022, 276.1405, 277.1180, 293.2099, 294.0978, 294.1443 | 294.1448 | 294.1451 | 2 | POS | 14162.87946 | 14954.01114 | 15133.48274 | 0.001894827 | 0.002036231 | 0.001986137 | 0.001972398 | KLAONOISLHWJEE-QWRGUYRKSA-N | N[C@@H](CC1=CC=CC=C1)C(=O)N[C@@H](CCC(N)=O)C(O)=O | HMDB0028993 | 23659 |  |  | 11779156 | 39537-24-1 | 苯丙氨酰谷氨酰胺 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00093 | 4.53\_594.1584n | M+H, M+Na | C27H30O15 | 53.3 | 60.2 | -0.1 | Meloside A | 343.0801, 349.0698, 367.0807, 379.0810, 397.0913, 415.1019, 433.1125, 449.1075, 594.3967, 595.1681 | 595.1657 | 595.1657 | 4.53 | POS | 500315.5494 | 467241.721 | 460821.6154 | 0.066936348 | 0.063622544 | 0.060478799 | 0.06367923 | RQTTXGQDIROLTQ-FASGCTRLSA-N | C1(O)=CC2OC(C3C=CC(O)=CC=3)=CC(=O)C=2C(O)=C1[C@H]1[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)[C@@H](O)[C@H](O)[C@@H](CO)O1 | HMDB0302583 | 48648 | LMPK12110217 | C04199 | 185995 |  | 异牡荆素-2''-O-葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N5124 | HPLC≥98% | level1 |
| compound00094 | 8.04\_261.1120m/z | M+H | C15H16O4 | 69.7 | 91.3 | -0.65 | Meranzin | 189.0544, 243.1014, 261.1122 | 261.1121 | 261.112 | 8.04 | POS | 26155.0974 | 25937.88136 | 25489.75845 | 0.003499245 | 0.003531864 | 0.003345307 | 0.003458805 | LSZONYLDFHGRDP-LBPRGKRZSA-N | COc1ccc2ccc(=O)oc2c1C[C@@H]1OC1(C)C |  |  |  |  |  | 23971-42-8 | 橙皮内酯水合物 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N3298 | HPLC≥98% | level1 |
| compound00095 | 5.42\_430.3312m/z | M+H | C27H43NO3 | 64.2 | 79.2 | -0.75 | Peiminine | 98.0967, 412.3205, 414.336, 430.3305 | 430.3316 | 430.3312 | 5.42 | POS | 2025436.355 | 1981301.039 | 1985792.132 | 0.270979609 | 0.269786294 | 0.260617816 | 0.267127906 | IQDIERHFZVCNRZ-YUYPDVIUSA-N | CC1CCC2C(C3CCC4C(C3CN2C1)CC5C4CC(=O)C6C5(CCC(C6)O)C)(C)O |  |  |  | C10808 | 167691 |  | 贝母素乙 | 生物碱 |  | Alkaloids |  | HY-N0213 | HPLC≥98% | level1 |
| compound00096 | 5.72\_194.0579n | M+H-H2O, M+H | C10H10O4 | 58.9 | 53.7 | 0.19 | Methyl caffeic acid | 89.0388, 117.0335, 135.044, 145.0282, 149.0595, 159.0439, 163.0387, 177.0541 | 177.0546 | 177.0547 | 5.72 | POS | 307225.7412 | 307330.8239 | 312854.8186 | 0.041103198 | 0.04184808 | 0.041059453 | 0.04133691 | OCNYGKNIVPVPPX-HWKANZROSA-N | COC(=O)C=CC1=CC(=C(C=C1)O)O |  | 68350 |  | C10477 | 689075 | 3843-74-1 | 咖啡酸甲酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N6005 | HPLC≥98% | level1 |
| compound00097 | 0.88\_191.0192m/z | M+FA-H | C5H6O5 | 57.9 | 76.3 | -3.28 | Oxoglutaric acid | 85.0284, 87.0077, 111.0076, 117.0183, 129.0183, 154.9977, 173.0082, 191.019 | 191.0199 | 191.0192 | 0.88 | NEG | 14854062.07 | 15662136.03 | 15386342.4 | 1.987299143 | 2.132654024 | 2.019322612 | 2.04642526 | KPGXRSRHYNQIFN-UHFFFAOYSA-N | OC(=O)CCC(=O)C(O)=O | HMDB0000208 | 119 |  | C00026 | 51 | 328-50-7 | 氧戊二酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | HY-W013636 | HPLC≥98% | level1 |
| compound00098 | 1.34\_159.0291m/z | M-H | C6H8O5 | 52.7 | 69 | -4.82 | Oxoadipic acid | 59.0128, 71.0490, 73.0283, 85.0285, 87.0443, 99.0441, 101.0234, 115.0390, 158.0813, 159.0290 | 159.0299 | 159.0291 | 1.34 | NEG | 193100.2559 | 190505.1882 | 197648.0208 | 0.025834548 | 0.025940373 | 0.025939571 | 0.025904831 | FGSBNBBHOZHUBO-UHFFFAOYSA-N | C(=O)(O)C(=O)CCCC(=O)O | HMDB0000225 | 322 | LMFA01170121 | C00322 | 71 | 3184-35-8 | 氧代己二酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | HY-113227 | HPLC≥98% | level1 |
| compound00099 | 11.69\_282.1614n | M+H, M+Na | C19H22O2 | 56.5 | 70 | -2.07 | Miltirone | 223.1114, 240.1144, 265.1576, 283.1689 | 305.1512 | 305.1506 | 11.69 | POS | 147408.7256 | 163223.1511 | 178024.4092 | 0.019721557 | 0.022225481 | 0.023364144 | 0.021770394 | FEFAIBOZOKSLJR-UHFFFAOYSA-N | CC(C)C1=CC2=C(C(=O)C1=O)C1=C(C=C2)C(C)(C)CCC1 | HMDB0035080 | 69654 |  | C13715 | 160142 | 27210-57-7 | 丹参新酮 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N1951 | HPLC≥98% | level1 |
| compound00100 | 2.78\_246.1450m/z | M+H | C10H19N3O4 | 58 | 78.3 | 0.68 | Asparaginyl-Leucine | 211.1078, 212.0916, 217.9905, 224.9839, 228.1358, 229.1180, 245.0979, 246.0753, 246.1113, 246.1453 | 246.1448 | 246.145 | 2.78 | POS | 16321.05216 | 16784.20275 | 16870.42391 | 0.002183565 | 0.002285442 | 0.002214095 | 0.002227701 | HXWUJJADFMXNKA-UHFFFAOYSA-N | CC(C)CC(NC(=O)C(N)CC(N)=O)C(O)=O | HMDB0028735 | 23810 |  |  | 18218182 |  | 天冬酰胺酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00101 | 0.73\_683.2246m/z | 2M-H | C12H22O11 | 60.5 | 83.9 | -0.86 | Alpha-Lactose | 59.0128, 71.0128, 89.0233, 101.0247, 179.0553, 341.1086, 683.226 | 683.2251 | 683.2246 | 0.73 | NEG | 1384736.155 | 1321519.345 | 1357127.616 | 0.185261443 | 0.179946308 | 0.178111107 | 0.181106286 | GUBGYTABKSRVRQ-XLOQQCSPSA-N | OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)[C@H](O)[C@@H](O)[C@H]1O | HMDB0000186 | 984806 |  | C00243 | 84571 | 63-42-3 | α-乳糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-B2123 | HPLC≥98% | level1 |
| compound00102 | 4.97\_193.0497m/z | M-H | C10H10O4 | 63.1 | 92.7 | -4.64 | Ferulic acid | 134.0363, 137.0235, 149.0598, 178.0264, 193.05 | 193.0506 | 193.0497 | 4.97 | NEG | 27377.15792 | 24725.38366 | 27438.52277 | 0.003662742 | 0.003366762 | 0.003601066 | 0.003543523 | KSEBMYQBYZTDHS-HWKANZROSA-N | COC1=C(O)C=CC(\C=C\C(O)=O)=C1 | HMDB0000954 | 4156 |  | C01494 | 445858 | 537-98-4 | 阿魏酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | msmls-lot-230-01 | HPLC≥98% | level1 |
| compound00103 | 3.73\_204.0893n | M-H, 2M-H | C11H12N2O2 | 60.7 | 78.1 | -3.06 | L-Tryptophan | 72.008, 74.0237, 116.0495, 142.0653, 159.0918, 160.0394, 203.0818 | 203.0826 | 203.082 | 3.73 | NEG | 53381.07368 | 59650.03993 | 55928.46124 | 0.007141761 | 0.008122321 | 0.00734012 | 0.007534734 | QIVBCDIJIAJPQS-VIFPVBQESA-N | N[C@@H](CC1=CNC2=C1C=CC=C2)C(O)=O | HMDB0000929 | 33 |  | C00078 | 6305 | 73-22-3 | L-色氨酸 | 吲哚及其衍生物 |  | Indoles and derivatives |  | HY-N0623 | HPLC≥98% | level1 |
| compound00104 | 2.70\_198.0526n | M-H2O-H, M+FA-H, M-H, 2M-H | C9H10O5 | 64.7 | 61.6 | -1.16 | 3-(3,4-Dihydroxyphenyl)lactic acid | 59.0128, 71.0128, 107.0492, 135.0442, 179.0344 | 395.0984 | 395.0979 | 2.7 | NEG | 15691168.09 | 15785319 | 15833110.21 | 2.099294103 | 2.149427385 | 2.077956972 | 2.10889282 | PAFLSMZLRSPALU-UHFFFAOYSA-N | OC(CC1=CC(O)=C(O)C=C1)C(O)=O | HMDB0003503 | 6942 |  | C01207 | 439435 | 23028-17-3 | 3-(3,4-二羟基苯基)乳酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | HY-N0106 | HPLC≥98% | level1 |
| compound00105 | 1.89\_282.1199m/z | M+H | C11H15N5O4 | 49.7 | 51.8 | 0.83 | 2'-O-Methyladenosine | 136.0617, 265.1292, 282.1197 | 282.1197 | 282.1199 | 1.89 | POS | 63265.93349 | 66381.88544 | 63072.96625 | 0.008464239 | 0.009038971 | 0.008277774 | 0.008593662 | FPUGCISOLXNPPC-UHFFFAOYSA-N | COC1C(O)C(CO)OC1N1C=NC2=C(N)N=CN=C12 | HMDB0004326 | 58235 |  | C04779 | 317398 | 2140-79-6 | 2'-O-甲基腺苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives | Purine nucleosides | HY-W011552 | HPLC≥98% | level1 |
| compound00106 | 11.50\_294.1252n | M+Na, M+K, M+H | C19H18O3 | 57 | 72.3 | -1.29 | Tanshinone IIA | 316.3204, 317.1144 | 317.1148 | 317.1144 | 11.5 | POS | 4092789.942 | 4650133.063 | 5143360.357 | 0.547567252 | 0.63319109 | 0.675020976 | 0.618593106 | HYXITZLLTYIPOF-UHFFFAOYSA-N | CC1=COC2=C1C(=O)C(=O)C1=C3CCCC(C)(C)C3=CC=C21 | HMDB0258715 |  |  |  |  |  | 丹参酮 IIA | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N0135 | HPLC≥98% | level1 |
| compound00107 | 10.77\_277.0855m/z | M+H | C18H12O3 | 59.1 | 79.5 | -1.45 | Tanshinone I | 249.0906, 277.0857 | 277.0859 | 277.0855 | 10.77 | POS | 922354.5461 | 932711.6535 | 987879.0341 | 0.123400211 | 0.12700383 | 0.129650467 | 0.126684836 | AIGAZQPHXLWMOJ-UHFFFAOYSA-N | CC1=COC2=C1C(=O)C(=O)C1=C2C=CC2=C1C=CC=C2C | HMDB0258714 |  |  |  |  |  | 丹参酮 I | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N0134 | HPLC≥98% | level1 |
| compound00108 | 3.86\_229.1554m/z | M-H | C11H22N2O3 | 55.5 | 69.5 | -1.71 | Valylisoleucine | 130.0864, 185.1654, 229.1555 | 229.1558 | 229.1554 | 3.86 | NEG | 12304.3528 | 12703.18447 | 12692.24524 | 0.001646178 | 0.001729745 | 0.001665746 | 0.001680556 | PNVLWFYAPWAQMU-CIUDSAMLSA-N | CC[C@H](C)[C@H](NC(=O)[C@@H](N)C(C)C)C(O)=O | HMDB0029130 | 23923 |  |  | 7010531 | 20556-14-3 | 缬氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00109 | 5.33\_139.0387m/z | M+H | C7H6O3 | 51.1 | 52.4 | -1.64 | 2,4-Dihydroxybenzaldehyde | 93.0338, 93.0702, 94.0655, 95.0859, 97.0652, 111.0443, 134.0601, 138.0546, 138.9948, 139.0391 | 139.039 | 139.0387 | 5.33 | POS | 25625.85127 | 25558.32457 | 26156.46243 | 0.003428438 | 0.003480181 | 0.003432806 | 0.003447142 | IUNJCFABHJZSKB-UHFFFAOYSA-N | OC1=CC=C(C=O)C(O)=C1 | HMDB0062484 |  |  |  | 7213 | 95-01-2 | 2，4-二羟基苯甲醛 | 其他 |  | Others |  | HY-W007539 | HPLC≥98% | level1 |
| compound00110 | 1.74\_169.0136m/z | M-H | C7H6O5 | 57.4 | 84 | -3.97 | Gallic acid | 125.0234, 169.0134 | 169.0142 | 169.0136 | 1.74 | NEG | 9508.679334 | 9354.465591 | 9468.779885 | 0.00127215 | 0.001273762 | 0.001242694 | 0.001262869 | LNTHITQWFMADLM-UHFFFAOYSA-N | OC(=O)C1=CC(O)=C(O)C(O)=C1 | HMDB0005807 | 3295 |  | C01424 | 370 | 149-91-7 | 没食子酸 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0523 | HPLC≥98% | level1 |
| compound00111 | 5.33\_153.0544m/z | M+H | C8H8O3 | 54 | 55.3 | -1.22 | 2',4'-dihydroxyacetophenone | 126.0551, 134.0601, 135.0440, 135.0812, 135.1167, 136.0389, 136.0754, 152.0703, 152.1066, 153.0544 | 153.0546 | 153.0544 | 5.33 | POS | 28499.7166 | 29114.82932 | 28403.44266 | 0.003812928 | 0.003964457 | 0.003727703 | 0.003835029 | SULYEHHGGXARJS-UHFFFAOYSA-N | CC(=O)C1=C(O)C=C(O)C=C1 | HMDB0029659 | 66018 |  | C03663 | 6990 | 89-84-9 | 2',4'-二羟基苯乙酮 | 其他 |  | Others |  | msmls-lot-230-01 | HPLC≥98% | level1 |
| compound00112 | 4.22\_265.1547m/z | M+H | C14H20N2O3 | 60.5 | 55.9 | 0.19 | Valylphenylalanine | 72.0813, 120.0808, 166.0861, 265.1041, 265.1537 | 265.1547 | 265.1547 | 4.22 | POS | 98327.08515 | 100807.2028 | 96047.18375 | 0.01315501 | 0.013726537 | 0.012605351 | 0.013162299 | GJNDXQBALKCYSZ-RYUDHWBXSA-N | CC(C)[C@H](N)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)=O | HMDB0029134 | 24009 |  |  | 6993119 | 3918-92-1 | 缬氨酰苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-107378 | HPLC≥98% | level1 |
| compound00113 | 4.33\_677.2298m/z | M-H | C29H42O18 | 60.4 | 93 | -0.11 | Tangshenoside I | 99.0441, 261.0976, 453.1769, 497.166, 677.2277 | 677.2298 | 677.2298 | 4.33 | NEG | 65368.42168 | 65752.45797 | 63123.37681 | 0.008745528 | 0.008953264 | 0.00828439 | 0.008661061 | ABKPQICIFGNRAA-FPFGLZQYSA-N | COc1cc(/C=C/COC(=O)C[C@](C)(CC(=O)O)O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)cc(OC)c1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 117278-74-7 | 党参苷I | 萜类 | 单萜类 | Terpenes | Monoterpenes | DD0190-0010 | HPLC≥98% | level1 |
| compound00114 | 9.37\_372.1204n | M+H, M+K, M+Na | C20H20O7 | 58.9 | 86.4 | -1.36 | Tangeretin | 343.0806, 358.1042, 373.1284 | 373.1282 | 373.1277 | 9.37 | POS | 3311109.274 | 3371840.09 | 3326910.223 | 0.442987554 | 0.459130755 | 0.436627814 | 0.446248707 | ULSUXBXHSYSGDT-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=CC(OC)=CC=3)=CC(=O)C=2C(OC)=C1OC | HMDB0030539 | 44437 | LMPK12111443 | C10190 | 68077 | 481-53-8 | 桔皮素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0133 | HPLC≥98% | level1 |
| compound00115 | 4.72\_206.0814m/z | M+H | C11H11NO3 | 50.5 | 53.3 | 1.26 | Indolelactic acid | 118.0652, 120.0808, 146.0599, 147.0439, 149.0232, 161.0958, 175.0388, 188.0703, 206.0808 | 206.0812 | 206.0814 | 4.72 | POS | 12204.3427 | 13467.95616 | 12274.74995 | 0.001632798 | 0.001833881 | 0.001610953 | 0.001692544 | XGILAAMKEQUXLS-JTQLQIEISA-N | O[C@@H](CC1=CNC2=C1C=CC=C2)C(O)=O | HMDB0000671 |  |  | C02043 | 676157 | 7417-65-4 | 吲哚乳酸 | 吲哚及其衍生物 |  | Indoles and derivatives |  | HY-113099 | HPLC≥98% | level1 |
| compound00116 | 6.25\_307.0722m/z | M+FA-H | C16H10N2O2 | 60.9 | 80.9 | -0.72 | Indigotin | 102.9558, 112.9843, 205.0773, 233.0715, 263.0822, 307.0005, 307.0718 | 307.0725 | 307.0722 | 6.25 | NEG | 9668.488412 | 9942.509478 | 10300.2063 | 0.00129353 | 0.001353834 | 0.001351812 | 0.001333059 | QQILFGKZUJYXGS-UHFFFAOYSA-N | O=C1C(c2[nH]c3ccccc3c2O)=Nc2ccccc21 |  |  |  |  |  | 482-89-3 | 靛蓝 | 生物碱 |  | Alkaloids |  | DD0088-0100 | HPLC≥98% | level1 |
| compound00117 | 4.85\_653.1728m/z | M-H | C29H34O17 | 53.7 | 67.1 | 0.72 | Syringetin-3-O-rutinoside | 61.9873, 329.0301, 345.0612, 653.1722 | 653.1723 | 653.1728 | 4.85 | NEG | 71768.67526 | 75885.79559 | 74964.19454 | 0.009601806 | 0.010333083 | 0.009838394 | 0.009924428 | BWDMLCWSGGUHGK-MWLOISQDSA-N | C1(O)=CC2OC(C3C=C(OC)C(O)=C(OC)C=3)=C(O[C@H]3[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)O3)C(=O)C=2C(O)=C1 |  |  | LMPK12112489 |  | 102402404 |  | 丁香亭-3-O-芸香糖苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DD0219 | HPLC≥98% | level1 |
| compound00118 | 7.10\_345.0615m/z | M-H | C17H14O8 | 58 | 64.6 | -0.14 | Syringetin | 171.1021, 185.1177, 201.1117, 215.128, 315.0148, 327.2174, 330.038, 345.0615 | 345.0616 | 345.0615 | 7.1 | NEG | 22971.81348 | 22505.98104 | 23592.89845 | 0.003073359 | 0.003064555 | 0.003096361 | 0.003078092 | UZMAPBJVXOGOFT-UHFFFAOYSA-N | C1(O)=CC2OC(C3C=C(OC)C(O)=C(OC)C=3)=C(O)C(=O)C=2C(O)=C1 | HMDB0304558 | 50914 | LMPK12112498 | C11620 | 5281953 |  | 丁香亭 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DD0210 | HPLC≥98% | level1 |
| compound00119 | 3.04\_330.0951n | M-H, M+FA-H | C14H18O9 | 58.6 | 85.4 | -0.07 | Vanillic acid 4-beta-D-glucopyranoside | 108.0208, 123.044, 152.0106, 167.0342, 329.0875 | 329.0878 | 329.0878 | 3.04 | NEG | 78757.07203 | 73717.2423 | 76199.73489 | 0.010536772 | 0.010037799 | 0.010000547 | 0.010191706 | JYFOSWJYZIVJPO-YGEZULPYSA-N | COC1=CC(=CC=C1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)C(O)=O | HMDB0302469 | 710956 |  |  | 14132337 |  | 香草酸-4-Β-D-葡萄糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | STC1580105 | HPLC≥98% | level1 |
| compound00120 | 5.95\_264.1364n | M+H-H2O, M+Na, M+H | C15H20O4 | 55.7 | 57 | 0.73 | (S)-Abscisic acid | 187.1114, 191.0696, 201.1270, 205.1220, 211.1116, 219.1373, 229.0851, 229.1218, 247.0930, 247.1316 | 287.1254 | 287.1256 | 5.95 | POS | 177601.2599 | 172862.2759 | 171043.3775 | 0.023760964 | 0.023538005 | 0.022447944 | 0.023248971 | JLIDBLDQVAYHNE-IBPUIESWSA-N | C1(=O)C=C(C)[C@](O)(/C=C/C(/C)=C/C(=O)O)C(C)(C)C1 | HMDB0035140 | 45378 | LMPR0103050001 | C06082 | 5702609 | 21293-29-8 | (S)-脱落酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | S18005 | HPLC≥98% | level1 |
| compound00121 | 4.01\_295.1293m/z | M+H | C14H18N2O5 | 58.7 | 86.5 | 1.66 | gamma-Glu-Phe | 84.0448, 120.0808, 130.0498, 136.0756, 166.0861, 186.0912, 232.0965, 278.1021, 295.1292 | 295.1288 | 295.1293 | 4.01 | POS | 148512.9514 | 143684.6353 | 153844.3279 | 0.01986929 | 0.019564995 | 0.02019072 | 0.019875002 | XHHOHZPNYFQJKL-QWRGUYRKSA-N | N[C@@H](CCC(=O)N[C@@H](CC1=CC=CC=C1)C(O)=O)C(O)=O | HMDB0000594 |  |  |  | 111299 | 7432-24-8 | γ-谷氨酰苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-101399 | HPLC≥98% | level1 |
| compound00122 | 1.32\_283.0916n | M-H, M+FA-H, 2M-H | C10H13N5O5 | 58 | 87.8 | -0.19 | Guanosine | 133.0145, 150.0412, 282.084 | 282.0844 | 282.0843 | 1.32 | NEG | 385836.8713 | 392078.5904 | 385337.1394 | 0.051620444 | 0.053387864 | 0.050572123 | 0.051860144 | NYHBQMYGNKIUIF-UUOKFMHZSA-N | NC1=NC2=C(N=CN2[C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N1 | HMDB0000133 | 87 |  | C00387 | 6802 | 118-00-3 | 鸟苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives | Purine nucleosides | HY-N0097 | HPLC≥98% | level1 |
| compound00123 | 3.70\_223.1078m/z | M+H | C11H14N2O3 | 53.9 | 82.4 | 0.25 | Glycyl-Phenylalanine | 86.0967, 120.0808, 166.0861, 177.1021, 206.0444, 223.0603, 223.1109 | 223.1077 | 223.1078 | 3.7 | POS | 29190.19647 | 30905.04081 | 30017.59128 | 0.003905306 | 0.004208223 | 0.003939546 | 0.004017691 | JBCLFWXMTIKCCB-UHFFFAOYSA-N | NCC(O)=NC(CC1=CC=CC=C1)C(O)=O | HMDB0028848 |  |  |  | 97415 |  | 甘氨酰苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | S46050 |  | level1 |
| compound00124 | 1.86\_239.1029m/z | M+H | C11H14N2O4 | 50.1 | 54.9 | 1.09 | Glycyl-L-tyrosine | 179.1179, 182.0812, 193.0972, 204.1134, 221.0927, 221.1394, 222.0746, 238.1165, 239.0926, 239.1021 | 239.1026 | 239.1029 | 1.86 | POS | 20055.1388 | 20514.74327 | 20009.10425 | 0.002683142 | 0.002793415 | 0.00262602 | 0.002700859 | XBGGUPMXALFZOT-VIFPVBQESA-N | NCC(=O)N[C@@H](CC1=CC=C(O)C=C1)C(O)=O | HMDB0028853 | 85762 |  |  | 92829 | 658-79-7 | 甘氨酰-L-酪氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-W009592 | HPLC≥98% | level1 |
| compound00125 | 0.70\_549.1666m/z | M+FA-H | C18H32O16 | 58.1 | 95.7 | -1.17 | 1-Kestose | 59.0128, 71.0127, 89.0234, 101.0234, 179.0554, 221.0662, 503.1616, 549.1673 | 549.1673 | 549.1666 | 0.7 | NEG | 4110997.443 | 4083112.403 | 4346848.035 | 0.550003202 | 0.555982025 | 0.570485714 | 0.558823647 | VAWYEUIPHLMNNF-OESPXIITSA-N | OC[C@H]1O[C@@](CO)(OC[C@@]2(O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)O[C@H](CO)[C@@H](O)[C@@H]2O)[C@@H](O)[C@@H]1O | HMDB0011729 |  |  | C03661 | 440080 | 470-69-9 | 蔗果三糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N2579 | HPLC≥98% | level1 |
| compound00126 | 3.34\_260.1375n | M+H-H2O, M+H | C11H20N2O5 | 54.8 | 56.7 | 1.16 | Glutamylleucine | 129.1019, 132.1019, 141.0650, 197.1283, 225.1248, 225.1596, 242.1865, 243.0234, 243.0829, 243.1352 | 243.134 | 243.1342 | 3.34 | POS | 42330.02695 | 44493.68512 | 43663.77531 | 0.005663261 | 0.006058537 | 0.005730488 | 0.005817429 | YBAFDPFAUTYYRW-YUMQZZPRSA-N | CC(C)C[C@H](NC(=O)[C@@H](N)CCC(O)=O)C(O)=O | HMDB0028823 | 44684 |  |  | 9856500 | 5969-52-8 | 谷氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00127 | 0.73\_365.1052m/z | M+Na | C12H22O11 | 61.5 | 81.5 | -0.82 | Trehalose | 185.042, 203.0524, 365.1051 | 365.1055 | 365.1052 | 0.73 | POS | 3582274.179 | 3603105.371 | 3582888.975 | 0.479266235 | 0.490621276 | 0.470222782 | 0.480036765 | HDTRYLNUVZCQOY-LIZSDCNHSA-N | OC[C@H]1O[C@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O | HMDB0000975 | 5913 |  | C01083 | 7427 | 99-20-7 | 海藻糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N1132 | HPLC≥98% | level1 |
| compound00128 | 7.05\_227.1284m/z | M-H | C12H20O4 | 54.8 | 68.8 | -2.24 | Traumatic acid | 142.9916, 158.9775, 162.9984, 165.1276, 183.1384, 186.9982, 209.116, 226.9929, 227.1055, 227.1278 | 227.1289 | 227.1284 | 7.05 | NEG | 24814.98204 | 24450.66873 | 23908.93776 | 0.003319953 | 0.003329355 | 0.003137839 | 0.003262382 | MAZWDMBCPDUFDJ-VQHVLOKHSA-N | C(CC(=O)O)CCCCCC/C=C/C(=O)O | HMDB0000933 | 5882 | LMFA01170002 | C16308 | 5283028 | 6402-36-4 | 愈伤酸 | 脂肪酰类 | 脂肪酸及其衍生物 | Fatty Acyls | Fatty acid and derivatives | HY-119358 | HPLC≥98% | level1 |
| compound00129 | 0.96\_177.0397m/z | M-H | C6H10O6 | 51.9 | 61.3 | -4.54 | 1,4-D-Gulonolactone | 89.0234, 99.0077, 105.0182, 115.0389, 129.0184, 131.0338, 147.0287, 158.0452, 159.0290, 177.0397 | 177.0405 | 177.0397 | 0.96 | NEG | 31213.1384 | 32204.22519 | 32894.36214 | 0.004175952 | 0.004385128 | 0.004317097 | 0.004292725 | SXZYCXMUPBBULW-LECHCGJUSA-N | C(C(C1C(C(C(=O)O1)O)O)O)O |  | 3314 |  | C01040 | 165105 | 3327-64-8 | D-谷洛糖酸γ-内酯 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-118840 | HPLC≥98% | level1 |
| compound00130 | 3.37\_279.1344m/z | M+H | C14H18N2O4 | 57.9 | 76.7 | 1.56 | Tyrosyl-Proline | 70.0656, 116.0708, 136.0756, 149.0232, 262.1073, 279.1335 | 279.1339 | 279.1344 | 3.37 | POS | 44465.32406 | 44349.84457 | 45129.1293 | 0.005948938 | 0.006038951 | 0.005922803 | 0.005970231 | VNYDHJARLHNEGA-UHFFFAOYSA-N | NC(CC1=CC=C(O)C=C1)C(=O)N1CCCC1C(O)=O | HMDB0029113 | 86005 |  |  | 13055260 |  | 酪氨酰脯氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00131 | 0.87\_684.2553m/z | M+NH4 | C24H42O21 | 67.1 | 73.1 | -0.61 | Isomaltotetraose | 91.0393, 97.0287, 127.0389, 145.0494, 163.0599, 289.0914, 325.1125, 343.1227, 487.1651, 505.1754 | 684.2557 | 684.2553 | 0.87 | POS | 1493227.291 | 1562495.982 | 1510041.535 | 0.199776284 | 0.212759188 | 0.198179719 | 0.20357173 | DFKPJBWUFOESDV-NGZVDTABSA-N | OC[C@H]([C@H]([C@@H]([C@H]1O)O)O)O[C@@H]1OC[C@H]([C@H]([C@@H]([C@H]2O)O)O)O[C@@H]2OC[C@H]([C@H]([C@@H]([C@H]3O)O)O)O[C@@H]3OC[C@H]([C@H]([C@@H]([C@H]4O)O)O)O[C@@H]4O |  |  |  |  |  | 35997-20-7 | 异麦芽四糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N7948 | HPLC≥98% | level1 |
| compound00132 | 3.78\_267.1341m/z | M+H | C13H18N2O4 | 54.8 | 56 | 0.58 | Threonylphenylalanine | 166.0860, 178.0578, 221.1281, 225.1341, 249.1234, 250.0821, 266.1572, 267.0398, 267.0767, 267.1359 | 267.1339 | 267.1341 | 3.78 | POS | 20198.93738 | 22253.53093 | 23167.79863 | 0.002702381 | 0.003030179 | 0.003040571 | 0.002924377 | IQHUITKNHOKGFC-MIMYLULJSA-N | C[C@@H](O)[C@H](N)C(=O)N[C@@H](CC1=CC=CC=C1)C(O)=O | HMDB0029068 | 85961 |  |  | 7010579 | 16875-27-7 | 苏氨酰苯丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00133 | 3.11\_233.1497m/z | M+H | C10H20N2O4 | 59.4 | 84.8 | 0.55 | Threonylleucine | 56.0501, 74.0606, 86.0969, 132.1019, 187.1441, 215.1394, 233.09, 233.1497 | 233.1496 | 233.1497 | 3.11 | POS | 96215.09872 | 98230.41179 | 100234.0602 | 0.012872451 | 0.013375665 | 0.013154842 | 0.013134319 | BQBCIBCLXBKYHW-CSMHCCOUSA-N | CC(C)C[C@H](NC(=O)[C@@H](N)[C@@H](C)O)C(O)=O | HMDB0029065 | 24000 |  |  | 7021827 | 50299-12-2 | 苏氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00134 | 15.07\_338.3414m/z | M+H | C22H43NO | 67.1 | 91.6 | -1.1 | 13-Docosenamide | 83.0858, 97.1015, 303.3043, 321.3139, 338.3412 | 338.3417 | 338.3414 | 15.07 | POS | 81886.6802 | 77302.99417 | 98322.04625 | 0.010955477 | 0.010526057 | 0.012903907 | 0.011461814 | UAUDZVJPLUQNMU-UHFFFAOYSA-N | CCCCCCCCC=CCCCCCCCCCCCC(N)=O | HMDB0244507 |  |  |  | 8214 |  | 13-二十二碳烯酰胺 | 脂肪酰类 | 脂肪酰胺类 | Fatty Acyls | Fatty acylamides | A01146042 |  | level1 |
| compound00135 | 6.67\_215.1283m/z | M-H | C11H20O4 | 59.2 | 81.6 | -2.65 | Undecanedioic acid | 153.1275, 194.9871, 197.1177, 214.9919, 215.0095, 215.1284 | 215.1289 | 215.1283 | 6.67 | NEG | 14999.34454 | 15033.8207 | 15408.96296 | 0.002006736 | 0.002047099 | 0.002022291 | 0.002025375 | LWBHHRRTOZQPDM-UHFFFAOYSA-N | C(CCCCCCCCCC(=O)O)(=O)O | HMDB0000888 | 5846 | LMFA01170007 |  | 15816 | 1852-04-6 | 十一烷二酸 | 脂肪酰类 | 脂肪酸及其衍生物 | Fatty Acyls | Fatty acid and derivatives | HY-W014125 | HPLC≥98% | level1 |
| compound00136 | 1.08\_244.0692n | M-H, M+FA-H | C9H12N2O6 | 54.9 | 57.8 | -1.44 | Uridine | 66.0339, 82.0287, 110.0237, 111.019, 128.0344, 140.0343, 152.0344, 153.0293, 200.0558, 243.062 | 243.0623 | 243.0619 | 1.08 | NEG | 172053.808 | 170903.2839 | 168314.2279 | 0.02301878 | 0.023271256 | 0.022089768 | 0.022793268 | DRTQHJPVMGBUCF-XVFCMESISA-N | OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=CC(=O)NC1=O | HMDB0000296 | 90 |  | C00299 | 6029 | 58-96-8 | 尿苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives | Pyrimidine nucleosides | HY-B1449 | HPLC≥98% | level1 |
| compound00137 | 3.78\_259.1297m/z | M-H | C11H20N2O5 | 57.4 | 81.5 | -0.96 | gamma-Glutamylleucine | 130.0863, 146.9378, 190.9269, 197.1289, 215.1064, 223.1082, 241.1190, 258.1451, 259.0742, 259.1289 | 259.1299 | 259.1297 | 3.78 | NEG | 8418.547565 | 7892.512793 | 8027.943902 | 0.001126303 | 0.001074694 | 0.001053597 | 0.001084865 | MYFMARDICOWMQP-YUMQZZPRSA-N | CC(C)C[C@H](NC(=O)CC[C@H](N)C(O)=O)C(O)=O | HMDB0011171 | 23750 |  |  | 151023 | 2566-39-4 | γ-谷氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | 130645 |  | level1 |
| compound00138 | 6.08\_418.1630n | M+H-H2O, M+Na | C22H26O8 | 53.7 | 65.6 | 0.58 | Syringaresinol | 315.0854, 323.1267, 330.1092, 339.1219, 343.1147, 351.1216, 369.1335, 383.1487, 400.3203, 401.1596 | 401.1595 | 401.1597 | 6.08 | POS | 32125.27748 | 31905.67137 | 30786.9041 | 0.004297985 | 0.004344475 | 0.004040511 | 0.004227657 | KOWMJRJXZMEZLD-UHFFFAOYSA-N | COC1=CC(=CC(OC)=C1O)C1OCC2C1COC2C1=CC(OC)=C(O)C(OC)=C1 | HMDB0038928 | 93540 |  |  | 100067 | 21453-71-4 | L-丁香脂素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-126066 | HPLC≥98% | level1 |
| compound00139 | 4.96\_183.0651m/z | M+H | C9H10O4 | 54.9 | 66 | -0.47 | Syringaldehyde | 123.0442, 136.0756, 137.0597, 140.0468, 141.9585, 154.9902, 155.0702, 182.1175, 182.9851, 183.0648 | 183.0652 | 183.0651 | 4.96 | POS | 11025.61458 | 11278.07741 | 11218.24091 | 0.001475098 | 0.001535693 | 0.001472296 | 0.001494362 | KCDXJAYRVLXPFO-UHFFFAOYSA-N | COC1=CC(C=O)=CC(OC)=C1O | HMDB0258653 | 335983 |  |  | 8655 |  | 丁香醛 | 酚类 | 单酚类 | Phenols | Monophenols | HY-N1390 | HPLC≥98% | level1 |
| compound00140 | 3.67\_231.1707m/z | M+H | C11H22N2O3 | 54.9 | 74.3 | 1.56 | Valylleucine | 72.0813, 86.0968, 116.0708, 132.1019, 185.1648, 231.1201, 231.1701 | 231.1703 | 231.1707 | 3.67 | POS | 95462.85773 | 96142.77232 | 95762.66777 | 0.01277181 | 0.013091399 | 0.012568011 | 0.012810407 | XCTHZFGSVQBHBW-IUCAKERBSA-N | CC(C)C[C@H](NC(=O)[C@@H](N)C(C)C)C(O)=O | HMDB0029131 | 23950 |  |  | 6993117 | 3989-97-7 | 缬氨酰亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides |  |  | level1 |
| compound00141 | 0.80\_342.1159n | M+H-H2O, M+H, M+NH4 | C12H22O11 | 53.9 | 51.7 | -0.87 | Sucrose | 91.0393, 97.0288, 99.0444, 109.0287, 112.0506, 127.0390, 145.0495, 163.0600, 182.0577, 306.1174 | 325.1129 | 325.1126 | 0.8 | POS | 1512242.35 | 1586343.979 | 1580728.646 | 0.202320275 | 0.21600648 | 0.207456783 | 0.208594513 | CZMRCDWAGMRECN-UGDNZRGBSA-N | OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O | HMDB0000258 | 137 |  | C00089 | 5988 | 57-50-1 | 蔗糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-B1779 | HPLC≥98% | level1 |
| compound00142 | 4.61\_565.1555m/z | M+H | C26H28O14 | 65.1 | 85.5 | 0.61 | Isovitexin 2''-O-arabinoside | 323.0908, 337.0703, 343.0799, 351.0862, 367.0806, 379.0806, 397.0914, 415.1019, 433.1122, 565.1544 | 565.1552 | 565.1555 | 4.61 | POS | 112560.4338 | 107784.6913 | 103378.1362 | 0.015059265 | 0.014676635 | 0.013567474 | 0.014434458 | ACRIYYKEWCXQOS-XAYOXWHSSA-N | C1C(C(C(C(O1)OC2C(C(C(OC2C3=C(C4=C(C=C3O)OC(=CC4=O)C5=CC=C(C=C5)O)O)CO)O)O)O)O)O | HMDB0037569 | 92425 |  |  | 44468060 | 53382-71-1 | 异牡荆素-2''-O-阿拉伯糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N5114 | HPLC≥98% | level1 |
| compound00143 | 6.34\_357.1328m/z | M+H | C20H20O6 | 59.5 | 89.7 | -1.33 | (+)-Balanophonin | 261.0909, 279.1009, 289.0859, 307.0960, 309.1114, 321.1116, 327.1229, 339.1223, 356.1518, 357.1290 | 357.1333 | 357.1328 | 6.34 | POS | 28905.45919 | 29263.21529 | 28210.61686 | 0.003867211 | 0.003984662 | 0.003702396 | 0.003851423 | GWCSSLSMGCFIFR-LNFBDUAVSA-N | COc1cc([C@H]2Oc3c(OC)cc(/C=C/C=O)cc3[C@@H]2CO)ccc1O |  |  |  |  |  | 215319-47-4 | 右旋蛇菰宁 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DY0169 | HPLC≥98% | level1 |
| compound00144 | 4.93\_430.3314m/z | M+H | C27H43NO3 | 57.6 | 84.9 | -0.44 | Yubeinine | 412.3205, 430.331 | 430.3316 | 430.3314 | 4.93 | POS | 174901.3774 | 184555.1911 | 187550.6769 | 0.023399751 | 0.025130185 | 0.024614383 | 0.02438144 | IQDIERHFZVCNRZ-UUSLGJCMSA-N | CC1CCC2N(C1)CC1C3CC4C(CC(=O)C5C[C@H](O)CC[C@@]54C)C3CCC1[C@]2(C)O |  |  |  |  |  | 157478-01-8 | 裕贝甲素 | 生物碱 |  | Alkaloids |  | HY-107276 | HPLC≥98% | level1 |
| compound00145 | 4.87\_153.0546m/z | M+H | C8H8O3 | 58.8 | 66.5 | -0.01 | Isovanillin | 97.0652, 107.0858, 110.0365, 111.0443, 111.9686, 125.0598, 134.0600, 135.1167, 153.0183, 153.0547 | 153.0546 | 153.0546 | 4.87 | POS | 27713.3893 | 28829.8012 | 28221.75721 | 0.003707726 | 0.003925645 | 0.003703858 | 0.003779077 | JVTZFYYHCGSXJV-UHFFFAOYSA-N | COC1=C(C=C(C=C1)C=O)O |  | 324054 |  |  | 12127 |  | 异香兰素 | 酚类 | 单酚类 | Phenols | Monophenols | HY-I0637 | HPLC≥98% | level1 |
| compound00146 | 7.44\_372.1209n | M+Na, M+K, M+H | C20H20O7 | 59.9 | 89.9 | -0.09 | Isosinensetin | 395.1094 | 395.1101 | 395.1101 | 7.44 | POS | 656068.713 | 683305.9097 | 767816.0272 | 0.087774293 | 0.09304319 | 0.100769125 | 0.093862203 | UYCWETIUOAGWIL-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=C(OC)C(OC)=CC=3)=CC(=O)C=2C(OC)=C1 | HMDB0037599 | 49827 | LMPK12111403 |  | 632135 | 17290-70-9 | 异甜橙黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | B21516-10mg | HPLC≥98% | level1 |
| compound00147 | 6.28\_308.0798n | M+H, M+Na | C17H12N2O4 | 61.7 | 78.7 | 0.21 | Flazin | 263.0811, 281.0914, 309.084 | 309.087 | 309.087 | 6.28 | POS | 40010.65253 | 40067.46445 | 39183.3155 | 0.005352956 | 0.005455836 | 0.005142467 | 0.005317086 | USBWYUYKHHILLZ-UHFFFAOYSA-N | OCC1=CC=C(O1)C1=C2NC3=CC=CC=C3C2=CC(=N1)C(O)=O | HMDB0033459 | 89289 |  |  | 5377686 | 100041-05-2 | 酒渣碱 | 生物碱 |  | Alkaloids |  | DJ0344 | HPLC≥98% | level1 |
| compound00148 | 4.98\_610.1894n | M-H, M+FA-H | C28H34O15 | 58.9 | 84.2 | -0.68 | Hesperidin | 286.0481, 301.0715, 609.1823 | 609.1825 | 609.1821 | 4.98 | NEG | 16231876.29 | 16815118.49 | 16133443.78 | 2.171634514 | 2.289651301 | 2.117373121 | 2.192886312 | QUQPHWDTPGMPEX-HPUKAVHFSA-N | COc1ccc(C2CC(=O)c3c(O)cc(O[C@@H]4OC(CO[C@@H]5OC(C)[C@H](O)[C@@H](O)C5O)[C@@H](O)[C@@H](O)C4O)cc3O2)cc1O |  |  |  |  |  | 520-26-3 | 橙皮甙 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-15337 | HPLC≥98% | level1 |
| compound00149 | 3.98\_139.0392m/z | M+H | C7H6O3 | 61.1 | 75.5 | 1.7 | 3,4-Dihydroxybenzaldehyde | 65.0391, 93.0338, 111.0442, 134.0599, 138.0549, 139.0388 | 139.039 | 139.0392 | 3.98 | POS | 110906.828 | 118607.8838 | 132728.1972 | 0.014838032 | 0.016150388 | 0.017419413 | 0.016135944 | IBGBGRVKPALMCQ-UHFFFAOYSA-N | OC1=CC=C(C=O)C=C1O | HMDB0059965 | 63101 |  | C16700 | 8768 | 139-85-5 | 3,4-二羟基苯甲醛 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0295 | HPLC≥98% | level1 |
| compound00150 | 4.83\_461.1089m/z | M-H | C22H22O11 | 62.9 | 89.6 | -0.06 | Isoscoparin | 298.0479, 341.0663, 371.0772, 461.1082 | 461.1089 | 461.1089 | 4.83 | NEG | 73472.6264 | 73812.37228 | 74731.29228 | 0.009829775 | 0.010050752 | 0.009807827 | 0.009896118 | KOMUHHCFAXYRPO-DGHBBABESA-N | C1(O)=CC2OC(C3C=CC(O)=C(OC)C=3)=CC(=O)C=2C(O)=C1[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 |  | 49168 | LMPK12110738 | C05990 | 442611 |  | 异金雀花素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | B28064-10mg | HPLC≥98% | level1 |
| compound00151 | 4.61\_608.1745n | M+H, M+Na | C28H32O15 | 57.8 | 73.9 | 0.64 | Spinosin | 285.0752, 297.0753, 323.0907, 327.0857, 351.0855, 381.0962, 411.1064, 429.1171, 447.1278, 609.1804 | 609.1814 | 609.1818 | 4.61 | POS | 2345933.608 | 2251362.086 | 2062794.522 | 0.31385838 | 0.306559489 | 0.270723705 | 0.297047191 | VGGSULWDCMWZPO-ODEMIOGVSA-N | COC1=C(C(=C2C(=C1)OC(=CC2=O)C3=CC=C(C=C3)O)O)C4C(C(C(C(O4)CO)O)O)OC5C(C(C(C(O5)CO)O)O)O |  | 49416 |  | C17834 | 155692 |  | 斯皮诺素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0651 | HPLC≥98% | level1 |
| compound00152 | 3.72\_182.0572n | M-H2O-H, M-H | C9H10O4 | 57 | 50.1 | -3.95 | Hydroxyphenyllactic acid | 72.9921, 93.0334, 101.0232, 112.9846, 119.0492, 135.0442, 137.0236, 163.0392, 181.0126, 181.0499 | 181.0506 | 181.0499 | 3.72 | NEG | 58363.80506 | 59350.19262 | 58846.30058 | 0.007808392 | 0.008081492 | 0.007723061 | 0.007870982 | JVGVDSSUAVXRDY-UHFFFAOYSA-N | OC(CC1=CC=C(O)C=C1)C(O)=O | HMDB0000755 | 34515 |  | C03672 | 9378 | 306-23-0 | 羟苯基乳酸 | 苯丙素类 | 苯丙酸类 | Phenylpropanoids | Phenylpropionates | HY-113219 | HPLC≥98% | level1 |
| compound00153 | 7.55\_388.1156n | M+H, M+Na | C20H20O8 | 52.7 | 57.6 | -0.49 | 3'-Demethylnobiletin | 251.1061, 311.1269, 355.1171, 359.0755, 374.0998, 389.1234 | 411.105 | 411.1048 | 7.55 | POS | 67502.84835 | 73057.41033 | 79491.57103 | 0.009031089 | 0.009947952 | 0.010432572 | 0.009803871 | XFYYZBJXMSDKCV-UHFFFAOYSA-N | C1(OC)=C(OC)C2OC(C3C=C(O)C(OC)=CC=3)=CC(=O)C=2C(OC)=C1OC | HMDB0029545 | 49900 | LMPK12111478 |  | 183466 | 112448-39-2 | 3'-去甲川陈皮素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4127 | HPLC≥98% | level1 |
| compound00154 | 4.27\_435.1285m/z | M+H | C21H22O10 | 56.5 | 82.9 | -0.13 | Isocoreopsin | 147.0438, 153.018, 273.0753 | 435.1286 | 435.1285 | 4.27 | POS | 53257.99643 | 51105.86072 | 51860.25574 | 0.007125295 | 0.006958892 | 0.006806204 | 0.006963464 | AWENDZQUFCJISN-ZRWXNEIDSA-N | O=C1C[C@@H](c2ccc(O)c(O)c2)Oc2cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)ccc21 |  |  |  |  |  | 30382-18-4 | 紫铆黄素-7-O-β-D-吡喃葡萄糖苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | DZ0163-0005 | HPLC≥98% | level1 |
| compound00155 | 4.39\_298.1440m/z | M+H | C18H19NO3 | 61.9 | 87.9 | 0.85 | Stepharine | 161.0833, 192.1018, 269.1171, 298.1432 | 298.1438 | 298.144 | 4.39 | POS | 84409.52283 | 87120.35603 | 85662.36605 | 0.011293003 | 0.01186285 | 0.011242435 | 0.011466096 | OGJKMZVUJJYWKO-UHFFFAOYSA-N | O=C1C=CC2(C=C1)C=3C(OC)=C(OC)C=C4C3C(NCC4)C2 |  |  |  |  | 98455 | 2810-21-1 | 光千金藤碱 | 生物碱 |  | Alkaloids |  | DG0237 | HPLC≥98% | level1 |
| compound00156 | 1.31\_205.0348m/z | M-H | C7H10O7 | 52 | 63.2 | -2.75 | 2-Methylcitric acid | 99.0441, 101.0233, 111.0078, 121.0434, 125.0234, 143.0340, 145.0133, 187.0241, 204.9749, 205.0347 | 205.0354 | 205.0348 | 1.31 | NEG | 81853.42144 | 83550.8527 | 87185.7186 | 0.010951027 | 0.011376805 | 0.011442362 | 0.011256731 | YNOXCRMFGMSKIJ-UHFFFAOYSA-N | CC(C(O)=O)C(O)(CC(O)=O)C(O)=O | HMDB0000379 | 5368 |  |  | 515 | 6061-96-7 | 2-甲基柠檬酸 | 有机酸及其衍生物 |  | Organic acids and derivatives |  | HY-113371 | HPLC≥98% | level1 |
| compound00157 | 3.17\_384.1149m/z | M+H | C14H17N5O8 | 58.4 | 81.8 | -0.23 | Succinyladenosine | 162.0772, 234.062, 252.0723, 384.1148 | 384.115 | 384.1149 | 3.17 | POS | 44450.84171 | 45393.54001 | 48196.02087 | 0.005947001 | 0.006181067 | 0.006325305 | 0.006151124 | VKGZCEJTCKHMRL-VWJPMABRSA-N | OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=C(N[C@@H](CC(O)=O)C(O)=O)N=CN=C12 | HMDB0000912 | 5867 |  |  | 20849086 | 4542-23-8 | 琥珀酰腺苷 | 核苷酸及其衍生物 |  | Nucleotides and derivatives | Purine nucleosides | S688825 |  | level1 |
| compound00158 | 4.22\_594.1588n | M+H, M+Na | C27H30O15 | 69.5 | 80 | 0.61 | Vicenin 2 | 457.1121, 475.1233, 481.1125, 499.1220, 511.1234, 541.1327, 559.1451, 577.1540, 594.3569, 595.1644 | 595.1657 | 595.1661 | 4.22 | POS | 811062.1351 | 796875.3061 | 773116.3266 | 0.108510593 | 0.108507507 | 0.101464743 | 0.106160948 | FIAAVMJLAGNUKW-VQVVXJKKSA-N | C1(O)=C([C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C2OC(C3C=CC(O)=CC=3)=CC(=O)C=2C(O)=C1[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 |  | 48649 | LMPK12110218 | C10195 | 442664 |  | 维采宁-2 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N2165 | HPLC≥98% | level1 |
| compound00159 | 1.81\_257.0779m/z | M-H | C10H14N2O6 | 56.2 | 83.5 | -0.06 | 2′-O-Methyluridine | 61.9872, 124.0395, 166.0494, 173.044, 214.0715, 257.0787 | 257.0779 | 257.0779 | 1.81 | NEG | 16663.96648 | 15711.56868 | 15204.08944 | 0.002229443 | 0.002139385 | 0.001995404 | 0.002121411 | SXUXMRMBWZCMEN-ZOQUXTDFSA-N | CO[C@@H]1[C@H](O)[C@@H](CO)O[C@H]1N1C=CC(=O)NC1=O | HMDB0240328 |  |  |  | 102212 | 2140-76-3 | 2'-甲氧基尿苷 | 其他 |  | Others |  | HY-W011824 | HPLC≥98% | level1 |
| compound00160 | 0.68\_666.2214n | M-H, M+FA-H | C24H42O21 | 58.1 | 86.3 | -0.65 | Stachyose | 59.0128, 71.0128, 89.0234, 101.0234, 179.0554, 341.1087, 383.1191, 485.1509, 665.2147 | 711.2201 | 711.2196 | 0.68 | NEG | 31017435.32 | 31773476.99 | 36977657.8 | 4.149768755 | 4.326474591 | 4.852993557 | 4.443078968 | UQZIYBXSHAGNOE-XNSRJBNMSA-N | OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO[C@H]3O[C@H](CO[C@H]4O[C@H](CO)[C@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O | HMDB0003553 | 6951 |  | C01613 | 439531 | 470-55-3 | 水苏糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | msmls-lot-230-01 | HPLC≥98% | level1 |
| compound00161 | 4.98\_369.1172m/z | M+H | C17H20O9 | 40.2 | 7.18 | -2.11 | Methyl chlorogenate | 175.0389, 177.0545, 191.0337, 207.065, 219.0286, 369.0966 | 369.118 | 369.1172 | 4.98 | POS | 35053.56634 | 32813.57137 | 37253.99412 | 0.004689756 | 0.0044681 | 0.00488926 | 0.004682372 | MZNIJRAPCCELQX-SMKXDYDZSA-N | COC(=O)[C@]1(O)C[C@@H](O)[C@@H](O)[C@H](OC(=O)C=Cc2ccc(O)c(O)c2)C1 |  |  |  |  |  | 29708-87-0 | 绿原酸甲酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | DL0215-0020 | HPLC≥98% | level2 |
| compound00162 | 4.92\_493.1332m/z | M+H | C23H24O12 | 40 | 0 | -1.72 | Iristectorin A |  | 493.1341 | 493.1332 | 4.92 | POS | 25011.99135 | 25306.44034 | 27053.62631 | 0.003346311 | 0.003445883 | 0.003550551 | 0.003447582 | HFODKTZIQVSGJO-UHFFFAOYSA-N | COc1ccc(-c2coc3cc(OC4OC(CO)C(O)C(O)C4O)c(OC)c(O)c3c2=O)cc1O |  |  |  |  |  | 37744-61-9 | 鸢尾甲苷 A | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N6820 | HPLC≥98% | level2 |
| compound00163 | 0.78\_134.0449m/z | M+H | C4H7NO4 | 42.6 | 14.9 | 0.82 | Iminodiacetic acid | 113.5319, 116.0343, 116.0707, 119.0190, 122.5370, 123.0403, 124.0244, 125.0393, 133.0607, 134.0449 | 134.0448 | 134.0449 | 0.78 | POS | 24089.15839 | 23933.3507 | 26350.02541 | 0.003222847 | 0.003258914 | 0.00345821 | 0.003313324 | NBZBKCUXIYYUSX-UHFFFAOYSA-N | OC(=O)CNCC(O)=O | HMDB0011753 | 34481 |  | C19911 | 8897 | 142-73-4 | 亚氨基二乙酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-W012683 | HPLC≥98% | level2 |
| compound00164 | 10.76\_483.3477m/z | M-H2O-H | C31H50O5 | 58 | 0 | -0.56 | Methyl arjunolate |  | 483.348 | 483.3477 | 10.76 | NEG | 10758.76831 | 9195.610244 | 9696.970446 | 0.001439397 | 0.001252132 | 0.001272642 | 0.00132139 | PQQIABJSQBQEFM-UHFFFAOYSA-N | CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)CO)O)O)C)C)C2C1)C)C(=O)OC)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00165 | 4.15\_153.0428n | M+H, M+Na | C7H7NO3 | 41.1 | 0 | 1.42 | Methyl 5-hydroxypyridine-2-carboxylate |  | 154.0499 | 154.0501 | 4.15 | POS | 6308.055342 | 6364.320273 | 6104.346565 | 0.000843944 | 0.000866606 | 0.000801142 | 0.00083723 | YYAYXDDHGPXWTA-UHFFFAOYSA-N | COC(=O)c1ccc(O)cn1 |  |  |  |  |  | 30766-12-2 | 5-羟基-2-吡啶甲酸甲酯 | 生物碱 |  | Alkaloids |  | HY-W005963 | HPLC≥98% | level2 |
| compound00166 | 5.33\_199.0598m/z | M+H | C9H10O5 | 42.3 | 7.6 | -1.4 | Methyl 3-O-methylgallate | 163.0875, 163.1116, 171.1158, 180.1105, 181.0492, 181.0986, 181.1223, 198.1192, 198.1491, 199.0398 | 199.0601 | 199.0598 | 5.33 | POS | 105169.618 | 112056.3833 | 106472.4531 | 0.01407046 | 0.015258295 | 0.013973576 | 0.014434111 | LVVUKXKEXOTUPV-UHFFFAOYSA-N | COC(=O)c1cc(O)c(O)c(OC)c1 |  |  |  |  |  | 3934-86-9 | 3,4-二羟基-5-甲氧基苯甲酸甲酯 | 羧酸及衍生物 |  | Carboxylic acid and derivatives |  | HY-N6669 | HPLC≥98% | level2 |
| compound00167 | 6.53\_348.1572n | M+H-H2O, M+Na, M+H | C19H24O6 | 50.2 | 33.4 | -0.37 | nagilactone e | 98.9844, 215.1069, 243.0658, 267.1372, 277.2159, 285.1484, 295.1324, 295.2271, 313.1429, 331.1523 | 331.154 | 331.1539 | 6.53 | POS | 85327.01357 | 85711.69366 | 79868.95987 | 0.011415753 | 0.011671038 | 0.010482101 | 0.011189631 | JOTPYRMNAYGVBN-TYQYQVCMSA-N | CC(C)[C@@H]1C23[C@H](O2)[C@@H]4[C@@H]5[C@@](C3=CC(=O)O1)(CC[C@@H]([C@@]5(C(=O)O4)C)O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00168 | 4.59\_292.0826m/z | M-H | C14H15NO6 | 56.9 | 77.8 | -0.33 | Isatan B | 59.0128, 164.0706, 186.0913, 188.0711, 207.9808, 225.1127, 230.0821, 274.072, 291.145, 292.0826 | 292.0827 | 292.0826 | 4.59 | NEG | 10661.8632 | 10756.33821 | 10302.22345 | 0.001426432 | 0.00146465 | 0.001352077 | 0.001414386 | AHWQTWBZNABQTO-UHFFFAOYSA-N | C1=CC=C2C(=C1)C(=CN2)OC3C(C(=O)C(C(O3)CO)O)O |  |  |  |  | 101529308 |  |  |  |  |  |  |  |  | level2 |
| compound00169 | 5.01\_642.2375m/z | M+NH4 | C29H36O15 | 44.9 | 0 | -2.86 | Isoacteoside |  | 642.2393 | 642.2375 | 5.01 | POS | 10867.32339 | 10376.87738 | 7715.58594 | 0.00145392 | 0.00141298 | 0.001012603 | 0.001293168 | FNMHEHXNBNCPCI-QEOJJFGVSA-N | CC1C(C(C(C(O1)OC2C(C(OC(C2O)OCCC3=CC(=C(C=C3)O)O)COC(=O)C=CC4=CC(=C(C=C4)O)O)O)O)O)O | HMDB0041025 | 95459 |  |  | 6476333 | 61303-13-7 | 异麦角甾苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N0022 | HPLC≥98% | level2 |
| compound00170 | 9.83\_422.1726n | M+H, M+Na | C25H26O6 | 41.5 | 0 | -0.7 | Mulberrin |  | 423.1802 | 423.1799 | 9.83 | POS | 34701.8674 | 34154.17673 | 34563.02698 | 0.004642703 | 0.004650646 | 0.004536094 | 0.004609814 | UWQYBLOHTQWSQD-UHFFFAOYSA-N | C1(O)=C(C/C=C(\C)/C)C2OC(C3C(O)=CC(O)=CC=3)=C(C/C=C(\C)/C)C(=O)C=2C(O)=C1 | HMDB0029507 | 49323 | LMPK12110895 |  | 5481958 | 62949-79-5 | 桑黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N3513 | HPLC≥98% | level2 |
| compound00171 | 5.09\_317.1028m/z | M-H | C17H18O6 | 48.7 | 19.6 | -0.87 | Isoagarotetrol | 59.0128, 112.9846, 180.9725, 201.0918, 201.1272, 227.1072, 229.123, 273.113, 317.1029 | 317.1031 | 317.1028 | 5.09 | NEG | 12880.15333 | 12770.55076 | 13884.71304 | 0.001723213 | 0.001738918 | 0.001822247 | 0.001761459 | CWMIROLCTHMEEO-XUWVNRHRSA-N | C1=CC=C(C=C1)CCC2=CC(=O)C3=C(O2)[C@@H]([C@H]([C@@H]([C@H]3O)O)O)O |  |  |  |  |  | 104060-61-9 | 异沉香四醇 | 酚类 | 多酚类 | Phenols | Polyphenols | B27396-10mg | HPLC≥98% | level2 |
| compound00172 | 6.23\_371.1484m/z | M+H-H2O | C21H24O7 | 40.7 | 0 | -1.44 | Medioresil |  | 371.1489 | 371.1484 | 6.23 | POS | 5606.002244 | 6010.209609 | 5552.966519 | 0.000750017 | 0.000818388 | 0.000728778 | 0.000765728 | VJOBNGRIBLNUKN-BMHXQBNDSA-N | COc1cc([C@H]2OC[C@@H]3[C@@H](c4cc(OC)c(O)c(OC)c4)OC[C@H]23)ccc1O |  |  |  |  |  | 40957-99-1 | 5'-甲氧基松脂素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DJ0140 | HPLC≥98% | level2 |
| compound00173 | 4.63\_739.2095m/z | M-H | C33H40O19 | 46.8 | 0 | 0.53 | Mauritianin |  | 739.2091 | 739.2095 | 4.63 | NEG | 25547.81981 | 21083.6857 | 21074.72787 | 0.003417998 | 0.002870886 | 0.002765873 | 0.003018253 | WRXVPTMENPZUIZ-UHFFFAOYSA-N | CC1OC(OCC2OC(OC3=C(OC4=CC(O)=CC(O)=C4C3=O)C3=CC=C(O)C=C3)C(OC3OC(C)C(O)C(O)C3O)C(O)C2O)C(O)C(O)C1O | HMDB0040562 | 50095 |  |  | 5459192 | 109008-28-8 | 毛里求斯排草素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N5038 | HPLC≥98% | level2 |
| compound00174 | 10.14\_315.1946m/z | M+H-H2O | C20H28O4 | 43.3 | 0 | -2.47 | Marrubiin |  | 315.1954 | 315.1946 | 10.14 | POS | 15644.19982 | 15342.49945 | 16367.60327 | 0.00209301 | 0.00208913 | 0.002148105 | 0.002110082 | HQLLRHCTVDVUJB-OBHOOXMTSA-N | CC1CC2C3C(CCCC3(C1(CCC4=COC=C4)O)C)(C(=O)O2)C |  | 67450 |  | C09128 | 73401 | 465-92-9 | 夏至草素 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N6995 | HPLC≥98% | level2 |
| compound00175 | 5.17\_159.0440m/z | M+H-H2O | C10H8O3 | 55.1 | 0 | -0.4 | Naphthalene-1,4,5-triol |  | 159.044 | 159.044 | 5.17 | POS | 5929.156409 | 6146.195248 | 5679.901193 | 0.000793252 | 0.000836904 | 0.000745437 | 0.000791864 | NHEVNUARLCWEED-UHFFFAOYSA-N | OC1=CC=CC2=C(O)C=CC(O)=C12 | HMDB0032883 | 88797 |  |  | 3083585 | 481-40-3 |  |  |  |  |  |  |  | level2 |
| compound00176 | 7.91\_313.1445m/z | M-H2O-H | C19H24O5 | 40.7 | 0 | -0.2 | Marmin |  | 313.1445 | 313.1445 | 7.91 | NEG | 9299.504102 | 9683.207944 | 9248.350974 | 0.001244164 | 0.001318526 | 0.001213765 | 0.001258818 | QYYKWTUUCOTGNS-JIIJFUIFSA-N | C/C(=C\COc1ccc2ccc(=O)oc2c1)CC[C@@H](O)C(C)(C)O |  |  |  |  |  | 14957-38-1 | 马尔敏 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DM0102 | HPLC≥98% | level2 |
| compound00177 | 5.79\_373.0927m/z | M+FA-H | C18H16O6 | 63.4 | 75.1 | -0.5 | isoamericanin a | 135.0442, 175.0393, 179.0343, 197.045, 373.092 | 373.0929 | 373.0927 | 5.79 | NEG | 322563.7236 | 313045.8918 | 317505.4461 | 0.04315524 | 0.042626279 | 0.041669808 | 0.042483775 | SDDXIQONGFZHJH-ZHEVZCJESA-N | C1=CC2=C(C=C1C=CC=O)OC(C(O2)CO)C3=CC(=C(C=C3)O)O | HMDB0033318 | 89172 |  |  | 11324912 | 109063-85-6 |  |  |  |  |  |  |  | level2 |
| compound00178 | 9.72\_489.3569m/z | M+H | C30H48O5 | 55.4 | 0 | -1.16 | Ilexolic acid A |  | 489.3575 | 489.3569 | 9.72 | POS | 27965.9969 | 29541.16014 | 29632.47465 | 0.003741522 | 0.004022508 | 0.003889003 | 0.003884344 | YLHQFGOOMKJFLP-UHFFFAOYSA-N | CC1CCC2(CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(CO)C5CCC34C)C2C1(C)O)C(O)=O | HMDB0257316 |  |  |  | 12315074 |  |  |  |  |  |  |  |  | level2 |
| compound00179 | 4.55\_448.1006n | M-H, M+FA-H | C21H20O11 | 59.1 | 81.2 | 0.14 | Maritimein with hplc | 61.9873, 197.0439, 297.0403, 299.0557, 327.0507, 357.0611, 379.0409, 447.0925 | 447.0933 | 447.0933 | 4.55 | NEG | 75670.58151 | 78929.08332 | 76181.82471 | 0.010123836 | 0.010747476 | 0.009998197 | 0.010289836 | SYRURBPRFQUYQS-UHFFFAOYSA-N | O=C1C(OC2=C(O)C(OC3OC(CO)C(O)C(O)C3O)=CC=C12)=CC4=CC=C(O)C(O)=C4 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00180 | 4.50\_360.1800m/z | M+H | C20H25NO5 | 57.1 | 66.4 | -1.52 | Homostephanoline | 58.0657, 86.0968, 163.0387, 200.1391, 228.134, 265.0853, 297.1115, 342.169, 359.169, 359.2268 | 360.1806 | 360.18 | 4.5 | POS | 69733.61703 | 72234.17433 | 72514.47925 | 0.009329539 | 0.009835855 | 0.00951689 | 0.009560762 | VCOZOQJXGDDART-UHFFFAOYSA-N | CN1CCC23C1(CCC4=C2C(=C(C=C4)O)OC)C(=C(C(=O)C3)OC)OC |  |  |  |  | 101673474 |  |  |  |  |  |  |  |  | level2 |
| compound00181 | 0.79\_162.0759m/z | M+H-H2O | C6H13NO5 | 43.9 | 0 | -0.92 | Manosamine |  | 162.0761 | 162.0759 | 0.79 | POS | 139285.7531 | 139138.9046 | 140018.5129 | 0.018634799 | 0.01894602 | 0.018376203 | 0.018652341 | FZHXIRIBWMQPQF-UHFFFAOYSA-N | NC(C=O)C(O)C(O)C(O)CO | HMDB0242589 |  |  |  | 318324 |  | 盐酸 D-甘露糖胺 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-W021425 | HPLC≥98% | level2 |
| compound00182 | 4.25\_371.0984m/z | M+FA-H | C15H18O8 | 50 | 13.1 | 0.16 | Melilotoside | 113.0234, 121.0285, 249.0611, 371.0977 | 371.0984 | 371.0984 | 4.25 | NEG | 17969.12868 | 18031.45771 | 17864.4815 | 0.002404058 | 0.002455276 | 0.002344557 | 0.002401297 | GVRIYIMNJGULCZ-ZMKUSUEASA-N | OC[C@H]1O[C@@H](OC2=C(\C=C\C(O)=O)C=CC=C2)[C@H](O)[C@@H](O)[C@@H]1O | HMDB0033581 | 984972 |  | C05158 | 5280759 | 618-67-7 |  |  |  |  |  |  |  | level2 |
| compound00183 | 9.84\_315.1237m/z | M-H2O-H | C18H22O6 | 43.3 | 0 | -0.31 | Methyl mycophenolate |  | 315.1238 | 315.1237 | 9.84 | NEG | 5433.708523 | 5552.750927 | 5212.211963 | 0.000726966 | 0.000756097 | 0.000684057 | 0.000722374 | ZPXRQFLATDNYSS-BJMVGYQFSA-N | COC(=O)CC/C(C)=C/Cc1c(O)c2c(c(C)c1OC)COC2=O |  |  |  |  |  | 31858-66-9 | 霉酚酸酯杂质E | 酚类 | 单酚类 | Phenols | Monophenols | HY-113972 | HPLC≥98% | level2 |
| compound00184 | 6.33\_313.1082m/z | M-H2O-H | C18H20O6 | 58.6 | 83 | 0.05 | nagilactone d | 161.0236, 221.0966, 283.0952, 313.1078 | 313.1081 | 313.1082 | 6.33 | NEG | 203623.699 | 207560.7178 | 208501.6042 | 0.027242461 | 0.028262761 | 0.027364008 | 0.027623077 | UEZYUDAMQBJVJP-CQVMLLNQSA-N | CCC1=C2CC3C4C(C(C5C(C4(C2=CC(=O)O1)C)O5)O)(C(=O)O3)C |  | 448913 |  |  | 3084330 |  |  |  |  |  |  |  |  | level2 |
| compound00185 | 4.97\_223.0604m/z | M-H2O-H | C11H14O6 | 57.1 | 81.7 | -3.22 | methyl syramuraldehydate | 158.9866, 163.0357, 164.0474, 179.0705, 182.9872, 193.0140, 202.9933, 208.0371, 222.0479, 223.0605 | 223.0611 | 223.0604 | 4.97 | NEG | 2577.173577 | 2453.308811 | 3284.206455 | 0.000344796 | 0.000334058 | 0.000431023 | 0.000369959 | JFWVMXPACNWBCB-UHFFFAOYSA-N | CC1C(C(C(=CO1)C(=O)O)CC(=O)OC)C=O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00186 | 4.13\_196.0971m/z | M+H | C10H13NO3 | 42.6 | 11 | 1.37 | N-acetyldopamine | 70.0656, 72.0812, 150.0911, 177.1635, 178.0581, 196.0964 | 196.0968 | 196.0971 | 4.13 | POS | 11141.99162 | 10795.90362 | 10560.25742 | 0.001490668 | 0.001470038 | 0.001385941 | 0.001448882 | OFSAJYZMIPNPHE-UHFFFAOYSA-N | CC(O)=NCCC1=CC(O)=C(O)C=C1 | HMDB0041943 | 96187 |  |  | 100526 | 2494-12-4 | N-乙酰多巴胺 | 生物碱 |  | Alkaloids |  | HY-N7493 | HPLC≥98% | level2 |
| compound00187 | 0.74\_191.0553m/z | M-H2O-H | C7H14O7 | 41 | 8.17 | -3.77 | Mannoheptulose | 117.0183, 118.0218, 129.0185, 130.0218, 131.0338, 156.0012, 173.0083, 174.0118, 191.0193, 191.0556 | 191.056 | 191.0553 | 0.74 | NEG | 1590275.624 | 1569607.939 | 1559396.205 | 0.212760211 | 0.213727596 | 0.204657087 | 0.210381632 | HSNZZMHEPUFJNZ-QMTIVRBISA-N | O=C(CO)[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO |  |  |  |  |  | 3615-44-9 | 甘露庚酮糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-U00462 | HPLC≥98% | level2 |
| compound00188 | 9.25\_285.1494m/z | M-H2O-H | C18H24O4 | 52.2 | 0 | -0.73 | hydroxypiloselloidone | 244.9828, 264.9889, 284.9973, 285.1494 | 285.1496 | 285.1494 | 9.25 | NEG | 23866.41146 | 22494.13622 | 22337.70399 | 0.003193046 | 0.003062942 | 0.002931628 | 0.003062538 | BQPCSMCCVBBMJR-UHFFFAOYSA-N | CC(C)CC(=O)C1=C(C(=CC(=C1)C(=O)C)C(C=C(C)C)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00189 | 4.93\_192.0422n | M+H-H2O, M+H | C10H8O4 | 50.9 | 46.7 | -0.27 | Hydrangetin | 60.0562, 70.0657, 116.0707, 119.0492, 147.0439, 175.0389 | 193.0495 | 193.0495 | 4.93 | POS | 82390.4514 | 87234.34597 | 83043.44282 | 0.011022875 | 0.011878372 | 0.010898724 | 0.011266657 | HAQWEMHXSIRYBE-UHFFFAOYSA-N | COC1=C(C=CC2=C1OC(=O)C=C2)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00190 | 7.28\_326.1139n | M+H-H2O, M+H | C19H18O5 | 45.3 | 19.3 | -4.74 | Moracin O | 265.1216, 291.1946, 309.1113 | 309.1121 | 309.1106 | 7.28 | POS | 415751.2802 | 422453.7448 | 417807.6309 | 0.055622641 | 0.057523934 | 0.05483359 | 0.055993388 | HMTMYIWMPJSCAZ-UHFFFAOYSA-N | CC(C)(O)C1CC2=C(O1)C=C1OC(=CC1=C2)C1=CC(O)=CC(O)=C1 | HMDB0040313 | 94834 |  |  | 14539883 | 123702-97-6 | 桑辛素 O | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N3244 | HPLC≥98% | level2 |
| compound00191 | 5.85\_313.1321n | M+H, M+Na | C18H19NO4 | 43.6 | 0 | 2.06 | N-Feruloyltyramine |  | 314.1387 | 314.1393 | 5.85 | POS | 9382.887514 | 9211.251043 | 8742.768933 | 0.00125532 | 0.001254261 | 0.001147412 | 0.001218998 | NPNNKDMSXVRADT-WEVVVXLNSA-N | COC1=CC(\C=C\C(=O)NCCC2=CC=C(O)C=C2)=CC=C1O | HMDB0029365 | 65816 |  | C02717 | 5280537 | 66648-43-9 | N-反式-阿魏酰酪胺 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N2410 | HPLC≥98% | level2 |
| compound00192 | 1.85\_115.0393m/z | M+H-H2O | C5H8O4 | 50.2 | 0 | 2.87 | Monomethyl succinate | 69.0341, 69.0704, 70.0657, 72.9377, 87.0444, 113.9638, 114.0553, 114.0665, 114.0917, 115.0393 | 115.039 | 115.0393 | 1.85 | POS | 120813.8301 | 127694.6655 | 134837.2558 | 0.016163472 | 0.017387701 | 0.017696208 | 0.017082461 | JDRMYOQETPMYQX-UHFFFAOYSA-N | COC(=O)CCC(O)=O | HMDB0246492 |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00193 | 5.61\_578.4040m/z | M+H | C33H55NO7 | 55.3 | 0 | -1.93 | Hupeheninoside | 578.4047 | 578.4051 | 578.404 | 5.61 | POS | 236922.3123 | 230284.9179 | 227154.7147 | 0.031697424 | 0.031357029 | 0.029812066 | 0.030955506 | YPEOJRRZBDHCLW-UHFFFAOYSA-N | CC1CCC2C(C3CCC4C(C3CN2C1)CC5C4CC(C6C5(CC(CC6)OC7C(C(C(C(O7)CO)O)O)O)C)O)C |  |  |  |  | 134611786 | 98985-22-9 |  |  |  |  |  |  |  | level2 |
| compound00194 | 5.55\_551.1190m/z | M-H | C28H24O12 | 64.7 | 90.8 | -0.82 | Monomethyl lithospermate | 197.0449, 266.0589, 277.0499, 291.0634, 294.0533, 309.0767, 327.0870, 507.1289, 515.0959, 551.1195 | 551.1195 | 551.119 | 5.55 | NEG | 486428.6852 | 479969.2617 | 473068.3153 | 0.065078448 | 0.065355605 | 0.062086071 | 0.064173375 | NFOCYHUCMXEHDG-PDLQCWERSA-N | COC(=O)[C@@H]1[C@H](OC2=C(C=CC(=C12)/C=C/C(=O)O[C@@H](CC3=CC(=C(C=C3)O)O)C(=O)O)O)C4=CC(=C(C=C4)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00195 | 10.97\_471.3476m/z | M-H | C30H48O4 | 48.9 | 0 | -0.79 | Momordicine I |  | 471.348 | 471.3476 | 10.97 | NEG | 14014.08891 | 14254.76097 | 15914.45428 | 0.001874921 | 0.001941017 | 0.002088633 | 0.00196819 | QBXNBPFTVLJTMK-MKVXWLNSSA-N | CC(C)=C[C@H](O)C[C@@H](C)[C@H]1CC[C@@]2(C)[C@@H]3[C@@H](O)C=C4[C@@H](CC[C@H](O)C4(C)C)[C@]3(C=O)CC[C@]12C |  |  |  |  |  | 91590-76-0 | 苦瓜素 I | 萜类 | 三萜类 | Terpenes | Triterpenes | DK0047 | HPLC≥98% | level2 |
| compound00196 | 5.93\_416.3520m/z | M+H | C27H45NO2 | 40.6 | 0 | -0.74 | Hupehenine |  | 416.3523 | 416.352 | 5.93 | POS | 10261.86644 | 12368.38259 | 10534.52021 | 0.001372917 | 0.001684156 | 0.001382563 | 0.001479879 | NEMWYOKGHGSVSC-MSSYMPDSSA-N | C[C@H]1CC[C@H]2[C@H](C)[C@@H]3CC[C@H]4[C@@H]5C[C@@H](O)[C@H]6C[C@@H](O)CC[C@]6(C)[C@H]5C[C@H]4[C@@H]3CN2C1 |  |  |  |  |  | 98243-57-3 | 湖贝甲素 | 生物碱 |  | Alkaloids |  | HY-N0413 | HPLC≥98% | level2 |
| compound00197 | 6.21\_385.0927m/z | M-H | C20H18O8 | 45.9 | 0.06 | -0.5 | Moluccanin | 112.9846, 180.9724, 248.9603, 297.113, 316.947, 341.1025 | 385.0929 | 385.0927 | 6.21 | NEG | 14171.29037 | 13730.04527 | 13798.09552 | 0.001895952 | 0.001869569 | 0.001810879 | 0.0018588 | GBLZBLJGCQTQMB-PXNSSMCTSA-N | COc1cc([C@@H]2Oc3cc4oc(=O)ccc4cc3O[C@H]2CO)cc(OC)c1O |  |  |  |  |  | 116521-73-4 | 反式-2，3-二氢-3-(4-羟基-3，5-二甲氧基苯基)-2-(羟基甲基)-7H-吡喃并[2，3-G]-1，4-苯并二氧六环-7-酮 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DM0069 | HPLC≥98% | level2 |
| compound00198 | 5.80\_347.1125m/z | M+H | C18H18O7 | 60.9 | 90.8 | 0.05 | Inumakilactone B | 275.1997, 283.0965, 287.0910, 293.2100, 299.0922, 301.1066, 311.0911, 311.2214, 329.1015, 347.1123 | 347.1125 | 347.1125 | 5.8 | POS | 24064.08818 | 23442.80605 | 21939.08078 | 0.003219493 | 0.003192119 | 0.002879312 | 0.003096974 | VLRYBJQMQSJMHB-UHFFFAOYSA-N | CC12C3C(C4C5(O4)C(OC(=O)C=C5C3(C6C(C1O)O6)C)C=C)OC2=O |  |  |  |  | 44179301 |  |  |  |  |  |  |  |  | level2 |
| compound00199 | 4.43\_360.1928m/z | M+NH4 | C19H22N2O4 | 40.4 | 0 | 2.84 | HuMantenidine |  | 360.1917 | 360.1928 | 4.43 | POS | 3672.599486 | 3827.825853 | 4047.254263 | 0.000491351 | 0.000521221 | 0.000531167 | 0.000514579 | FLDAHLDTMBMPJD-SEEUIANRSA-N | CCC1=N[C@H]2C[C@@]3(C(=O)N(OC)c4ccccc43)[C@@H]3OC[C@@H]2[C@H]1[C@H]3O |  |  |  |  |  | 114027-39-3 | 胡蔓藤碱丙 | 生物碱 |  | Alkaloids |  | DH0197 | HPLC≥98% | level2 |
| compound00200 | 4.80\_464.0957n | M+H, M+Na | C21H20O12 | 46.6 | 0 | 0.43 | Hyperoside |  | 465.1028 | 465.103 | 4.8 | POS | 17679.07847 | 16586.27886 | 15613.60548 | 0.002365253 | 0.002258491 | 0.002049149 | 0.002224298 | OVSQVDMCBVZWGM-DTGCRPNFSA-N | C1(O)=CC2OC(C3C=C(O)C(O)=CC=3)=C(O[C@H]3[C@H](O)[C@@H](O)[C@@H](O)[C@@H](CO)O3)C(=O)C=2C(O)=C1 | HMDB0030775 | 87190 | LMPK12112041 | C10073 | 5281643 | 482-36-0 | 金丝桃苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N0452 | HPLC≥98% | level2 |
| compound00201 | 10.40\_308.2216m/z | M+H | C18H29NO3 | 41.7 | 0 | -1.29 | N-Vanillyldecanamide |  | 308.222 | 308.2216 | 10.4 | POS | 5788.62836 | 5075.114065 | 5753.920226 | 0.000774451 | 0.000691059 | 0.000755152 | 0.00074022 | QLHTWDQJPOTDMV-UHFFFAOYSA-N | CCCCCCCCCC(O)=NCc1ccc(O)c(OC)c1 |  |  |  |  |  | 31078-36-1 | 癸酸香草酰胺 | 生物碱 |  | Alkaloids |  | HY-N5099 | HPLC≥98% | level2 |
| compound00202 | 1.99\_297.1075n | M+H, M+Na | C11H15N5O5 | 43.6 | 23.7 | 0.72 | N2-Methylguanosine | 136.0756, 143.1180, 152.0566, 166.0722, 182.0808, 251.1032, 281.0505, 297.1167, 297.1519, 298.0012 | 298.1146 | 298.1148 | 1.99 | POS | 22218.05628 | 23800.2072 | 23411.12917 | 0.002972515 | 0.003240784 | 0.003072506 | 0.003095268 | SLEHROROQDYRAW-KQYNXXCUSA-N | CNC1=NC(=O)C2=C(N1)N(C=N2)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O | HMDB0005862 | 58332 |  |  | 3035422 | 2140-77-4 | N2-甲基鸟苷 | 其他 |  | Others |  | HY-111647 | HPLC≥98% | level2 |
| compound00203 | 4.55\_387.2011m/z | M+H | C19H30O8 | 52.4 | 0 | -0.65 | icariside b2 |  | 387.2013 | 387.2011 | 4.55 | POS | 14653.24816 | 16367.39229 | 16393.50421 | 0.001960433 | 0.002228686 | 0.002151504 | 0.002113541 | RZPOXAOUEYNXNO-VLSJDARNSA-N | CC(=O)/C=C/[C@]12[C@](O1)(C[C@H](CC2(C)C)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00204 | 6.96\_331.0811m/z | M+H | C17H14O7 | 48.5 | 35.8 | -0.46 | Iristectorigenin A | 98.9845, 313.1448, 315.0491, 331.0817 | 331.0812 | 331.0811 | 6.96 | POS | 36983.14454 | 35780.24838 | 35600.24283 | 0.004947911 | 0.004872062 | 0.00467222 | 0.004830731 | CCRPIWFQMLICCY-UHFFFAOYSA-N | C1(O)=CC2OC=C(C3C=CC(O)=C(OC)C=3)C(=O)C=2C(O)=C1OC |  | 47906 | LMPK12050403 |  | 5491637 |  | 鸢尾甲黄素 A | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N2505 | HPLC≥98% | level2 |
| compound00205 | 4.51\_243.0508m/z | M+FA-H | C9H10O5 | 53.3 | 0 | -1.21 | Methyl-4-O-methylgallate |  | 243.0511 | 243.0508 | 4.51 | NEG | 2976.525514 | 3635.907411 | 3162.48367 | 0.000398224 | 0.000495088 | 0.000415048 | 0.00043612 | SUGIJIFASYORQN-UHFFFAOYSA-N | COC1=C(C=C(C=C1O)C(=O)OC)O |  |  |  |  | 5319726 |  |  |  |  |  |  |  |  | level2 |
| compound00206 | 4.93\_446.3261m/z | M+H | C27H43NO4 | 63 | 87.7 | -0.97 | Imperialine beta-N-oxide | 98.0966, 428.3151, 446.3258 | 446.3265 | 446.3261 | 4.93 | POS | 774770.4747 | 787461.8285 | 794535.0427 | 0.103655195 | 0.107225709 | 0.104275762 | 0.105052222 | RTQDXHMAHWNJLQ-SDWOMLPSSA-N | C[C@H]1CC[C@H]2C([C@@H]3CC[C@@H]4[C@H]([C@@H]3C[N+]2(C1)[O-])C[C@H]5[C@H]4CC(=O)[C@@H]6[C@@]5(CC[C@@H](C6)O)C)(C)O |  |  |  |  | 3730728 |  |  |  |  |  |  |  |  | level2 |
| compound00207 | 6.22\_373.0932m/z | M-H | C19H18O8 | 41.7 | 0 | 0.74 | Methyl rosmarinic acid |  | 373.0929 | 373.0932 | 6.22 | NEG | 8825.603306 | 9274.027718 | 8939.527037 | 0.001180762 | 0.001262809 | 0.001173235 | 0.001205602 | XHALVRQBZGZHFE-BBOMDTFKSA-N | COC(=O)[C@@H](CC1=CC(O)=C(O)C=C1)OC(=O)\C=C\C1=CC(O)=C(O)C=C1 | HMDB0035446 | 90732 |  |  | 6479915 | 99353-00-1 | 迷迭香酸甲酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N3266 | HPLC≥98% | level2 |
| compound00208 | 9.10\_269.1168m/z | M+H-H2O | C17H18O4 | 45 | 0 | -1.61 | Loureirin A |  | 269.1172 | 269.1168 | 9.1 | POS | 11392.30231 | 12390.95725 | 11600.45387 | 0.001524156 | 0.00168723 | 0.001522458 | 0.001577948 | RSAIVLRELNGZEY-UHFFFAOYSA-N | C1(O)C=CC(C(=O)CCC2C=CC(OC)=CC=2OC)=CC=1 | HMDB0254174 | 52404 | LMPK12120602 |  | 5319081 |  | 龙血素A | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | HY-N1505 | HPLC≥98% | level2 |
| compound00209 | 10.77\_235.1689m/z | M+H | C15H22O2 | 46.8 | 27.4 | -1.38 | Isocurcumenol | 179.1064, 235.169 | 235.1693 | 235.1689 | 10.77 | POS | 26313.74758 | 26865.47672 | 28492.5466 | 0.003520471 | 0.003658171 | 0.003739397 | 0.003639346 | DEBDFZGNZTYPMF-NZBPQXDJSA-N | C=C1C[C@@]2(O)O[C@@]3(CC2=C(C)C)[C@@H](C)CC[C@@H]13 |  |  |  |  |  | 24063-71-6 | 异莪术烯醇 | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | HY-N4121 | HPLC≥98% | level2 |
| compound00210 | 6.14\_375.1449m/z | M-H | C20H24O7 | 40.5 | 2.09 | -0.06 | Leocarpinolide F | 102.9559, 112.9843, 227.1437, 238.9316, 239.0907, 283.1337, 331.1565, 375.095, 375.1451 | 375.1449 | 375.1449 | 6.14 | NEG | 9891.715251 | 9887.531439 | 9707.029865 | 0.001323395 | 0.001346348 | 0.001273963 | 0.001314569 | RGDZQGAEJIRTEC-RJBZGIITSA-N | C/C=C(/C)\C(=O)O[C@H]1[C@@H]2[C@@H](C=C(CC/C=C(\[C@@H]1O)/C=O)CO)OC(=O)C2=C |  |  |  |  |  | 145042-08-6 |  | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | DL0397 | HPLC≥95% | level2 |
| compound00211 | 5.68\_175.0389m/z | M+H | C10H6O3 | 43.7 | 0 | -0.15 | Lawsone |  | 175.039 | 175.0389 | 5.68 | POS | 3960.954961 | 4538.462497 | 4981.250158 | 0.000529929 | 0.000617985 | 0.000653745 | 0.000600553 | WVCHIGAIXREVNS-UHFFFAOYSA-N | OC1=CC(=O)C(=O)C2=CC=CC=C12 | HMDB0253997 | 44321 |  | C10368 | 6755 | 83-72-7 | 2-羟基-1,4-萘醌 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-N2493 | HPLC≥98% | level2 |
| compound00212 | 5.78\_383.1467m/z | M+Na | C20H24O6 | 44.5 | 0 | 0.55 | Lariciresinol |  | 383.1465 | 383.1467 | 5.78 | POS | 6552.473559 | 6474.216677 | 6682.545907 | 0.000876644 | 0.00088157 | 0.000877026 | 0.000878413 | MHXCIKYXNYCMHY-SXGZJXTBSA-N | COC1=C(C=CC(=C1)CC2COC(C2CO)C3=CC(=C(C=C3)O)OC)O |  |  |  | C20454 | 23815394 |  | (-)-落叶松脂醇 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | B50409-1mg | HPLC≥95% | level2 |
| compound00213 | 4.56\_449.1075m/z | M+H | C21H20O11 | 51.3 | 22 | -0.68 | Isoorientin | 85.0288, 329.0648, 430.3306, 448.3416, 449.1074 | 449.1078 | 449.1075 | 4.56 | POS | 25354.61391 | 24463.42725 | 23935.88064 | 0.00339215 | 0.003331093 | 0.003141375 | 0.003288206 | ODBRNZZJSYPIDI-VJXVFPJBSA-N | C1(O)=CC2OC(C3C=CC(O)=C(O)C=3)=CC(=O)C=2C(O)=C1[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 | HMDB0301981 | 48900 | LMPK12110469 | C01821 | 114776 |  | 异荭草素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0767 | HPLC≥98% | level2 |
| compound00214 | 1.09\_365.1055m/z | M+Na | C12H22O11 | 52.3 | 63.3 | 0.23 | Lactose | 185.0419, 203.0523, 365.1048 | 365.1054 | 365.1055 | 1.09 | POS | 823796.7153 | 808207.1259 | 791324.7939 | 0.110214331 | 0.110050518 | 0.103854445 | 0.108039764 | GUBGYTABKSRVRQ-PICCSMPSSA-N | OCC1OC(OC2C(O)C(O)C(O)OC2CO)C(O)C(O)C1O |  |  |  | C00208 |  | 69-79-4 |  |  |  |  |  |  |  | level2 |
| compound00215 | 7.07\_884.4769n | M+H-H2O, M+Na | C45H72O17 | 44.2 | 0 | -0.07 | Isoproprotogracillin B |  | 867.4737 | 867.4736 | 7.07 | POS | 43895.05135 | 40669.33023 | 37724.11283 | 0.005872643 | 0.005537789 | 0.004950959 | 0.005453797 | IKWOPELBOIFGSX-YSKFQSCVSA-N | C1[C@@H](CC2=CC[C@@H]3[C@@H]([C@]2(C1)C)CC[C@]1([C@H]3C[C@H]2[C@@H]1C(=C(O2)CC[C@H](CO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O)C)C)C)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O[C@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)C)O)O)O)CO |  |  |  |  |  | 117457-34-8 | 异原纤细薯蓣次皂苷 | 甾体类 | 其他甾体类 | Steroids | Other steroids | DY0502 | HPLC≥98% | level2 |
| compound00216 | 9.90\_311.1289m/z | M-H2O-H | C19H22O5 | 51.3 | 0 | -0.04 | lactiflorasyne | 239.1438, 243.1962, 267.1388, 275.2013, 281.1182, 293.2119, 310.2102, 311.0103, 311.0945, 311.1286 | 311.1289 | 311.1289 | 9.9 | NEG | 46245.1023 | 50539.61388 | 50222.46512 | 0.006187052 | 0.006881789 | 0.006591258 | 0.006553366 | RYAXKMRZPSXCFZ-LEWXTWDNSA-N | CC#CC#COC1=C[C@]2(CCC(CO2)OC(=O)CC(C)C)[C@H]3[C@@H]1O3 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00217 | 2.46\_178.0864m/z | M+H-H2O | C10H13NO3 | 41.9 | 10.1 | 0.99 | L-Tyrosine methyl ester | 177.1635, 178.0859 | 178.0863 | 178.0864 | 2.46 | POS | 48662.25556 | 49053.98642 | 52644.75231 | 0.006510439 | 0.006679496 | 0.006909162 | 0.006699699 | MWZPENIJLUWBSY-VIFPVBQESA-N | COC(=O)[C@@H](N)CC1=CC=C(O)C=C1 | HMDB0029217 | 65971 |  | C03404 | 70652 | 1080-06-4 | L-酪氨酸甲酯 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino acids | HY-W007671 | HPLC≥98% | level2 |
| compound00218 | 7.57\_302.1021m/z | M+NH4 | C16H12O5 | 52.8 | 0 | -0.77 | Isoprunetin |  | 302.1023 | 302.1021 | 7.57 | POS | 2512.7794 | 3377.979924 | 2718.572692 | 0.00033618 | 0.000459967 | 0.000356789 | 0.000384312 | YSINCDVRUMTOPK-UHFFFAOYSA-N | C1(O)=CC2OC=C(C3C=CC(O)=CC=3)C(=O)C=2C(OC)=C1 | HMDB0301940 | 47845 | LMPK12050338 |  | 5748551 |  |  |  |  |  |  |  |  | level2 |
| compound00219 | 4.69\_347.0772m/z | M-H2O-H | C17H18O9 | 45.3 | 0.119 | -0.05 | Isopsoralenoside | 72.992, 149.0236, 179.0341, 197.045, 347.0757 | 347.0772 | 347.0772 | 4.69 | NEG | 32978.78761 | 33848.65072 | 32182.67498 | 0.004412175 | 0.004609043 | 0.004223694 | 0.004414971 | CAMYXILYLXYDFE-MIVOEOINSA-N | O=C(O)/C=C\c1ccc2occc2c1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 905954-18-9 | 异补骨脂苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N7504 | HPLC≥98% | level2 |
| compound00220 | 4.26\_785.2151m/z | M-H | C34H42O21 | 51.6 | 2.6 | 0.61 | Isorhamnetin 3-sophoroside-7-rhamnoside | 269.0455, 315.0505, 577.1567, 739.2125, 785.2033 | 785.2146 | 785.2151 | 4.26 | NEG | 60282.7226 | 53221.75553 | 54052.15411 | 0.008065121 | 0.007247006 | 0.007093872 | 0.007468666 | FJQKXKNZQQBTDD-IOCIRFPBSA-N | C1(O[C@H]2[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O2)=CC2OC(C3C=C(OC)C(O)=CC=3)=C(O[C@H]3[C@H](O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)[C@@H](O)[C@H](O)[C@@H](CO)O3)C(=O)C=2C(O)=C1 |  | 50769 | LMPK12112353 |  | 102004843 |  | 异鼠李素-3-O-槐二糖-7-O-鼠李糖苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DY0159 | HPLC≥98% | level2 |
| compound00221 | 4.89\_579.1709m/z | M+H-H2O | C27H32O15 | 52.4 | 0 | 0.17 | Isorubrofusarin-6-O-beta-gentiobioside |  | 579.1708 | 579.1709 | 4.89 | POS | 87317.07058 | 86939.67089 | 88793.0573 | 0.011681999 | 0.011838247 | 0.011653311 | 0.011724519 | CREWSFDYWMXJQL-UHFFFAOYSA-N | COC1=CC(OC2OC(COC3OC(CO)C(O)C(O)C3O)C(O)C(O)C2O)=C2C(C=C(O)C3=C2OC(C)=CC3=O)=C1 | HMDB0034609 | 90072 |  |  | 85211061 | 200127-93-1 | 异红镰霉素龙胆二糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | B22026-10mg | HPLC≥98% | level2 |
| compound00222 | 8.96\_172.1694m/z | M+NH4 | C10H18O | 49.3 | 0 | -1.11 | L-Borneol |  | 172.1696 | 172.1694 | 8.96 | POS | 2275.541582 | 2115.864943 | 2311.176049 | 0.000304441 | 0.000288109 | 0.000303322 | 0.000298624 | DTGKSKDOIYIVQL-NQMVMOMDSA-N | CC1(C)[C@@H]2CC[C@]1(C)[C@H](O)C2 |  |  |  |  |  | 464-45-9 | 左旋龙脑 | 萜类 | 单萜类 | Terpenes | Monoterpenes | JOT-10228 | HPLC≥98% | level2 |
| compound00223 | 5.74\_432.1420n | M+H-H2O, M+H | C22H24O9 | 55.2 | 71.5 | -0.18 | isosakuranetin-7-rutinoside | 164.1433, 219.0284, 245.0445, 263.0548, 281.0656, 353.1013, 397.1271, 398.3049, 414.3293, 415.1373 | 433.1493 | 433.1492 | 5.74 | POS | 280818.6172 | 268094.386 | 273556.9847 | 0.037570235 | 0.036505402 | 0.035901957 | 0.036659198 | LBGSZVCVDNTPPJ-WLFXGSQNSA-N | C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC2=CC(=C3C(=O)C[C@H](OC3=C2)C4=CC=C(C=C4)OC)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00224 | 5.20\_432.3469m/z | M+H | C27H45NO3 | 73.6 | 96.8 | -0.74 | Korseveriline | 414.336, 432.3466 | 432.3472 | 432.3469 | 5.2 | POS | 836995.7501 | 827041.3939 | 831773.7359 | 0.111980206 | 0.112615109 | 0.109163014 | 0.111252777 | NQGYOUYEGZOZBN-UHFFFAOYSA-N | CC1CCC2C(C3CCC4(C(C3CN2C1)CC5C4CC(C6C5(CCC(C6)O)C)O)O)C |  |  |  |  | 101316984 |  |  |  |  |  |  |  |  | level2 |
| compound00225 | 4.43\_344.1859m/z | M+H | C20H25NO4 | 60.9 | 64.4 | 0.68 | Kodamin | 58.0658, 137.0596, 175.0752, 344.1855 | 344.1856 | 344.1859 | 4.43 | POS | 167292.1748 | 166235.2988 | 155598.6571 | 0.022381729 | 0.022635634 | 0.02042096 | 0.021812775 | OKORHWXYDBSYNO-UHFFFAOYSA-N | COC1=C(OC)C=C(CC2N(C)CCC3=CC(OC)=C(O)C=C23)C=C1 | HMDB0034593 | 90056 |  |  | 89421 | 21040-59-5 |  |  |  |  |  |  |  | level2 |
| compound00226 | 5.75\_426.3002m/z | M+H | C27H39NO3 | 45.8 | 17.2 | -0.19 | Jervine | 98.0967, 120.0809, 233.1646, 261.1594, 408.2892, 426.2994 | 426.3003 | 426.3002 | 5.75 | POS | 90842.09018 | 91012.03584 | 90407.29032 | 0.012153605 | 0.012392766 | 0.011865165 | 0.012137179 | CLEXYFLHGFJONT-DNMILWOZSA-N | CC1CC2C(C(C3(O2)CCC4C5CC=C6CC(CCC6(C5C(=O)C4=C3C)C)O)C)NC1 |  | 68599 |  | C10811 | 10098 | 469-59-0 | 蒜黎芦碱 | 生物碱 |  | Alkaloids |  | HY-N0836 | HPLC≥98% | level2 |
| compound00227 | 5.90\_432.3480m/z | M+H | C27H45NO3 | 45 | 0 | 1.76 | Isoverticine |  | 432.3472 | 432.348 | 5.9 | POS | 15016.16063 | 14542.75128 | 14744.24281 | 0.002008986 | 0.001980232 | 0.001935053 | 0.001974757 | IUKLSMSEHKDIIP-RZNVUHDWSA-N | C[C@H]1CC[C@@H]2N(C1)C[C@@H]1[C@H](CC[C@H]3[C@@H]4C[C@@H](O)[C@H]5C[C@@H](O)CC[C@]5(C)[C@H]4C[C@H]31)[C@]2(C)O |  |  |  |  |  | 23496-43-7 | 异浙贝甲素 | 生物碱 |  | Alkaloids |  | HY-N7596 | HPLC≥98% | level2 |
| compound00228 | 11.12\_313.1807m/z | M-H | C20H26O3 | 58.3 | 73.9 | -0.61 | Jolkinolide A | 298.1572, 313.1076, 313.1807 | 313.1809 | 313.1807 | 11.12 | NEG | 29023.1568 | 33330.50203 | 27733.00848 | 0.003882958 | 0.004538489 | 0.003639714 | 0.004020387 | OYXDHOVYZKWSRM-PHJMNMFVSA-N | CC1=C2[C@@H]3[C@]4(O3)CC[C@H]5[C@]([C@@H]4C=C2OC1=O)(CCCC5(C)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00229 | 10.94\_329.1757m/z | M-H | C20H26O4 | 43.9 | 0 | -0.4 | Jolkinolide B |  | 329.1758 | 329.1757 | 10.94 | NEG | 4791.78648 | 3895.759504 | 4377.457977 | 0.000641085 | 0.000530471 | 0.000574503 | 0.00058202 | SOVOCMGDFRGRKF-MCDHERAVSA-N | CC1=C2[C@H]3O[C@]34CC[C@@H]3C(C)(C)CCC[C@@]3(C)[C@@H]4[C@H]3O[C@@]23OC1=O |  |  |  |  |  | 37905-08-1 | 岩大戟内酯B | 萜类 | 二萜类 | Terpenes | Diterpenes | DY0043-0020 | HPLC≥98% | level2 |
| compound00230 | 4.39\_169.0498m/z | M+H | C8H8O4 | 40.2 | 0 | 1.47 | Isovanillic acid |  | 169.0495 | 169.0498 | 4.39 | POS | 5381.689299 | 5555.481638 | 5524.771265 | 0.000720007 | 0.000756469 | 0.000725078 | 0.000733851 | LBKFGYZQBSGRHY-UHFFFAOYSA-N | COC1=CC=C(C=C1O)C(O)=O | HMDB0060003 | 349613 |  |  | 12575 |  | 异香草酸 | 酚类 | 单酚类 | Phenols | Monophenols | HY-N6864 | HPLC≥98% | level2 |
| compound00231 | 4.88\_577.1557m/z | M-H | C27H30O14 | 53.4 | 0 | -0.92 | Kaempferitrin |  | 577.1563 | 577.1557 | 4.88 | NEG | 35498.71376 | 34480.72333 | 34227.40556 | 0.004749311 | 0.00469511 | 0.004492047 | 0.004645489 | PUPKKEQDLNREIM-NZOUPAKWSA-N | C[C@@H]1O[C@@H](Oc2cc(O)c3c(=O)c(O[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)c(-c4ccc(O)cc4)oc3c2)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 482-38-2 | 山奈苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N0628 | HPLC≥98% | level2 |
| compound00232 | 5.66\_223.0598m/z | M+H | C11H10O5 | 56.7 | 0 | -1.19 | Leptodactylone |  | 223.0601 | 223.0598 | 5.66 | POS | 7636.036271 | 8635.645234 | 8757.253114 | 0.001021612 | 0.001175883 | 0.001149313 | 0.001115603 | TUFLVKBJDSZLAW-UHFFFAOYSA-N | COC1=CC(=C(C2=C1C=CC(=O)O2)O)OC |  | 67566 |  | C09271 | 442134 | 61899-44-3 |  |  |  |  |  |  |  | level2 |
| compound00233 | 4.75\_589.1176m/z | M-H2O-H | C27H28O16 | 59.7 | 91.6 | -3.7 | kaempferol 3-o-(2''-α-rhamnopyranosyl)-β-glucuronopyranoside | 135.0441, 161.0231, 179.0343, 201.0162, 219.0269, 341.0864, 381.0586, 543.1118 | 589.1198 | 589.1176 | 4.75 | NEG | 102061.079 | 102066.7799 | 103743.3208 | 0.013654574 | 0.013898049 | 0.013615402 | 0.013722675 | NQSVMEYOIVETBP-UHFFFAOYSA-N | CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC=C(C=C5)O)C(=O)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00234 | 6.14\_575.1173m/z | M-H2O-H | C30H26O13 | 41.7 | 0 | -3.63 | Kaempferol-3-o-(6''-o-cis-coumaryl)glucoside |  | 575.1194 | 575.1173 | 6.14 | NEG | 12609.93682 | 12412.8782 | 11423.65732 | 0.001687062 | 0.001690215 | 0.001499255 | 0.00162551 | DVGGLGXQSFURLP-PYFXTMFGSA-N | O=C(/C=C\c1ccc(O)cc1)OC[C@H]1O[C@@H](Oc2c(-c3ccc(O)cc3)oc3cc(O)cc(O)c3c2=O)[C@H](O)[C@@H](O)[C@@H]1O |  |  |  |  |  | 163956-16-9 | 顺式银椴苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | B50315-5mg | HPLC≥95% | level2 |
| compound00235 | 2.62\_236.0903m/z | M+Na | C10H15NO4 | 40.7 | 0 | 4.67 | Kainic acid |  | 236.0892 | 236.0903 | 2.62 | POS | 1239.570964 | 943.4045035 | 1297.598077 | 0.00016584 | 0.00012846 | 0.000170298 | 0.000154866 | VLSMHEGGTFMBBZ-OOZYFLPDSA-N | CC(=C)C1CNC(C1CC(=O)O)C(=O)O |  | 44252 |  | C12819 | 10255 | 487-79-6 | 红藻氨酸 | 生物碱 |  | Alkaloids |  | HY-N2309 | HPLC≥98% | level2 |
| compound00236 | 6.40\_491.0982m/z | M-H | C26H20O10 | 65.6 | 93 | -0.4 | isosalvianolic acid c | 135.0443, 197.0448, 265.0501, 293.0453, 311.0558, 491.0986 | 491.0984 | 491.0982 | 6.4 | NEG | 699014.379 | 716402.6107 | 720444.6659 | 0.093519919 | 0.097549843 | 0.094552049 | 0.09520727 | AVGRZVZQTALJJF-VURDRKPISA-N | C1=CC(=C(C=C1C[C@H](C(=O)O)OC(=O)/C=C/C2=C3C=CC4=CC(=C(C=C4OC3=C(C=C2)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00237 | 11.13\_315.1952m/z | M+H-H2O | C20H28O4 | 51.7 | 0 | -0.75 | kakispyrone |  | 315.1955 | 315.1952 | 11.13 | POS | 2471.79233 | 2098.558961 | 2661.458355 | 0.000330697 | 0.000285753 | 0.000349293 | 0.000321914 | ZMSSBNLNFAIVPK-UHFFFAOYSA-N | CC1=C(OC(=C(C1=O)C)OC)CC=C(C)CC=CC(=CC(C)O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00238 | 6.41\_429.1188m/z | M-H2O-H | C22H24O10 | 51.1 | 0 | -0.75 | Isosakuranin |  | 429.1191 | 429.1188 | 6.41 | NEG | 7999.226208 | 7756.959851 | 7014.613093 | 0.001070203 | 0.001056236 | 0.000920607 | 0.001015682 | KEEWIHDTSNESJZ-UHFFFAOYSA-N | COC1=CC=C(C=C1)C1CC(=O)C2=C(O1)C=C(OC1OC(CO)C(O)C(O)C1O)C=C2O | HMDB0029481 |  |  |  | 12304405 | 491-69-0 | 异樱花苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N4296 | HPLC≥98% | level2 |
| compound00239 | 4.26\_477.1615m/z | M-H | C20H30O13 | 52.1 | 0 | 0.31 | kelampayoside A |  | 477.1614 | 477.1615 | 4.26 | NEG | 4784.721466 | 5019.257026 | 4876.792884 | 0.00064014 | 0.000683453 | 0.000640036 | 0.000654543 | CKGKQISENBKOCA-FHXQZXMCSA-N | COC1=CC(O[C@@H]2O[C@H](CO[C@@H]3OC[C@](O)(CO)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)=CC(OC)=C1OC | HMDB0038714 | 93369 |  |  | 10552637 | 87562-76-3 |  |  |  |  |  |  |  | level2 |
| compound00240 | 4.11\_755.2037m/z | M-H | C33H40O20 | 41.6 | 0 | -0.45 | Kaempferol 3-sophoroside-7-rhamnoside |  | 755.204 | 755.2037 | 4.11 | NEG | 23116.38242 | 22528.36859 | 22048.33346 | 0.003092701 | 0.003067603 | 0.002893651 | 0.003017985 | VRYWDBDPXMHHGE-IAYTZLMWSA-N | CC1C(C(C(C(O1)OC2=CC(=C3C(=C2)OC(=C(C3=O)OC4C(C(C(C(O4)CO)O)O)OC5C(C(C(C(O5)CO)O)O)O)C6=CC=C(C=C6)O)O)O)O)O |  | 50174 |  |  | 102004842 |  | 山柰酚-3-槐二糖-7-鼠李糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DS0109 | HPLC≥98% | level2 |
| compound00241 | 4.48\_386.1610m/z | M+FA-H | C20H23NO4 | 67.9 | 87.7 | 0.32 | Isocopalmine | 310.1085, 325.1316, 340.155 | 386.1609 | 386.161 | 4.48 | NEG | 334837.3049 | 343525.9026 | 332123.385 | 0.044797301 | 0.046776627 | 0.043588284 | 0.045054071 | KDFKJOFJHSVROC-UHFFFAOYSA-N | COC1=CC2=C(C=C1O)C1CC3=C(CN1CC2)C(OC)=C(OC)C=C3 | HMDB0243515 |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00242 | 4.97\_507.1131m/z | M+FA-H | C22H22O11 | 57.6 | 0.682 | -2.91 | Leptosin | 135.044, 179.0346, 197.045, 301.0353, 309.0775, 329.0301, 344.0546, 507.116 | 507.1145 | 507.1131 | 4.97 | NEG | 27844.58253 | 37195.8901 | 32111.64647 | 0.003725278 | 0.005064824 | 0.004214372 | 0.004334825 | NXOKVARAWXQHGX-UHFFFAOYSA-N | C12C(=O)C(=CC3C=C(O)C(O)=CC=3)OC=1C(OC)=C(OC1OC(CO)C(O)C(O)C1O)C=C2 |  |  | LMPK12130015 |  | 42607750 |  |  |  |  |  |  |  |  | level2 |
| compound00243 | 4.72\_450.1159n | M-H2O-H, M-H | C21H22O11 | 53.7 | 69.7 | -0.73 | Isookaninglucoside | 161.0448, 197.0448, 205.1226, 283.0609, 311.0561, 341.0663, 367.1758, 431.0992 | 431.0984 | 431.098 | 4.72 | NEG | 45932.3328 | 47846.71306 | 46645.55156 | 0.006145207 | 0.006515107 | 0.00612182 | 0.006260711 | DGGOLFCPSUVVHX-UHFFFAOYSA-N | C1(OC2OC(CO)C(O)C(O)C2O)=C(O)C2OC(C3C=C(O)C(O)=CC=3)CC(=O)C=2C=C1 |  | 52582 | LMPK12140092 |  | 12309901 |  |  |  |  |  |  |  |  | level2 |
| compound00244 | 4.28\_467.0810m/z | M+FA-H | C19H18O11 | 43.4 | 0 | -4.98 | Mangiferin |  | 467.0833 | 467.081 | 4.28 | NEG | 4140.296908 | 3636.201857 | 3703.352891 | 0.000553923 | 0.000495128 | 0.000486033 | 0.000511695 | AEDDIBAIWPIIBD-ZJKJAXBQSA-N | [H][C@]1(CO)O[C@@]([H])(C2=C(O)C3=C(OC4=C(C=C(O)C(O)=C4)C3=O)C=C2O)[C@]([H])(O)[C@@]([H])(O)[C@]1([H])O | HMDB0302730 | 68115 |  | C10077 | 5281647 | 4773-96-0 | 芒果苷 | 苯丙素类 | 氧杂蒽酮 | Phenylpropanoids | Xanthones | HY-N0290 | HPLC≥98% | level2 |
| compound00245 | 10.61\_267.1376m/z | M+H | C18H18O2 | 48.6 | 0 | -1.21 | Magnolol |  | 267.138 | 267.1376 | 10.61 | POS | 2912.430459 | 2628.541516 | 2756.020337 | 0.000389649 | 0.000357919 | 0.000361704 | 0.000369757 | VVOAZFWZEDHOOU-UHFFFAOYSA-N | OC1=C(C=C(CC=C)C=C1)C1=C(O)C=CC(CC=C)=C1 | HMDB0254305 | 68465 |  | C10651 | 72300 | 528-43-8 | 厚朴酚 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | HY-N0163 | HPLC≥98% | level2 |
| compound00246 | 4.01\_399.0930m/z | M+FA-H | C16H18O9 | 42.3 | 4.49 | -0.88 | Magnolioside | 72.9921, 81.0335, 99.0077, 125.0235, 143.0341, 161.0447, 205.0348, 223.0454, 399.0921 | 399.0933 | 399.093 | 4.01 | NEG | 126400.4783 | 133798.7681 | 130993.5187 | 0.0169109 | 0.018218874 | 0.017191751 | 0.017440509 | WBAVLTNIRYDCPM-YMILTQATSA-N | COC1=C(C=C2C=CC(=O)OC2=C1)OC3C(C(C(C(O3)CO)O)O)O |  | 985238 |  |  | 3084335 |  | 6-甲氧基香豆素-7--β-D-吡喃葡萄糖苷 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N7034 | HPLC≥98% | level2 |
| compound00247 | 4.34\_300.1594m/z | M+H | C18H21NO3 | 57.3 | 0 | -0.03 | magnococline |  | 300.1594 | 300.1594 | 4.34 | POS | 9621.884193 | 9603.394653 | 10057.34638 | 0.001287295 | 0.001307658 | 0.001319939 | 0.001304964 | KRFKJAVTNDLYGI-UHFFFAOYSA-N | COC1=CC=C(C=C1)CC2C3=C(CCN2)C=CC(=C3O)OC |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00248 | 5.70\_307.0457m/z | M+FA-H | C13H10O6 | 56.6 | 0 | -1.08 | Macurin |  | 307.046 | 307.0457 | 5.7 | NEG | 6425.97351 | 6472.603978 | 5942.982948 | 0.00085972 | 0.00088135 | 0.000779964 | 0.000840345 | XNWPXDGRBWJIES-UHFFFAOYSA-N | OC1=CC(O)=C(C(=O)C2=CC(O)=C(O)C=C2)C(O)=C1 | HMDB0032644 | 68038 |  | C09951 | 68213 | 519-34-6 |  |  |  |  |  |  |  | level2 |
| compound00249 | 4.02\_261.1238m/z | M+H | C14H16N2O3 | 46.7 | 28.5 | 1.72 | Maculosin | 70.0656, 86.0967, 107.0493, 120.081, 136.0754, 260.0913, 260.1267, 261.1238 | 261.1234 | 261.1238 | 4.02 | POS | 12652.1035 | 13196.65898 | 14323.89019 | 0.001692703 | 0.001796939 | 0.001879885 | 0.001789842 | LSGOTAXPWMCUCK-RYUDHWBXSA-N | C1CC2C(=O)NC(C(=O)N2C1)CC3=CC=C(C=C3)O |  | 68423 |  | C10605 | 119404 | 4549-02-4 | 环(脯氨酸一酪氨酸) | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-P1940 | HPLC≥98% | level2 |
| compound00250 | 6.86\_205.0500m/z | M-H | C11H10O4 | 58.9 | 80.4 | -3.16 | Isoeugenitol | 135.044, 161.0236, 164.996, 204.9894, 205.0497 | 205.0506 | 205.05 | 6.86 | NEG | 15824.75429 | 15404.88319 | 16541.83208 | 0.002117166 | 0.002097625 | 0.002170971 | 0.002128587 | XSSGQRFNGHRFBC-UHFFFAOYSA-N | CC1=CC(=O)C2=C(O)C=C(O)C(C)=C2O1 | HMDB0029472 | 43925 |  |  | 5318562 | 479-06-1 |  |  |  |  |  |  |  | level2 |
| compound00251 | 1.00\_990.3271n | M-H, M+FA-H | C36H62O31 | 65.5 | 55.2 | -0.42 | lycopose | 89.0233, 101.0232, 179.055, 191.0186, 341.1065, 827.2589, 989.3188 | 1035.3257 | 1035.3253 | 1 | NEG | 88985.7673 | 104591.1087 | 83514.82209 | 0.011905251 | 0.014241777 | 0.010960589 | 0.012369206 | YMKYJQIVVYKNIO-UHFFFAOYSA-N | C(C1C(C(C(C(O1)OC2C(OC(C(C2O)O)OC3C(OC(C(C3O)O)OC4C(OC(C(C4O)O)OC5C(OC(C(C5O)O)OC6(C(C(C(O6)CO)O)O)CO)CO)CO)CO)CO)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00252 | 4.62\_289.0708m/z | M+Na | C16H12NO3+ | 42.5 | 0 | -0.58 | Lycobetaine |  | 289.071 | 289.0708 | 4.62 | POS | 10962.32872 | 11037.51162 | 10820.73289 | 0.001466631 | 0.001502936 | 0.001420126 | 0.001463231 | DFQOXFIPAAMFAU-UHFFFAOYSA-O | C1C[N+]2=CC3=CC4=C(C=C3C5=CC(=CC1=C52)O)OCO4 |  | 452352 |  |  | 159646 |  | 氧化石蒜碱 | 生物碱 |  | Alkaloids |  | DY0676 | HPLC≥98% | level2 |
| compound00253 | 8.87\_215.1066m/z | M+H-H2O | C14H16O3 | 54.7 | 0 | -0.41 | isofraxinellone |  | 215.1066 | 215.1066 | 8.87 | POS | 2796.352379 | 2709.152988 | 2756.117781 | 0.000374119 | 0.000368895 | 0.000361716 | 0.000368244 | CKJJQJLXFWVISP-VBVNFKHJSA-N | CC1=CCC[C@@]2(C1C(=O)O[C@H]2C3=COC=C3)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00254 | 5.95\_273.1707m/z | M+FA-H | C13H24O3 | 51.2 | 48.8 | -0.38 | japonicumin D | 124.0394, 169.0076, 232.9856, 255.1612, 273.172 | 273.1708 | 273.1707 | 5.95 | NEG | 12151.71633 | 11637.57644 | 12674.22709 | 0.001625757 | 0.001584645 | 0.001663381 | 0.001624594 | MNJZVIWXEFIIPW-CCJOIDDDSA-N | C[C@]12CCCC([C@@H]1[C@H]([C@H](C[C@@H]2O)O)O)(C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00255 | 5.29\_343.1533m/z | M+H-H2O | C20H24O6 | 42.3 | 5.32 | -1.83 | Isolariciresinol | 175.0751, 265.0850, 293.1166, 297.1110, 299.1268, 311.1271, 325.1428, 342.1684, 343.0728, 343.1526 | 343.154 | 343.1533 | 5.29 | POS | 202648.3127 | 205491.8947 | 202211.7389 | 0.027111965 | 0.027981057 | 0.026538519 | 0.027210514 | OGFXBIXJCWAUCH-KPHUOKFYSA-N | COC1=C(O)C=C2[C@@H]([C@@H](CO)[C@H](CO)CC2=C1)C1=CC(OC)=C(O)C=C1 | HMDB0301739 |  |  |  |  |  | 异落叶松脂素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DY0274 | HPLC≥95% | level2 |
| compound00256 | 5.26\_196.1098n | M+H, M+Na | C11H16O3 | 59.7 | 92.4 | -0.87 | isololiolide | 107.0858, 133.1011, 135.1167, 161.0959, 179.1064, 197.1168 | 197.1172 | 197.117 | 5.26 | POS | 80929.23072 | 76196.82802 | 77772.84453 | 0.010827381 | 0.010375435 | 0.010207004 | 0.01046994 | XEVQXKKKAVVSMW-CPCISQLKSA-N | C[C@]12C[C@H](CC(C1=CC(=O)O2)(C)C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00257 | 2.47\_246.1450m/z | M+NH4 | C10H16N2O4 | 55.8 | 0 | 0.88 | Longitubanine A |  | 246.1448 | 246.145 | 2.47 | POS | 6059.716309 | 6405.614525 | 6564.485988 | 0.000810719 | 0.000872228 | 0.000861531 | 0.00084816 | NWUDALIQMUEQSX-UHFFFAOYSA-N | CC1=CCOC1NC(=O)CCC(C(=O)O)N |  |  |  |  | 102377982 |  |  |  |  |  |  |  |  | level2 |
| compound00258 | 4.03\_357.1192m/z | M-H2O-H | C16H24O10 | 40.8 | 0 | 0.19 | Loganic acid |  | 357.1191 | 357.1192 | 4.03 | NEG | 7264.515885 | 6959.516385 | 6615.91543 | 0.000971907 | 0.000947651 | 0.000868281 | 0.00092928 | JNNGEAWILNVFFD-CDJYTOATSA-N | [C@@]12([H])[C@@H](C)[C@H](C[C@]1([H])C(C(=O)O)=CO[C@H]2O[C@H]1[C@H](O)[C@H]([C@H](O)[C@@H](CO)O1)O)O |  | 44647 | LMPR01020138 | C01512 | 89640 | 22255-40-9 | 马钱苷酸 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N0513 | HPLC≥98% | level2 |
| compound00259 | 0.81\_145.0496m/z | M+H-H2O | C6H10O5 | 45.3 | 22.7 | 0.12 | Levoglucosan | 84.0813, 86.0602, 87.0444, 99.0443, 144.1015 | 145.0495 | 145.0496 | 0.81 | POS | 332705.3091 | 362275.1067 | 390900.4575 | 0.044512065 | 0.049329636 | 0.05130226 | 0.04838132 | TWNIBLMWSKIRAT-VFUOTHLCSA-N | [H][C@@]12OC[C@@H](O1)[C@@H](O)[C@H](O)[C@H]2O | HMDB0000640 | 4132 |  |  | 2724705 | 498-07-7 | 1,6-脱水-β-D-葡萄糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-W050145 | HPLC≥98% | level2 |
| compound00260 | 4.69\_287.0560m/z | M-H | C15H12O6 | 40.6 | 0 | -0.33 | Isookanin |  | 287.0561 | 287.056 | 4.69 | NEG | 3766.900645 | 4058.001032 | 3984.812791 | 0.000503967 | 0.000552563 | 0.000522972 | 0.000526501 | ZPVNWCMRCGXRJD-ZDUSSCGKSA-N | C1C(OC2=C(C1=O)C=CC(=C2O)O)C3=CC(=C(C=C3)O)O |  | 52585 |  |  | 91196552 |  | 异奥卡宁 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | DY0453-0020 | HPLC≥98% | level2 |
| compound00261 | 10.61\_326.1514n | M+H, M+Na | C20H22O4 | 46.4 | 8.97 | -1.1 | Licarin A | 207.0802, 225.0912, 231.1168, 233.0362, 249.1272, 250.9998, 267.1377, 309.1125, 327.0780, 327.1550 | 349.1411 | 349.1407 | 10.61 | POS | 103632.1932 | 109602.3037 | 115851.1581 | 0.013864771 | 0.014924133 | 0.015204449 | 0.014664451 | ITDOFWOJEDZPCF-WSQXBVHWSA-N | C/C=C/c1cc(OC)c2c(c1)[C@H](C)C(c1ccc(O)c(OC)c1)O2 |  |  |  |  |  | 51020-86-1 | 利卡灵 A | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DL0082 | HPLC≥95% | level2 |
| compound00262 | 6.06\_285.0768m/z | M-H | C16H14O5 | 44.7 | 17.5 | -0.27 | Licochalcone B | 237.0922, 255.0659, 255.1019, 267.1016, 285.0404, 285.0762 | 285.0768 | 285.0768 | 6.06 | NEG | 15825.29468 | 15367.04881 | 16550.77775 | 0.002117239 | 0.002092473 | 0.002172145 | 0.002127285 | DRDRYGIIYOPBBZ-XBXARRHUSA-N | C1(O)=CC=C(C(=O)/C=C/C2C=CC(O)=C(O)C=2OC)C=C1 | HMDB0037320 | 52237 | LMPK12120434 |  | 5318999 | 58749-23-8 | 甘草查尔酮 B | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | HY-N0373 | HPLC≥98% | level2 |
| compound00263 | 4.85\_535.1456m/z | M-H2O-H | C25H30O14 | 43.5 | 16.3 | -0.26 | Ligustrosidic acid | 135.0441, 151.0393, 179.0340, 179.0550, 193.0498, 295.0970, 337.0358, 355.1184, 373.0921, 535.1545 | 535.1457 | 535.1456 | 4.85 | NEG | 111120.3968 | 114481.9694 | 110946.22 | 0.014866605 | 0.015588578 | 0.014560719 | 0.015005301 | DJAAGTPILCOZIR-MSISIIAVSA-N | COC(=O)C1=COC(O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)/C(=C/C(=O)O)C1CC(=O)OCCc1ccc(O)cc1 |  |  |  |  |  | 96382-89-7 | 女贞苷酸 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N6874 | HPLC≥98% | level2 |
| compound00264 | 4.99\_509.1282m/z | M+H | C23H24O13 | 52.7 | 52.9 | -1.5 | limocitrin-3-glucoside | 195.0287, 332.0523, 347.0755, 490.3427, 508.3538 | 509.129 | 509.1282 | 4.99 | POS | 101884.4663 | 101736.652 | 107579.0606 | 0.013630946 | 0.013853096 | 0.014118809 | 0.013867617 | XZGXHUKLGCOGII-YXTZPTRNSA-N | COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(O2)C(=C(C=C3O)O)OC)OC4C(C(C(C(O4)CO)O)O)O)O |  | 51601 |  |  | 44259988 |  |  |  |  |  |  |  |  | level2 |
| compound00265 | 1.68\_201.1240m/z | M-H | C9H18N2O3 | 46.7 | 33 | -2.52 | Leu-ala | 88.0394, 98.024, 113.0599, 133.0132, 157.1337, 201.0401, 201.1242 | 201.1245 | 201.124 | 1.68 | NEG | 4884.821654 | 5293.315557 | 5249.820555 | 0.000653532 | 0.000720771 | 0.000688993 | 0.000687765 | HSQGMTRYSIHDAC-BQBZGAKWSA-N | CC(C)C[C@H](N)C(=O)N[C@@H](C)C(O)=O | HMDB0028922 |  |  |  | 81721 | 7298-84-2 | 亮氨酸-丙氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-128434 | HPLC≥98% | level2 |
| compound00266 | 4.87\_461.1442m/z | M+H-H2O | C23H26O11 | 54.5 | 0 | -0.08 | Lindleyin |  | 461.1442 | 461.1442 | 4.87 | POS | 9736.882046 | 10761.23518 | 8591.483298 | 0.001302681 | 0.001465317 | 0.001127557 | 0.001298518 | BJYRNIFAMMOVGW-OXUVVOBNSA-N | CC(=O)CCc1ccc(O[C@@H]2O[C@H](COC(=O)c3cc(O)c(O)c(O)c3)[C@@H](O)[C@H](O)[C@H]2O)cc1 |  |  |  |  |  | 59282-56-3 | 叶酸 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DL0141 | HPLC≥98% | level2 |
| compound00267 | 1.03\_123.0555m/z | M+H | C6H6N2O | 47.8 | 39.4 | 1.66 | Isonicotinamide | 80.0499, 96.0447, 123.0553 | 123.0553 | 123.0555 | 1.03 | POS | 80090.85508 | 78303.43742 | 82901.54686 | 0.010715216 | 0.010662284 | 0.010880102 | 0.010752534 | VFQXVTODMYMSMJ-UHFFFAOYSA-N | NC(=O)C1=CC=NC=C1 | HMDB0253663 | 65768 |  | C02421 | 15074 | 1453-82-3 | 异烟酰胺 | 生物碱 |  | Alkaloids |  | STC0560100 | HPLC≥98% | level2 |
| compound00268 | 8.06\_285.1119m/z | M+H-H2O | C17H18O5 | 42 | 0 | -0.82 | Isomucronulatol |  | 285.1121 | 285.1119 | 8.06 | POS | 2954.549397 | 3041.718458 | 2891.620605 | 0.000395284 | 0.000414179 | 0.0003795 | 0.000396321 | NQRBAPDEZYMKFL-UHFFFAOYSA-N | C1(O)C=CC2CC(C3C=CC(OC)=C(OC)C=3O)COC=2C=1 | HMDB0033189 | 48278 | LMPK12080033 |  | 602152 | 64474-51-7 | 7,2'-二羟基-3',4'-二甲氧基异黄烷 | 黄酮类 | 其他黄酮类 | Flavonoids | Other flavonoids | HY-N2495 | HPLC≥98% | level2 |
| compound00269 | 4.87\_418.1261n | M+H-H2O, M+H | C21H22O9 | 56.3 | 0.264 | -0.66 | Liquiritin | 273.0752, 281.0653, 285.0755, 297.0757, 323.0903, 339.0859, 365.1016, 383.1115, 400.1438, 401.1192 | 419.1337 | 419.1334 | 4.87 | POS | 539790.1245 | 532389.1005 | 529250.9749 | 0.072217582 | 0.072493417 | 0.069459553 | 0.071390184 | DEMKZLAVQYISIA-ZRWXNEIDSA-N | C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)OC4C(C(C(C(O4)CO)O)O)O |  | 52511 |  | C16989 | 503737 |  | 甘草苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0376 | HPLC≥98% | level2 |
| compound00270 | 10.45\_282.1252n | M+H, M+Na | C18H18O3 | 41.8 | 0 | -1.27 | Isomaglone |  | 305.1148 | 305.1145 | 10.45 | POS | 16314.76368 | 16864.55082 | 17247.65607 | 0.002182724 | 0.002296382 | 0.002263604 | 0.00224757 | LVHHYWFCRQIOJG-UHFFFAOYSA-N | C=CCc1ccc(O)c(Oc2ccc(C(=O)CC)cc2)c1 |  |  |  |  |  | 155709-41-4 | 异木兰花碱 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DY0682 | HPLC≥98% | level2 |
| compound00271 | 5.21\_441.1760m/z | M+FA-H | C20H28O8 | 47.3 | 31.2 | -1.47 | Lobetyolin | 179.0346, 179.0552, 185.0965, 197.0449, 215.1071, 233.1179, 305.1237, 359.0771, 441.0009, 441.1767 | 441.1767 | 441.176 | 5.21 | NEG | 261784.598 | 256838.144 | 261255.0505 | 0.035023706 | 0.034972682 | 0.034287436 | 0.034761275 | MMMUDYVKKPDZHS-UPPVCQNNSA-N | CC=CC#CC#CC(C(C=CCCCO)OC1C(C(C(C(O1)CO)O)O)O)O |  | 830495 |  |  | 53486204 |  | 党参炔苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N0327 | HPLC≥98% | level2 |
| compound00272 | 4.85\_603.2292m/z | M+FA-H | C26H38O13 | 48.8 | 37.8 | -0.36 | Lobetyolinin | 323.0986, 341.1094, 377.1607, 423.0094, 467.1772, 557.2242, 602.3000, 603.0430, 603.2253, 603.2459 | 603.2295 | 603.2292 | 4.85 | NEG | 234236.0032 | 237132.6419 | 237706.6278 | 0.031338028 | 0.032289458 | 0.031196912 | 0.031608133 | GDLSOFWVVAOUJI-MZCJGBHSSA-N | C/C=C/C#CC#CC(O)C(/C=C/CCCO)OC1O[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 142451-48-7 | 党参炔苷宁 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | B50850-5mg | HPLC≥95% | level2 |
| compound00273 | 8.08\_287.1288m/z | M-H2O-H | C17H22O5 | 56.3 | 0 | -0.25 | LIPIFEROLIDE | 241.1233, 243.1385, 243.1736, 246.9992, 257.1187, 257.1540, 266.9828, 286.9864, 287.0179, 287.1274 | 287.1289 | 287.1288 | 8.08 | NEG | 13168.37716 | 12851.21322 | 12860.23036 | 0.001761774 | 0.001749901 | 0.001687793 | 0.001733156 | ODYJJNFWFYUXSS-UHFFFAOYSA-N | CC1=CCCC2(C(O2)C3C(C(C1)OC(=O)C)C(=C)C(=O)O3)C |  |  |  |  | 101241953 |  |  |  |  |  |  |  |  | level2 |
| compound00274 | 6.77\_273.0757m/z | M+H | C15H12O5 | 61.1 | 26 | -0.26 | Naringenin | 147.0439, 153.0181, 273.0755 | 273.0758 | 273.0757 | 6.77 | POS | 13738.07489 | 13942.57795 | 14444.32358 | 0.001837993 | 0.001898508 | 0.001895691 | 0.001877397 | FTVWIRXFELQLPI-UHFFFAOYSA-N | OC1=CC=C(C=C1)C1CC(=O)C2=C(O)C=C(O)C=C2O1 | HMDB0242579 | 3401 |  | C00509 | 932 | 480-41-1 | 柚皮素 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-W011641 | HPLC≥98% | level2 |
| compound00275 | 4.92\_536.1893n | M+NH4, M+Na | C26H32O12 | 56.6 | 0 | -0.06 | (+)-1-hydroxypinoresinol-4'-o-β-d-glucopyra noside |  | 559.1786 | 559.1786 | 4.92 | POS | 48894.52813 | 52700.60247 | 50747.44627 | 0.006541514 | 0.007176042 | 0.006660158 | 0.006792571 | GQLQVPZSTWXDBQ-UHFFFAOYSA-N | COC1=C(C=CC(=C1)C2C3COC(C3(CO2)O)C4=CC(=C(C=C4)O)OC)OC5C(C(C(C(O5)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00276 | 4.26\_742.2321n | M-H, M+FA-H | C33H42O19 | 55.9 | 71.4 | 0.14 | Narirutin 4'-glucoside | 271.061, 433.1136, 579.171, 741.2239 | 787.2302 | 787.2303 | 4.26 | NEG | 1267235.941 | 1301800.742 | 1242293.711 | 0.169541294 | 0.1772613 | 0.163040164 | 0.169947586 | KQUWJUNIYQVHCG-UHFFFAOYSA-N | CC1OC(OCC2OC(OC3=CC4=C(C(=O)CC(O4)C4=CC=C(OC5OC(CO)C(O)C(O)C5O)C=C4)C(O)=C3)C(O)C(O)C2O)C(O)C(O)C1O | HMDB0037584 |  |  |  | 14375140 | 17257-22-6 |  |  |  |  |  |  |  | level2 |
| compound00277 | 5.64\_505.1127m/z | M+Na | C25H22O10 | 52.1 | 5.91 | 4.57 | Silychristin | 281.0440, 295.0594, 297.0750, 307.0595, 313.0700, 323.0544, 341.0650, 486.3186, 504.3315, 505.1117 | 505.1104 | 505.1127 | 5.64 | POS | 244302.282 | 254927.3874 | 254292.2064 | 0.032684778 | 0.034712501 | 0.033373624 | 0.033590301 | BMLIIPOXVWESJG-LMBCONBSSA-N | C1(O)C=C(O)C2C(=O)[C@@H]([C@@H](C3=CC4[C@@H](CO)[C@H](C5=CC=C(O)C(OC)=C5)OC=4C(O)=C3)OC=2C=1)O |  | 67150 | LMPK12140717 | C08717 | 441764 | 33889-69-9 | 水飞蓟亭 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0647 | HPLC≥98% | level2 |
| compound00278 | 6.01\_537.0773m/z | M+K | C25H22O11 | 50.7 | 0 | -4.21 | silymandin |  | 537.0795 | 537.0773 | 6.01 | POS | 9195.115217 | 7392.638528 | 6825.780093 | 0.001230198 | 0.001006628 | 0.000895824 | 0.001044217 | BVNNAIYNHUXFCR-QRVGLHCZSA-N | COC1=C(C=CC(=C1)C2C3COC(=O)C3C(=CC2C(=O)O)C4C(C(=O)C5=C(C=C(C=C5O4)O)O)O)O |  | 984145 |  |  | 23634490 |  |  |  |  |  |  |  |  | level2 |
| compound00279 | 3.95\_352.1505m/z | M+Na | C19H23NO4 | 46.8 | 0 | -4.37 | Sinomenine |  | 352.152 | 352.1505 | 3.95 | POS | 5897.856074 | 5392.660029 | 6574.888115 | 0.000789064 | 0.000734298 | 0.000862896 | 0.00079542 | INYYVPJSBIVGPH-QHRIQVFBSA-N | CN1CCC23CC(=O)C(=CC2C1CC4=C3C(=C(C=C4)OC)O)OC |  | 44251 |  | C09643 | 5459308 | 115-53-7 | 盐酸青藤碱 | 生物碱 |  | Alkaloids |  | HY-15122 | HPLC≥98% | level2 |
| compound00280 | 4.12\_369.0826m/z | M+FA-H | C15H16O8 | 43.4 | 0.0583 | -0.3 | Skimmin | 57.0335, 85.0284, 111.0076, 128.0342, 129.0184, 163.0391, 205.0347, 223.0455, 369.0807 | 369.0827 | 369.0826 | 4.12 | NEG | 70765.62446 | 68976.56162 | 69524.79663 | 0.00946761 | 0.009392278 | 0.00912452 | 0.009328136 | VPAOSFFTKWUGAD-TVKJYDDYSA-N | O=C1OC=2C=C(OC3OC(CO)C(O)C(O)C3O)C=CC2C=C1 |  |  |  |  |  |  | 茵芋苷 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N2263 | HPLC≥98% | level2 |
| compound00281 | 4.61\_295.0459m/z | M+FA-H | C12H10O6 | 60.3 | 92.7 | -0.31 | sodium methylesculetin acetate | 71.0128, 72.9921, 85.0285, 121.0285, 129.0185, 251.056, 295.0461 | 295.046 | 295.0459 | 4.61 | NEG | 24939.51871 | 25277.63407 | 24308.29815 | 0.003336615 | 0.00344196 | 0.003190251 | 0.003322942 | PLEFEZPTTKWFDT-UHFFFAOYSA-N | CC1=CC(OC2=CC(OCC(O)=O)=C(O)C=C12)=O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00282 | 5.66\_868.5039m/z | M+H | C45H73NO15 | 50.5 | 0 | -1.62 | Solamargine |  | 868.5053 | 868.5039 | 5.66 | POS | 20972.55547 | 22654.60594 | 20191.11329 | 0.002805882 | 0.003084792 | 0.002649907 | 0.00284686 | MBWUSSKCCUMJHO-PUQINFEQSA-N | CC1OC(OC2C(CO)OC(O[C@H]3CC[C@@]4(C)C(=CC[C@H]5[C@@H]6C[C@@H]7O[C@]8(CC[C@@H](C)CN8)[C@@H](C)[C@@H]7[C@@]6(C)CC[C@@H]54)C3)C(OC3OC(C)C(O)C(O)C3O)C2O)C(O)C(O)C1O |  |  |  |  |  | 20311-51-7 | 澳洲茄边碱 | 生物碱 |  | Alkaloids |  | HY-N0069 | HPLC≥98% | level2 |
| compound00283 | 4.78\_363.1448m/z | M-H2O-H | C19H26O8 | 53.3 | 58.7 | -0.24 | Solaniol | 301.1076, 301.1443, 315.1239, 319.1180, 319.1922, 327.1239, 345.1332, 362.2267, 363.0988, 363.1464 | 363.1449 | 363.1448 | 4.78 | NEG | 26777.93334 | 29961.05631 | 27050.50125 | 0.003582573 | 0.004079684 | 0.003550141 | 0.003737466 | TVZHDVCTOCZDNE-UHFFFAOYSA-N | CC(=O)OCC12CC(O)C(C)=CC1OC1C(O)C(OC(C)=O)C2(C)C11CO1 | HMDB0255530 |  |  |  | 426719 |  |  |  |  |  |  |  |  | level2 |
| compound00284 | 5.10\_863.2040m/z | 2M-H | C21H20O10 | 43.8 | 0 | -0.05 | Sophoricoside |  | 863.204 | 863.204 | 5.1 | NEG | 41289.08362 | 44686.76716 | 42102.15358 | 0.005523995 | 0.006084829 | 0.005525539 | 0.005711454 | ISQRJFLLIDGZEP-CMWLGVBASA-N | C1(O)C=C(O)C2C(=O)C(C3C=CC(O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)=CC=3)=COC=2C=1 |  |  | LMPK12050168 |  | 5321398 |  | 槐角苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N0423 | HPLC≥98% | level2 |
| compound00285 | 4.86\_709.2328m/z | M+Na | C31H42O17 | 41 | 0 | 1.96 | Specneuzhenide |  | 709.2314 | 709.2328 | 4.86 | POS | 22365.92317 | 21132.79417 | 19224.01237 | 0.002992298 | 0.002877573 | 0.002522983 | 0.002797618 | STKUCSFEBXPTAY-GSUVRYNNSA-N | O=C(OC)C1=COC(OC2OC(CO)C(O)C(O)C2O)C(=CC)C1CC(=O)OCC3OC(OCCC4=CC=C(O)C=C4)C(O)C(O)C3O |  |  |  |  |  |  | 特女贞苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N6075 | HPLC≥98% | level2 |
| compound00286 | 5.64\_702.1581n | M+NH4, M+Na, M+H | C36H30O15 | 65.2 | 84.2 | -0.56 | spicataside | 277.0490, 279.0648, 281.0447, 295.0595, 307.0593, 313.0699, 323.0544, 341.0643, 505.1123, 521.1071 | 725.1477 | 725.1473 | 5.64 | POS | 1128465.257 | 1096831.914 | 1069076.802 | 0.150975405 | 0.149351467 | 0.140306962 | 0.146877945 | KJCNUIUQRDNXFM-YWYCBELZSA-N | C1=CC(=CC=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)C4=C(C=C(C5=C4OC(=CC5=O)C6=CC=C(C=C6)O)O)O[C@H]7[C@@H]([C@H]([C@@H]([C@H](O7)CO)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00287 | 0.66\_168.0767m/z | M+H | C7H9N3O2 | 42.8 | 20.7 | -0.12 | Spinacine | 105.9631, 110.0089, 123.0403, 124.0871, 125.9863, 128.0192, 146.0296, 151.0351, 167.0123, 168.0767 | 168.0768 | 168.0767 | 0.66 | POS | 7009.09296 | 6962.109298 | 6942.720347 | 0.000937734 | 0.000948004 | 0.000911171 | 0.000932303 | YCFJXOFFQLPCHD-UHFFFAOYSA-N | OC(=O)C1CC2=C(CN1)N=CN2 | HMDB0029873 | 86559 |  |  | 363935 | 59981-63-4 | (S)-4,5,6,7-四氢-3H-咪唑并[4,5-c]吡啶-6-羧酸 | 其他 |  | Others |  | HY-W067716 | HPLC≥98% | level2 |
| compound00288 | 0.77\_143.0946n | M+Na, M+K | C7H13NO2 | 40 | 0 | -0.32 | Stachydrine |  | 182.0578 | 182.0577 | 0.77 | POS | 233330.6803 | 236537.0899 | 242022.6267 | 0.031216906 | 0.032208364 | 0.031763349 | 0.03172954 | CMUNUTVVOOHQPW-LURJTMIESA-N | C[N+]1(C)CCC[C@H]1C([O-])=O | HMDB0004827 | 7089 |  | C10172 | 115244 | 471-87-4 | 盐酸水苏碱 | 生物碱 |  | Alkaloids |  | HY-N0298 | HPLC≥98% | level2 |
| compound00289 | 5.09\_431.1923m/z | M+FA-H | C19H30O8 | 55.6 | 0 | 0.06 | staphylionoside a |  | 431.1923 | 431.1923 | 5.09 | NEG | 3002.659262 | 1579.826181 | 4110.175262 | 0.000401721 | 0.000215119 | 0.000539424 | 0.000385421 | ZZMRRHANYHOIDL-RXZGHDNNSA-N | CC1=C(C(C[C@@H](C1=O)O)(C)C)/C=C\[C@H](C)O[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00290 | 8.41\_305.0454m/z | M-H2O-H | C18H12O6 | 60.6 | 70.7 | -0.31 | Sterigmatocystin, reference material | 264.0419, 264.9895, 265.0499, 277.0506, 279.0657, 284.9953, 293.0460, 304.9866, 305.0031, 305.0452 | 305.0455 | 305.0454 | 8.41 | NEG | 34312.42652 | 32085.71426 | 34494.35726 | 0.0045906 | 0.004368991 | 0.004527082 | 0.004495558 | UTSVPXMQSFGQTM-UHFFFAOYSA-N | COC1=CC2=C(C3C=COC3O2)C2=C1C(=O)C1=C(O)C=CC=C1O2 | HMDB0030588 |  |  | C00961 | 5284457 | 10048-13-2 |  |  |  |  |  |  |  | level2 |
| compound00291 | 4.86\_592.3843m/z | M+H | C33H53NO8 | 65.2 | 97.3 | -0.21 | STOCK1N-49993 | 98.0965, 114.0915, 574.3708, 592.3818 | 592.3844 | 592.3843 | 4.86 | POS | 6108158.23 | 6098896.464 | 5825232.37 | 0.817199872 | 0.830463742 | 0.764510703 | 0.804058106 | DHQFYEJMFMYGCV-VRSJZOOHSA-N | C[C@H]1CC[C@H]2[C@@]([C@H]3CC[C@@H]4[C@H]([C@@H]3CN2C1)C[C@H]5[C@H]4CC(=O)[C@@H]6[C@@]5(CC[C@H](C6)O[C@H]7[C@@H]([C@H]([C@@H]([C@H](O7)CO)O)O)O)C)(C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00292 | 4.90\_535.1213m/z | M+K | C23H28O12 | 40.9 | 0 | 0.06 | Swertiaside |  | 535.1212 | 535.1213 | 4.9 | POS | 29212.81616 | 30060.15676 | 29299.3533 | 0.003908332 | 0.004093178 | 0.003845283 | 0.003948931 | BSMWQZICWPFTBG-IFJHVRIVSA-N | C[C@H]1[C@@H](C[C@H]2[C@@H]1[C@@H](OC=C2C(=O)O)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)OC(=O)C4=CC(=CC=C4)O |  |  |  |  |  | 96087-14-8 |  | 萜类 | 单萜类 | Terpenes | Monoterpenes | DS0404 | HPLC≥98% | level2 |
| compound00293 | 4.86\_654.1794n | M+H, M+Na | C29H34O17 | 57.1 | 0 | -0.28 | syringetin-3-rutinoside |  | 655.1869 | 655.1867 | 4.86 | POS | 80214.03834 | 78616.11382 | 73223.236 | 0.010731697 | 0.01070486 | 0.009609908 | 0.010348822 | BWDMLCWSGGUHGK-PPKCOPKDSA-N | CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C(=C5)OC)O)OC)O)O)O)O)O)O |  | 50905 |  |  | 44259493 |  |  |  |  |  |  |  |  | level2 |
| compound00294 | 4.29\_547.1667m/z | M-H | C23H32O15 | 40.8 | 0 | -0.33 | Sibiricose A6 |  | 547.1668 | 547.1667 | 4.29 | NEG | 10612.06874 | 10749.3921 | 9944.897987 | 0.00141977 | 0.001463704 | 0.001305181 | 0.001396218 | WTCVROXOIQEIRC-UHFFFAOYSA-N | COc1cc(C=CC(=O)OC2C(O)C(CO)OC2(CO)OC2OC(CO)C(O)C(O)C2O)cc(OC)c1O |  |  |  |  |  | 241125-75-7 | 西伯利亚远志糖 A6 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DX0037 | HPLC≥98% | level2 |
| compound00295 | 4.28\_518.1635n | M-H, M+FA-H | C22H30O14 | 41 | 0 | -0.09 | Sibiricose A5 |  | 563.1618 | 563.1617 | 4.28 | NEG | 42132.11516 | 41837.65271 | 41913.94423 | 0.005636782 | 0.005696875 | 0.005500838 | 0.005611499 | ZPEADZHVGOCGKH-YQTDNFGYSA-N | COC1=C(C=CC(=C1)C=CC(=O)OC2C(C(OC2(CO)OC3C(C(C(C(O3)CO)O)O)O)CO)O)O |  | 985245 |  |  | 6326020 |  | 西伯利亚远志糖苷 A5 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N2167 | HPLC≥98% | level2 |
| compound00296 | 1.09\_689.2112m/z | M+Na | C24H42O21 | 57.3 | 86.6 | 0.23 | sesamose | 185.0423, 203.0526, 347.0949, 365.1049, 527.1577, 689.2102 | 689.2111 | 689.2112 | 1.09 | POS | 2881937.344 | 2926046.516 | 2801103.722 | 0.385569388 | 0.398428724 | 0.367620318 | 0.38387281 | LAOVEVDFIVNYLQ-QDQSDLQTSA-N | C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCC3C(C(C(O3)(CO)OC4C(C(C(C(O4)CO)O)O)O)O)O)O)O)O)O)O)O)O |  | 66864 |  | C08248 | 441430 | 58985-23-2 |  |  |  |  |  |  |  | level2 |
| compound00297 | 6.08\_519.0932m/z | M-H2O-H | C27H22O12 | 70.1 | 95 | -0.19 | salvianolic acid j | 109.0285, 185.0236, 277.0508, 279.0297, 293.0453, 295.0605, 321.0403, 339.0508, 519.0931 | 519.0933 | 519.0932 | 6.08 | NEG | 779268.6364 | 780602.2081 | 786404.9207 | 0.104256996 | 0.10629166 | 0.103208755 | 0.104585804 | KPKHMGUZUPELJC-OEKAYNNHSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)/C=C/C2=CC3=C(C=C2)O[C@@H]([C@@H](O3)C(=O)O)C4=CC(=C(C=C4)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00298 | 5.64\_494.1210n | M+NH4, M+K, M+Na, M+H, M+H-H2O | C26H22O10 | 63.5 | 77.5 | -0.64 | salvianolic acid n | 181.0492, 223.0751, 233.0593, 251.0697, 269.0805, 279.0644, 297.0753 | 495.1286 | 495.1283 | 5.64 | POS | 1487754.62 | 1501739.05 | 1471136.636 | 0.199044105 | 0.204486146 | 0.193073792 | 0.198868014 | JJRXOJCDDDQFCC-UHFFFAOYSA-N | C1=CC2=CC(=C(C=C2OC3C1C=C(C=C3O)C=CC(=O)OC(CC4=CC(=C(C=C4)O)O)C(=O)O)O)O |  |  |  |  | 49769102 |  |  |  |  |  |  |  |  | level2 |
| compound00299 | 4.92\_418.0897n | M-H, 2M-H | C20H18O10 | 59.8 | 80 | -0.66 | SALVIANOLICACID D | 72.992, 135.0441, 175.0392, 179.0341, 197.0449, 373.0928, 417.0824 | 417.0827 | 417.0824 | 4.92 | NEG | 25098932.03 | 24498710.9 | 24674743.7 | 3.357942488 | 3.335897115 | 3.23834389 | 3.310727831 | KFCMFABBVSIHTB-UHFFFAOYSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C=CC2=C(C(=C(C=C2)O)O)CC(=O)O)O)O |  |  |  |  | 75412558 | 142998-47-8 |  |  |  |  |  |  |  | level2 |
| compound00300 | 5.98\_330.1104n | M+H, M+Na | C18H18O6 | 53.7 | 57.6 | 0.31 | samaderin a | 295.0960, 295.1327, 301.1071, 313.1064, 313.1440, 313.2153, 314.1114, 330.2068, 331.0787, 331.1157 | 331.1176 | 331.1177 | 5.98 | POS | 47457.95613 | 46797.7586 | 45750.73149 | 0.006349317 | 0.006372274 | 0.006004383 | 0.006241991 | BHRGGWSNTHQGED-QNHMRRABSA-N | CC1=CC(=O)C2(C1=CC(=O)C34C2C(C5C(C3C(=O)O5)(OC4)C)O)C |  | 67198 |  | C08781 | 441807 | 64364-76-7 |  |  |  |  |  |  |  | level2 |
| compound00301 | 5.56\_355.0809m/z | M+Na | C20H14NO4+ | 49.1 | 0 | -1.76 | Sanguinarine |  | 355.0815 | 355.0809 | 5.56 | POS | 18521.4472 | 18773.06335 | 18914.11547 | 0.002477952 | 0.002556257 | 0.002482312 | 0.002505507 | INVGWHRKADIJHF-UHFFFAOYSA-N | C[N+]1=C2C3=CC4=C(OCO4)C=C3C=CC2=C2C=CC3=C(OCO3)C2=C1 | HMDB0029367 |  |  | C06162 | 5154 | 2447-54-3 | 血根碱 | 生物碱 |  | Alkaloids |  | HY-N0052A | HPLC≥98% | level2 |
| compound00302 | 5.74\_287.0912m/z | M+H | C16H14O5 | 49 | 12.1 | -0.74 | Sappanchalcone | 153.018, 161.0595, 171.0286, 286.1068, 287.0909 | 287.0914 | 287.0912 | 5.74 | POS | 98092.26317 | 94553.65033 | 96836.0305 | 0.013123593 | 0.012875014 | 0.01270888 | 0.012902496 | JVGNTXGHBHMJDO-QHHAFSJGSA-N | C1(O)=CC=C(C(=O)/C=C/C2C=CC(O)=C(O)C=2)C(OC)=C1 |  | 51918 | LMPK12120114 |  | 5319493 |  | 苏木查尔酮 | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | DS0367 | HPLC≥98% | level2 |
| compound00303 | 5.01\_303.0857m/z | M+H | C16H14O6 | 50.4 | 37.8 | -2 | sappanone b | 153.0181, 177.0544, 179.0336, 303.0858 | 303.0863 | 303.0857 | 5.01 | POS | 1241492.123 | 1209907.789 | 1248916.626 | 0.166097073 | 0.164748583 | 0.163909363 | 0.16491834 | BTLMXNHNFFXBHW-MRXNPFEDSA-N | C1[C@@](C(=O)C2=C(O1)C=C(C=C2)O)(CC3=CC(=C(C=C3)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00304 | 6.24\_209.0811m/z | M+H-H2O | C11H14O5 | 48.4 | 0 | 1.08 | Sarracenin |  | 209.0809 | 209.0811 | 6.24 | POS | 3769.582243 | 3815.74053 | 3895.25851 | 0.000504326 | 0.000519575 | 0.000511219 | 0.000511706 | QGBCGMGBGAHJIT-UHFFFAOYSA-N | CC1C2C3CC(O1)OC2OC=C3C(=O)OC |  | 322275 |  |  | 427877 |  | 脱水莫诺苷元 | 萜类 | 单萜类 | Terpenes | Monoterpenes | DT0054-0005 | HPLC≥98% | level2 |
| compound00305 | 8.95\_359.1483m/z | M+H | C20H22O6 | 42.9 | 7.93 | -1.6 | Scabertopin | 258.2272, 263.1064, 273.1849, 281.1171, 299.1275, 323.2663, 341.1380, 341.2770, 358.2815, 359.1490 | 359.1489 | 359.1483 | 8.95 | POS | 160370.4272 | 158961.5531 | 159723.7831 | 0.021455681 | 0.021645195 | 0.020962347 | 0.021354408 | FTPHYXGWMIZVMP-BAJPKFKCSA-N | C=C1C(=O)O[C@@H]2/C=C(/C)C[C@@H]3C=C(C[C@H](OC(=O)/C(C)=C\C)[C@@H]12)C(=O)O3 |  |  |  |  |  | 185213-52-9 | 地胆草种内酯 | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | HY-N1247 | HPLC≥98% | level2 |
| compound00306 | 5.29\_202.1434m/z | M+NH4 | C10H16O3 | 53.5 | 0 | -1.8 | schizonodiol |  | 202.1438 | 202.1434 | 5.29 | POS | 2451.816111 | 2350.631752 | 2371.70232 | 0.000328024 | 0.000320077 | 0.000311265 | 0.000319789 | GTUFHYHOPUHIKF-UHFFFAOYSA-N | CC1CC(=O)C(=CC1O)C(C)(C)O |  |  |  |  |  | 121693-13-8 |  |  |  |  |  |  |  | level2 |
| compound00307 | 4.44\_667.2608m/z | M-H2O-H | C32H46O16 | 40.4 | 0 | 0.02 | Secoisolariciresinol diglucoside |  | 667.2607 | 667.2608 | 4.44 | NEG | 17094.19952 | 18543.15923 | 15825.78797 | 0.002287003 | 0.002524952 | 0.002076996 | 0.002296317 | SBVBJPHMDABKJV-NNSPVXBOSA-N | COc1cc(C[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)Cc2ccc(O)c(OC)c2)ccc1O |  |  |  |  |  | 257930-74-8 | 亚麻木酚素 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | HY-105008 | HPLC≥98% | level2 |
| compound00308 | 4.39\_316.1546m/z | M+H-H2O | C18H23NO5 | 42.2 | 0 | 0.81 | Seneciphylline |  | 316.1543 | 316.1546 | 4.39 | POS | 3541.75849 | 4216.234225 | 4005.532321 | 0.000473846 | 0.000574109 | 0.000525691 | 0.000524548 | FCEVNJIUIMLVML-DVZMFYIRSA-N | C=C1C/C(=C\C)C(=O)O[C@@H]2CCN3CC=C(COC(=O)[C@@]1(C)O)[C@H]23 |  |  |  |  |  | 480-81-9 | 千里光菲灵碱 | 生物碱 |  | Alkaloids |  | HY-N1282 | HPLC≥98% | level2 |
| compound00309 | 7.97\_207.1020m/z | M-H | C12H16O3 | 55.1 | 21.1 | -3.35 | Senkyunolide G | 73.0284, 103.9193, 109.0283, 161.0446, 179.1071, 186.9987, 206.9883, 207.1019 | 207.1027 | 207.102 | 7.97 | NEG | 9812.738256 | 9967.235998 | 10005.66385 | 0.001312829 | 0.001357201 | 0.001313156 | 0.001327729 | JGIFAEPLZJPSHA-UHFFFAOYSA-N | CCCCC1(C2=C(C=CCC2)C(=O)O1)O |  |  |  |  | 10013283 | 94530-85-5 |  |  |  |  |  |  |  | level2 |
| compound00310 | 5.69\_207.1010m/z | M+H-H2O | C12H16O4 | 40.2 | 0 | -2.61 | Senkyunolide I |  | 207.1015 | 207.101 | 5.69 | POS | 16709.01462 | 17102.06108 | 17022.81157 | 0.00223547 | 0.002328723 | 0.002234095 | 0.002266096 | DQNGMIQSXNGHOA-JXQVETIVSA-N | CCC/C=C1\OC(=O)C2=C1CC[C@H](O)[C@H]2O |  |  |  |  |  | 94596-28-8 | 洋川芎内酯 I | 其他 |  | Others |  | HY-N0745 | HPLC≥98% | level2 |
| compound00311 | 4.28\_275.0565m/z | 2M-H | C7H6O3 | 41.4 | 0 | 1.3 | Sesamol |  | 275.0561 | 275.0565 | 4.28 | NEG | 1171.330849 | 1150.142923 | 999.8953701 | 0.00015671 | 0.000156611 | 0.000131228 | 0.000148183 | LUSZGTFNYDARNI-UHFFFAOYSA-N | OC1=CC2=C(OCO2)C=C1 | HMDB0033812 | 68615 |  | C10832 | 68289 | 533-31-3 | 芝麻酚 | 酚类 | 单酚类 | Phenols | Monophenols | HY-N1417 | HPLC≥98% | level2 |
| compound00312 | 7.52\_372.1206n | M+H-H2O, M+NH4 | C20H20O7 | 51.3 | 38.9 | -0.8 | Sesamolinol | 149.0233, 251.1066, 311.1275, 355.1173, 359.075, 389.1235 | 355.1176 | 355.1173 | 7.52 | POS | 98180.04468 | 97266.58123 | 95884.80979 | 0.013135338 | 0.013244424 | 0.012584041 | 0.012987934 | OJVGWDJIYBTWDS-AFHBHXEDSA-N | COC1=C(C=CC(=C1)OC2C3COC(C3CO2)C4=CC5=C(C=C4)OCO5)O |  | 68653 |  | C10883 | 443019 | 100016-94-2 |  |  |  |  |  |  |  | level2 |
| compound00313 | 8.34\_271.1316m/z | M+Na | C15H20O3 | 51.3 | 0 | 4.42 | SESQUITERPENE LACTONE TS-2 |  | 271.1304 | 271.1316 | 8.34 | POS | 7842.751894 | 8554.101544 | 7814.354363 | 0.001049268 | 0.00116478 | 0.001025566 | 0.001079871 | LIDPBIULZNRIJE-UHFFFAOYSA-N | CC12CCCC(=C)C1(CC3C(C2)OC(=O)C3=C)O |  |  |  |  | 12443309 |  |  |  |  |  |  |  |  | level2 |
| compound00314 | 7.97\_329.1394m/z | M-H2O-H | C19H24O6 | 52.6 | 0 | -0.09 | Tagitinin F | 171.1018, 201.1125, 281.1183, 329.1396 | 329.1394 | 329.1394 | 7.97 | NEG | 427160.4863 | 445038.6511 | 441324.8425 | 0.057149059 | 0.060599236 | 0.057920018 | 0.058556104 | XJUPOHKZSDZNBE-UHFFFAOYSA-N | CC1=CC2C(C(CC3(C=CC1(O3)O)C)OC(=O)C(C)C)C(=C)C(=O)O2 |  |  |  |  | 129316524 |  |  |  |  |  |  |  |  | level2 |
| compound00315 | 4.40\_417.1406m/z | M+FA-H | C17H24O9 | 51.5 | 0 | 0.89 | Tangshenoside II |  | 417.1402 | 417.1406 | 4.4 | NEG | 4914.012883 | 4569.551767 | 4379.488424 | 0.000657437 | 0.000622219 | 0.000574769 | 0.000618142 | MATKEAOBTGAMFZ-UHFFFAOYSA-N | COC1=CC(=CC(=C1OC2C(C(C(C(O2)CO)O)O)O)OC)C(C=C)O |  |  |  |  | 14135593 |  |  |  |  |  |  |  |  | level2 |
| compound00316 | 7.78\_313.1069m/z | M+H | C18H16O5 | 50.9 | 0 | -0.46 | tanshindiol a | 249.0909, 249.1266, 251.1425, 253.1218, 267.1371, 277.0857, 277.1219, 294.2147, 295.0957, 295.1319 | 313.1071 | 313.1069 | 7.78 | POS | 17125.48708 | 17174.28082 | 18091.90599 | 0.002291189 | 0.002338557 | 0.002374404 | 0.002334717 | TZHMQUSSYNZSTA-GOSISDBHSA-N | CC1=COC2=C1C(=O)C(=O)C3=C2C=CC4=C3CCC[C@]4(CO)O |  |  |  |  |  | 97411-46-6 |  |  |  |  |  |  |  | level2 |
| compound00317 | 1.03\_323.0282m/z | M-H | C9H13N2O9P | 56.1 | 91.4 | -1.11 | uridine-5-monophosphate | 78.958, 96.9686, 111.0189, 211.0008, 323.0285 | 323.0286 | 323.0282 | 1.03 | NEG | 34851.09497 | 34831.35024 | 35676.75185 | 0.004662667 | 0.004742854 | 0.004682261 | 0.004695927 | DJJCXFVJDGTHFX-UHFFFAOYSA-N | OC1C(COP(O)(O)=O)OC(C1O)N1C=CC(O)=NC1=O | HMDB0247871 |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00318 | 5.07\_243.0295m/z | M-H | C13H8O5 | 40.8 | 0 | -1.7 | Urolithin C |  | 243.0299 | 243.0295 | 5.07 | NEG | 3238.615861 | 3035.339932 | 3819.907808 | 0.000433289 | 0.000413311 | 0.000501329 | 0.00044931 | HHXMEXZVPJFAIJ-UHFFFAOYSA-N | OC1=CC2=C(C=C1)C1=C(C=C(O)C(O)=C1)C(=O)O2 | HMDB0029218 | 86097 |  |  | 60198001 |  | 尿石素C | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-135897 | HPLC≥98% | level2 |
| compound00319 | 4.23\_771.1985m/z | M+FA-H | C32H38O19 | 40 | 0 | -0.65 | Vaccarin |  | 771.199 | 771.1985 | 4.23 | NEG | 35995.6932 | 24217.28429 | 32684.91768 | 0.004815801 | 0.003297576 | 0.004289609 | 0.004134329 | GYIKGLVKALOGDP-HLEFUGOVSA-N | C1(C2C=CC(O[C@H]3[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O3)=CC=2)=CC(=O)C2C(O)=C([C@H]3[C@H](O[C@H]4[C@H](O)[C@@H](O)[C@@H](O)CO4)[C@@H](O)[C@H](O)[C@@H](CO)O3)C(O)=CC=2O1 |  |  | LMPK12110321 |  | 71307582 |  | 王不留行黄酮苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N1419 | HPLC≥98% | level2 |
| compound00320 | 0.92\_136.0754m/z | M+H-H2O | C8H11NO2 | 41.2 | 0.211 | -2.15 | Vanillylamine | 136.0616 | 136.0757 | 136.0754 | 0.92 | POS | 26645.70967 | 28896.40894 | 27040.88494 | 0.003564883 | 0.003934715 | 0.003548879 | 0.003682826 | WRPWWVNUCXQDQV-UHFFFAOYSA-N | COC1=CC(CN)=CC=C1O | HMDB0012309 | 62928 |  | C16666 | 70966 | 1196-92-5 | 4-(氨基甲基)-2-甲氧基苯酚 | 生物碱 |  | Alkaloids |  | HY-W097899 | HPLC≥98% | level2 |
| compound00321 | 5.93\_331.1179m/z | 2M-H | C9H10O3 | 43.1 | 0 | -2.45 | Veratraldehyde |  | 331.1187 | 331.1179 | 5.93 | NEG | 70748.91393 | 70302.59357 | 71424.6553 | 0.009465374 | 0.009572839 | 0.00937386 | 0.009470691 | WJUFSDZVCOTFON-UHFFFAOYSA-N | COC1=C(OC)C=C(C=O)C=C1 | HMDB0032138 | 44710 |  | C02201 | 8419 | 120-14-9 | 藜芦醛 | 其他 |  | Others |  | HY-N1096 | HPLC≥98% | level2 |
| compound00322 | 5.77\_410.3055m/z | M+H | C27H39NO2 | 40.9 | 0.119 | 0.35 | Veratramine | 410.3045 | 410.3054 | 410.3055 | 5.77 | POS | 205693.7816 | 200533.1849 | 202453.0007 | 0.027519413 | 0.027305848 | 0.026570182 | 0.027131815 | MALFODICFSIXPO-KFKQDBFTSA-N | CC1CC(C(NC1)C(C)C2=C(C3=C(C=C2)C4CC=C5CC(CCC5(C4C3)C)O)C)O |  | 68612 |  | C10829 | 6070 | 60-70-8 | 黎芦碱 | 生物碱 |  | Alkaloids |  | HY-N0837 | HPLC≥98% | level2 |
| compound00323 | 5.06\_572.3577m/z | M+H | C33H49NO7 | 46.2 | 5.94 | -0.9 | Veratrosine | 98.0967, 572.3574 | 572.3582 | 572.3577 | 5.06 | POS | 1212292.918 | 1231875.932 | 1218514.949 | 0.162190562 | 0.167739902 | 0.159919409 | 0.163283291 | WXQHVBNTINGJJR-NIFRNHPISA-N | OCC1OC(OC2CC3=CCC4C5=CC=C(C(=C5CC4C3(C)CC2)C)C(C)C6NCC(C)CC6O)C(O)C(O)C1O |  |  |  |  | 23616879 | 475-00-3 | 藜芦托素 | 生物碱 |  | Alkaloids |  | HY-N6243 | HPLC≥98% | level2 |
| compound00324 | 4.86\_669.2035m/z | M+FA-H | C29H36O15 | 42.7 | 0 | -0.19 | Verbascoside |  | 669.2036 | 669.2035 | 4.86 | NEG | 16943.13062 | 10733.74909 | 16801.75132 | 0.002266792 | 0.001461574 | 0.002205083 | 0.001977816 | FBSKJMQYURKNSU-UHFFFAOYSA-N | CC1OC(OC2C(O)C(OCCC3=CC=C(O)C(O)=C3)OC(CO)C2OC(=O)C=CC2=CC=C(O)C(O)=C2)C(O)C(O)C1O | HMDB0259785 |  |  |  | 354009 |  | 毛蕊花糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N0021 | HPLC≥98% | level2 |
| compound00325 | 4.58\_545.1306m/z | M-H2O-H | C26H28O14 | 49.3 | 0 | 0.94 | Vicenin 3 |  | 545.1301 | 545.1306 | 4.58 | NEG | 6631.056944 | 7120.878173 | 7170.675149 | 0.000887158 | 0.000969623 | 0.000941088 | 0.000932623 | MMDUKUSNQNWVET-MCIQUCDDSA-N | C1(O)=C([C@H]2[C@H](O)[C@@H](O)[C@H](O)CO2)C2OC(C3C=CC(O)=CC=3)=CC(=O)C=2C(O)=C1[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 |  | 48673 | LMPK12110242 | C10181 | 185958 |  | 维采宁-3 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4090 | HPLC≥98% | level2 |
| compound00326 | 5.01\_464.1312n | M+H-H2O, M+H | C22H24O11 | 58.2 | 78.5 | -1.43 | Viscumiside A | 98.0967, 114.0915, 219.0285, 315.0862, 327.0864, 369.0961, 428.3154, 446.323, 447.1279 | 465.1391 | 465.1385 | 5.01 | POS | 992471.3609 | 955239.2792 | 1017068.21 | 0.132781018 | 0.130071332 | 0.13348129 | 0.132111213 | KZQCCKUDYVSOLC-UHFFFAOYSA-N | C1C(OC2OC(CO)C(O)C(O)C2O)=CC2OC(C3C=C(OC)C(O)=CC=3)CC(=O)C=2C=1O |  | 52917 | LMPK12140435 |  | 14035424 |  |  |  |  |  |  |  |  | level2 |
| compound00327 | 4.36\_581.1512m/z | M+H | C26H28O15 | 52.4 | 0 | 1.9 | Vitexin xyloside |  | 581.1501 | 581.1512 | 4.36 | POS | 10751.90266 | 11879.36995 | 10979.19648 | 0.001438478 | 0.001617569 | 0.001440923 | 0.00149899 | JPMTYZSEANLMKJ-UHFFFAOYSA-N | OC1OC(OCC2OC(C(O)C(O)C2O)C2=C(O)C=C(O)C3=C2OC(=CC3=O)C2=CC=C(O)C=C2)C(O)C(O)C1O | HMDB0302559 |  |  |  | 5364006 |  |  |  |  |  |  |  |  | level2 |
| compound00328 | 4.61\_639.1578m/z | M+FA-H | C27H30O15 | 50.4 | 1.21 | 1.98 | Vitexin-4''-O-glucoside | 135.0442, 315.0148, 330.0386, 639.1556 | 639.1566 | 639.1578 | 4.61 | NEG | 71407.09216 | 76232.12705 | 69815.45139 | 0.009553431 | 0.010380241 | 0.009162666 | 0.009698779 | NDSUKTASTPEKBX-LXXMDOISSA-N | C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C(=C(C=C3O)O)C4C(C(C(C(O4)CO)OC5C(C(C(C(O5)CO)O)O)O)O)O)O |  | 843933 |  |  | 56776173 |  | 牡荆素-4''-O-葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N5073 | HPLC≥98% | level2 |
| compound00329 | 9.29\_197.0596m/z | M+H | C13H8O2 | 43.1 | 0 | -0.42 | Xanthone |  | 197.0597 | 197.0596 | 9.29 | POS | 950.5619963 | 1053.211187 | 1150.776808 | 0.000127174 | 0.000143412 | 0.000151029 | 0.000140538 | JNELGWHKGNBSMD-UHFFFAOYSA-N | O=C1C2=CC=CC=C2OC2=CC=CC=C12 | HMDB0259922 | 43571 |  |  | 7020 | 90-47-1 | 占吨酮 | 苯丙素类 | 氧杂蒽酮 | Phenylpropanoids | Xanthones | HY-N0126 | HPLC≥98% | level2 |
| compound00330 | 5.60\_409.1834m/z | M+Na | C19H30O8 | 54.6 | 0 | 0.29 | XTODSGVDHGMKSN-UHFFFAOYSA-N |  | 409.1833 | 409.1834 | 5.6 | POS | 4000.2148 | 3911.089543 | 2946.591546 | 0.000535182 | 0.000532558 | 0.000386714 | 0.000484818 | XTODSGVDHGMKSN-UHFFFAOYSA-N | CC(=O)C=C=C1C(C)(C)CC(O)CC1(C)OC1OC(CO)C(O)C(O)C1O | HMDB0030370 |  |  |  | 14312560 | 120330-44-1 |  |  |  |  |  |  |  | level2 |
| compound00331 | 4.75\_667.2608m/z | M-H2O-H | C32H46O16 | 56.8 | 82.3 | 0.01 | yadanzioside H | 607.2394, 667.2601 | 667.2607 | 667.2608 | 4.75 | NEG | 272344.2839 | 263045.4938 | 271646.3161 | 0.036436468 | 0.035817913 | 0.035651199 | 0.035968527 | DYJYHQPMHVMJIS-DXMXMRDXSA-N | CC1=C[C@@H]([C@H]([C@]2([C@H]1C[C@@H]3[C@]45[C@@H]2[C@H]([C@@H]([C@]([C@@H]4[C@H](C(=O)O3)OC(=O)CC(C)C)(OC5)C(=O)OC)O)O)C)O)O[C@H]6[C@@H]([C@H]([C@@H]([C@H](O6)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00332 | 4.69\_443.3037n | M+H-H2O, M+H | C27H41NO4 | 44.3 | 6.19 | 0.32 | Yibeissine | 408.289, 426.2995 | 444.3108 | 444.311 | 4.69 | POS | 534953.9932 | 534069.0005 | 532517.2721 | 0.071570565 | 0.072722163 | 0.069888226 | 0.071393651 | NURPXYQPDMVKOY-RUKZUWONSA-N | C[C@H]1C[C@@H]2[C@H]([C@H]([C@]3(O2)CC[C@H]4[C@@H]5CC(=O)[C@H]6C[C@H](CC[C@@]6([C@H]5[C@H](C4=C3C)O)C)O)C)NC1 |  |  |  |  |  | 143502-51-6 | 伊贝辛 | 生物碱 |  | Alkaloids |  | DY0512 | HPLC≥98% | level2 |
| compound00333 | 9.17\_301.1444m/z | M-H2O-H | C18H24O5 | 41.7 | 0 | -0.41 | Zearalanone |  | 301.1445 | 301.1444 | 9.17 | NEG | 12268.24526 | 13121.38639 | 13122.4976 | 0.001641347 | 0.00178669 | 0.001722213 | 0.00171675 | APJDQUGPCJRQRJ-UHFFFAOYSA-N | CC1CCCC(=O)CCCCCC2=CC(O)=CC(O)=C2C(=O)O1 | HMDB0259993 |  |  |  | 4371409 |  | 玉米赤霉酮 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N6678 | HPLC≥98% | level2 |
| compound00334 | 5.20\_145.0283m/z | M+H-H2O | C9H6O3 | 42.4 | 0 | -0.59 | Umbelliferone |  | 145.0284 | 145.0283 | 5.2 | POS | 6356.848766 | 6943.770832 | 6805.454098 | 0.000850472 | 0.000945507 | 0.000893156 | 0.000896378 | ORHBXUUXSCNDEV-UHFFFAOYSA-N | OC1=CC2=C(C=C1)C=CC(=O)O2 | HMDB0029865 | 44642 |  | C09315 | 5281426 | 93-35-6 | 7-羟基香豆素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0573 | HPLC≥98% | level2 |
| compound00335 | 9.43\_358.1643m/z | M+NH4 | C20H20O5 | 51.2 | 0 | -1.76 | ugonin e |  | 358.1649 | 358.1643 | 9.43 | POS | 22407.22608 | 22237.08034 | 17711.03338 | 0.002997824 | 0.003027939 | 0.002324418 | 0.002783394 | QEGKZPOCQRZIAS-INIZCTEOSA-N | C1(O)C(C(C)(C)C=C)=C2O[C@H](C3C=CC(O)=CC=3)CC(=O)C2=C(O)C=1 |  | 52781 | LMPK12140297 |  | 12114693 |  |  |  |  |  |  |  |  | level2 |
| compound00336 | 1.16\_341.1089m/z | M-H | C12H22O11 | 43.5 | 30.7 | 0.03 | Turanose | 101.0233, 111.0076, 113.0232, 119.0338, 143.0340, 161.0446, 179.0553, 191.0189, 341.0837, 341.1085 | 341.1089 | 341.1089 | 1.16 | NEG | 160540.581 | 159891.6528 | 163408.6633 | 0.021478445 | 0.021771844 | 0.021445955 | 0.021565415 | RULSWEULPANCDV-PIXUTMIVSA-N | OC[C@@H](O)[C@@H](O)[C@H](O[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)C(=O)CO | HMDB0011740 | 62463 |  | C19636 | 5460935 | 547-25-1 | 松二糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-113334 | HPLC≥98% | level2 |
| compound00337 | 4.56\_186.1129m/z | M+FA-H | C8H15NO | 40.2 | 0 | -4.69 | Tropine |  | 186.1138 | 186.1129 | 4.56 | NEG | 1794.527825 | 2049.668731 | 1826.359086 | 0.000240087 | 0.000279096 | 0.000239694 | 0.000252959 | CYHOMWAPJJPNMW-DHBOJHSNSA-N | CN1[C@H]2CC[C@@H]1CC(O)C2 |  |  |  |  |  | 120-29-6 | 托品醇 | 生物碱 |  | Alkaloids |  | HY-N7061 | HPLC≥98% | level2 |
| compound00338 | 8.12\_193.0863m/z | M+FA-H | C10H12O | 56.2 | 0 | -4.63 | Tarragon | 192.9889, 193.0862 | 193.0872 | 193.0863 | 8.12 | NEG | 33276.65053 | 32192.98618 | 33658.87938 | 0.004452025 | 0.004383598 | 0.004417433 | 0.004417685 | ZFMSMUAANRJZFM-UHFFFAOYSA-N | COC1=CC=C(CC=C)C=C1 | HMDB0034121 | 68335 |  | C10452 | 8815 | 140-67-0 |  |  |  |  |  |  |  | level2 |
| compound00339 | 8.71\_593.2580m/z | M+H-H2O | C30H42O13 | 56.5 | 0 | -1.98 | taxuspine v |  | 593.2592 | 593.258 | 8.71 | POS | 43028.83785 | 41240.76499 | 44135.96236 | 0.005756753 | 0.0056156 | 0.005792458 | 0.005721604 | KLIDFAOXPCGARX-UHFFFAOYSA-N | CC1=C2C(C(C3(C(CC(C4(C3C(C(C2(C)C)(CC1OC(=O)C)O)OC(=O)C)CO4)O)OC(=O)C)C)OC(=O)C)OC(=O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00340 | 4.84\_617.1477m/z | M+Na | C27H30O15 | 55.9 | 0 | 0.05 | Tectorigenin 7-O-Xylosyl Glucoside |  | 617.1477 | 617.1477 | 4.84 | POS | 51636.72113 | 55115.30112 | 47672.27283 | 0.006908387 | 0.007504843 | 0.006256568 | 0.006889933 | MCYJIRFKDCXYCX-YUPZTAPUSA-N | COc1c(O[C@@H]2O[C@H](CO[C@@H]3OC[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)cc2occ(-c3ccc(O)cc3)c(=O)c2c1O |  |  |  |  |  | 231288-19-0 | 鸢尾黄素-7-O-木糖基葡萄糖苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N4172 | HPLC≥98% | level2 |
| compound00341 | 8.07\_365.1345m/z | M+Na | C20H22O5 | 56.6 | 0 | -4.11 | Tetrahydrodemethoxycurcumin |  | 365.136 | 365.1345 | 8.07 | POS | 8048.295599 | 9776.181413 | 11109.40801 | 0.001076767 | 0.001331186 | 0.001458012 | 0.001288655 | HJFYFYWETUVIHT-UHFFFAOYSA-N | COC1=C(C=CC(=C1)CCC(=O)CC(=O)CCC2=CC=C(C=C2)O)O |  | 431455 |  |  | 9906039 |  |  |  |  |  |  |  |  | level2 |
| compound00342 | 9.39\_342.1098n | M+H-H2O, M+H | C19H18O6 | 43 | 0 | -1.62 | Tetramethylkaempferol |  | 343.1176 | 343.1171 | 9.39 | POS | 14730.00989 | 13908.76371 | 14535.8461 | 0.001970702 | 0.001893904 | 0.001907702 | 0.001924103 | YZWIIEJLESXODL-UHFFFAOYSA-N | C12C(=O)C(OC)=C(C3C=CC(OC)=CC=3)OC=1C=C(OC)C=C2OC |  | 51113 | LMPK12112699 |  | 631095 |  | 四甲基山奈酚 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DS0446 | HPLC≥98% | level2 |
| compound00343 | 5.45\_359.1949m/z | M+NH4 | C20H23NO4 | 51.7 | 0 | -4.82 | Thaliporphine |  | 359.1966 | 359.1949 | 5.45 | POS | 4403.388615 | 4838.967966 | 4843.457246 | 0.000589122 | 0.000658904 | 0.000635661 | 0.000627896 | SAERKXUSZPTMCQ-UHFFFAOYSA-N | COC1=CC2=C3C(CC4=CC(OC)=C(OC)C=C4C3=C1O)N(C)CC2 | HMDB0242264 |  |  |  | 100020 |  |  |  |  |  |  |  |  | level2 |
| compound00344 | 6.24\_291.1223m/z | M+H-H2O | C16H20O6 | 44.7 | 0 | -1.39 | Toddalolactone |  | 291.1227 | 291.1223 | 6.24 | POS | 3284.572605 | 3306.390932 | 3706.029569 | 0.000439437 | 0.000450219 | 0.000486384 | 0.00045868 | GLWPLQBQHWYKRK-UHFFFAOYSA-N | COc1cc2oc(=O)ccc2c(OC)c1CC(O)C(C)(C)O |  |  |  |  |  | 483-90-9 | 飞龙掌血内酯 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0518 | HPLC≥98% | level2 |
| compound00345 | 5.85\_399.1055m/z | M+H-H2O | C21H20O9 | 47 | 0 | -4.55 | Toringin |  | 399.1074 | 399.1055 | 5.85 | POS | 6655.100701 | 6419.585913 | 6375.082884 | 0.000890374 | 0.000874131 | 0.000836674 | 0.00086706 | IRHAYEHCEVRWSB-QNDFHXLGSA-N | C1(O)=CC2OC(C3C=CC=CC=3)=CC(=O)C=2C(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=C1 |  | 48579 | LMPK12110146 |  | 101686456 |  | 三叶海棠素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4192 | HPLC≥98% | level2 |
| compound00346 | 10.59\_525.3569m/z | M+Na | C31H50O5 | 57.7 | 0 | 3.77 | Tormentic acid, methyl ester |  | 525.355 | 525.3569 | 10.59 | POS | 16763.56988 | 16624.98609 | 17947.45945 | 0.002242769 | 0.002263762 | 0.002355447 | 0.002287326 | RQWXHGLRDYGNGZ-UHFFFAOYSA-N | CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C(C5(C)C)O)O)C)C)C2C1(C)O)C)C(=O)OC |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00347 | 5.17\_538.1107n | M+NH4, M+Na, M+K | C27H22O12 | 61.8 | 81.8 | -0.75 | salvianolic acid H | 139.0388, 181.0492, 233.0593, 251.0698, 253.0493, 279.0643, 295.0595, 297.0751, 323.0544, 341.065 | 556.145 | 556.1445 | 5.17 | POS | 6721579.948 | 6520570.155 | 6228090.241 | 0.899268497 | 0.887881459 | 0.817382268 | 0.868177408 | HFTLCJIFEZUOCR-JKXXRSRDSA-N | OC(=O)C(CC1=CC(O)=C(O)C=C1)OC(=O)\C=C\C1=CC(O\C(=C/C2=CC(O)=C(O)C=C2)C(O)=O)=C(O)C=C1 | HMDB0039523 | 94090 |  |  | 21582559 |  |  |  |  |  |  |  |  | level2 |
| compound00348 | 6.01\_312.0636n | M+H-H2O, M+H | C17H12O6 | 57.7 | 65.5 | 0.72 | TOURNEFOLIC ACID A | 239.0703, 267.0653, 295.0599 | 295.0601 | 295.0603 | 6.01 | POS | 300773.3823 | 297115.2162 | 304053.055 | 0.040239948 | 0.040457059 | 0.039904299 | 0.040200435 | KSKIGSUQYGWNAK-ZZXKWVIFSA-N | C1=CC(=C(C=C1C2=CC3=C(C=CC(=C3O2)O)/C=C/C(=O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00349 | 3.92\_356.1106n | M-H, M+FA-H | C16H20O9 | 51.2 | 40.9 | -0.4 | Trans-ferulic acid-4-beta-glucoside | 85.0284, 134.0362, 147.029, 149.0596, 178.0264, 191.019, 193.05, 209.0296, 355.0641 | 401.109 | 401.1088 | 3.92 | NEG | 69836.93087 | 71304.40948 | 69646.46576 | 0.009343362 | 0.009709253 | 0.009140488 | 0.009397701 | IEMIRSXOYFWPFD-BJGSYIFTSA-N | COC1=CC(\C=C\C(O)=O)=CC=C1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O | HMDB0301717 |  |  |  |  | 537-98-4 | (E)-阿魏酸-4-O-葡萄糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | Y69061-50mg | HPLC≥97% | level2 |
| compound00350 | 5.82\_311.0561m/z | M-H2O-H | C17H14O7 | 42.1 | 0 | -0.02 | Tricin |  | 311.0561 | 311.0561 | 5.82 | NEG | 22561.13586 | 22905.44328 | 22862.83156 | 0.003018415 | 0.003118948 | 0.003000546 | 0.00304597 | HRGUSFBJBOKSML-UHFFFAOYSA-N | C12C(=O)C=C(C3C=C(OC)C(O)=C(OC)C=3)OC=1C=C(O)C=C2O | HMDB0124861 | 49301 | LMPK12110873 | C10193 | 5281702 |  | 苜蓿素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N1127 | HPLC≥98% | level2 |
| compound00351 | 9.59\_263.1066m/z | M+H-H2O | C18H16O3 | 53.4 | 0 | -0.34 | Trijuganone B |  | 263.1067 | 263.1066 | 9.59 | POS | 1712.482692 | 1814.642567 | 1925.49267 | 0.00022911 | 0.000247093 | 0.000252704 | 0.000242969 | AZIUYJPOBCMPON-UHFFFAOYSA-N | O=C1C(=O)C2=C(OCC2C)C=3C=CC=4C(=CCCC4C13)C |  |  |  |  |  | 126979-84-8 |  |  |  |  |  |  |  | level2 |
| compound00352 | 10.69\_271.1327m/z | M+H | C17H18O3 | 43.4 | 9.37 | -0.7 | Trimethoxyresveratrol | 215.0696, 253.1219, 270.3145, 271.0608, 271.1327 | 271.1329 | 271.1327 | 10.69 | POS | 18357.79339 | 19353.0126 | 19796.03468 | 0.002456057 | 0.002635227 | 0.002598056 | 0.002563113 | GDHNBPHYVRHYCC-SNAWJCMRSA-N | O(C1=CC=C(C=C1)C=CC=2C=C(OC)C=C(OC)C2)C |  |  |  |  |  |  | 白藜芦醇三甲醚 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N1408 | HPLC≥98% | level2 |
| compound00353 | 10.59\_327.0776m/z | M+H | C18H15O4P | 46.3 | 18.8 | -1.47 | Triphenyl phosphate | 98.9845, 153.0695, 174.992, 207.0804, 225.0907, 231.1161, 233.036, 249.1273, 267.1378, 327.0782 | 327.0781 | 327.0776 | 10.59 | POS | 21884.27139 | 20993.03819 | 20400.05577 | 0.002927859 | 0.002858543 | 0.002677329 | 0.002821243 | XZZNDPSIHUTMOC-UHFFFAOYSA-N | O=P(OC1=CC=CC=C1)(OC1=CC=CC=C1)OC1=CC=CC=C1 | HMDB0259262 | 69897 |  | C14235 | 8289 | 115-86-6 | 磷酸三苯酯 | 其他 |  | Others |  | STC0470100 | HPLC≥98% | level2 |
| compound00354 | 9.15\_301.2157m/z | M+H-H2O | C20H30O3 | 44.4 | 0 | -1.65 | Tripterifordin |  | 301.2162 | 301.2157 | 9.15 | POS | 7609.609596 | 8098.111756 | 7461.822928 | 0.001018076 | 0.001102689 | 0.000979299 | 0.001033355 | KLMZPLYXGZZBCX-XGRAKDAMSA-N | C[C@@]1(O)C[C@@]23CC[C@@H]4[C@@]5(C)CCC[C@@]4(COC5=O)[C@@H]2CC[C@H]1C3 |  |  |  |  |  | 139122-81-9 | 雷公藤福定 | 萜类 | 二萜类 | Terpenes | Diterpenes | B31362-5mg | HPLC≥98% | level2 |
| compound00355 | 6.75\_383.1472m/z | M+Na | C20H24O6 | 44.1 | 0 | 1.96 | Triptolide |  | 383.1465 | 383.1472 | 6.75 | POS | 5588.665553 | 5305.896267 | 4797.540008 | 0.000747698 | 0.000722484 | 0.000629635 | 0.000699939 | DFBIRQPKNDILPW-CIVMWXNOSA-N | CC(C)C12C(O1)C3C4(O3)C5(CCC6=C(C5CC7C4(C2O)O7)COC6=O)C |  | 67513 |  | C09204 | 107985 | 38748-32-2 | 雷公藤甲素 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-32735 | HPLC≥98% | level2 |
| compound00356 | 10.76\_301.2154m/z | M+H | C20H28O2 | 45.3 | 14.5 | -2.56 | Triptonoterpene methyl ether | 300.1578, 301.076, 301.1787, 301.2157 | 301.2162 | 301.2154 | 10.76 | POS | 90788.0896 | 94073.15405 | 95226.68913 | 0.012146381 | 0.012809587 | 0.012497668 | 0.012484545 | WENIWZBFJBCNNG-OXJNMPFZSA-N | CC(C)c1ccc2c(c1O)CC[C@H]1C(C)(C)C(=O)CC[C@]21C |  |  |  |  |  | 99694-87-8 | 雷酚萜甲醚 | 萜类 | 二萜类 | Terpenes | Diterpenes | / | HPLC≥98% | level2 |
| compound00357 | 5.46\_179.0701m/z | M+H | C10H10O3 | 67.8 | 88.7 | -0.9 | trans-Ferulaldehyde | 55.0185, 105.07, 119.0492, 133.0646, 147.0438, 161.0595, 179.034, 179.07 | 179.0703 | 179.0701 | 5.46 | POS | 21011.14393 | 22372.87196 | 22678.78611 | 0.002811044 | 0.00304643 | 0.002976392 | 0.002944622 | DKZBBWMURDFHNE-UHFFFAOYSA-N | O=CC=CC1=CC=C(O)C(OC)=C1 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00358 | 4.39\_378.0950n | M-H, 2M-H | C18H18O9 | 62 | 93.5 | -0.29 | salvianic acid c | 72.992, 119.0492, 135.0441, 137.0234, 161.0235, 179.0342, 197.0448, 359.0771, 377.0876 | 377.0878 | 377.0877 | 4.39 | NEG | 329992.2596 | 332952.8564 | 330680.8479 | 0.044149091 | 0.045336935 | 0.043398964 | 0.044294997 | VTSYCUCOACFUEN-HZPDHXFCSA-N | C1=CC(=C(C=C1C[C@H](C(=O)O[C@H](CC2=CC(=C(C=C2)O)O)C(=O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00359 | 3.99\_208.1335m/z | M+H | C12H17NO2 | 45.1 | 0 | 1.49 | Salsolidine |  | 208.1332 | 208.1335 | 3.99 | POS | 1152.392427 | 1008.560032 | 958.1247308 | 0.000154177 | 0.000137332 | 0.000125745 | 0.000139085 | HMYJLVDKPJHJCF-UHFFFAOYSA-N | CC1C2=CC(=C(C=C2CCN1)OC)OC |  | 44388 |  |  | 10302 | 493-48-1 | 异喹啉,1,2,3,4-四氢-6,7-二甲氧基-1-甲基-,盐酸盐 | 生物碱 |  | Alkaloids |  | HY-22385 | HPLC≥98% | level2 |
| compound00360 | 4.31\_107.0495m/z | M+H-H2O | C7H8O2 | 42.2 | 0 | 2.54 | Salicyl alcohol |  | 107.0492 | 107.0495 | 4.31 | POS | 3061.694992 | 3087.430291 | 2940.545152 | 0.000409619 | 0.000420404 | 0.000385921 | 0.000405314 | CQRYARSYNCAZFO-UHFFFAOYSA-N | OCC1=C(O)C=CC=C1 | HMDB0059709 | 63123 |  | C02323 | 5146 | 90-01-7 | 水杨醇 | 酚类 | 单酚类 | Phenols | Monophenols | HY-B1419 | HPLC≥98% | level2 |
| compound00361 | 3.62\_299.0771m/z | M-H2O-H | C13H18O9 | 56 | 17.8 | -0.5 | opuntioside | 102.055, 137.0234, 232.1187, 254.1006, 299.0771 | 299.0772 | 299.0771 | 3.62 | NEG | 43235.62003 | 43746.06486 | 43970.45939 | 0.005784418 | 0.005956737 | 0.005770737 | 0.005837298 | OQVZJGGNKYGQLT-KABOQKQYSA-N | COC1=CC(=O)OC(=C1)CO[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00362 | 3.59\_448.1573n | M-H, M+FA-H | C19H28O12 | 41.4 | 0.602 | -1.72 | Orcinol gentiobioside | 152.0105, 153.0548, 447.1127 | 447.1508 | 447.15 | 3.59 | NEG | 28869.48472 | 27815.3504 | 26842.84771 | 0.003862398 | 0.003787511 | 0.003522889 | 0.003724266 | XZPNBJLXZMBECP-SKYGPZSASA-N | Cc1cc(O)cc(O[C@@H]2O[C@H](CO[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)c1 |  |  |  |  |  | 164991-86-0 | 苔黑酚龙胆二糖苷 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | DT0034-0020 | HPLC≥99% | level2 |
| compound00363 | 6.08\_459.0935m/z | M-H | C22H20O11 | 51.8 | 0 | 0.37 | Oroxylin A-7-O-glucuronide |  | 459.0933 | 459.0935 | 6.08 | NEG | 12152.08762 | 12247.18094 | 13010.95213 | 0.001625807 | 0.001667652 | 0.001707573 | 0.001667011 | QXIPXNZUEQYPLZ-QSUZLTIMSA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](C(=O)O)O2)=CC2OC(C3C=CC=CC=3)=CC(=O)C=2C(O)=C1OC |  |  | LMPK12111086 |  | 14655552 |  | 千层纸素A苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N2481 | HPLC≥98% | level2 |
| compound00364 | 4.78\_161.0598m/z | M+H-H2O | C10H10O3 | 46.9 | 33.2 | 0.56 | Osmundacetone | 103.0545, 105.0701, 114.0915, 115.0544, 117.07, 118.0416, 133.0647, 160.0968, 161.0594 | 161.0597 | 161.0598 | 4.78 | POS | 28063.31777 | 28267.31012 | 28922.68895 | 0.003754543 | 0.003849053 | 0.003795849 | 0.003799815 | YIFZKRGUGKLILR-NSCUHMNNSA-N | CC(=O)C=CC1=CC(=C(C=C1)O)O |  | 828933 |  |  | 9942292 |  | 紫萁酮 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1966 | HPLC≥98% | level2 |
| compound00365 | 8.35\_313.1081m/z | M-H | C18H18O5 | 41.7 | 0 | -0.3 | p-Hydroxyphenethyl trans-ferulate |  | 313.1081 | 313.1081 | 8.35 | NEG | 23108.26425 | 22628.77705 | 22546.9111 | 0.003091615 | 0.003081275 | 0.002959085 | 0.003043991 | JMSFLLZUCIXALN-WEVVVXLNSA-N | COC1=C(O)C=CC(\C=C\C(=O)OCCC2=CC=C(O)C=C2)=C1 | HMDB0032806 | 88728 |  |  | 637308 | 84873-15-4 | 4-羟基苯乙基 反式-阿魏酸酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | DH0304 | HPLC≥98% | level2 |
| compound00366 | 0.72\_189.1345m/z | M+H | C7H16N4O2 | 49.8 | 54.1 | -0.61 | homoarginin | 130.0499, 130.0862, 142.0862, 144.1129, 158.0925, 170.0807, 172.0967, 172.1084, 188.0914, 189.1349 | 189.1346 | 189.1345 | 0.72 | POS | 61549.99972 | 58805.81479 | 61305.99923 | 0.008234667 | 0.008007366 | 0.008045875 | 0.00809597 | QUOGESRFPZDMMT-UHFFFAOYSA-N | C(CCN=C(N)N)CC(C(=O)O)N |  |  |  |  | 9085 |  |  |  |  |  |  |  |  | level2 |
| compound00367 | 6.88\_341.1002m/z | M+Na | C17H18O6 | 43.3 | 10.3 | 1.96 | Paeoniflorigenone | 297.1114, 323.0898, 340.12, 341.0994 | 341.0995 | 341.1002 | 6.88 | POS | 20128.70703 | 19593.64842 | 20411.66679 | 0.002692985 | 0.002667993 | 0.002678852 | 0.002679943 | BANPEMKDTXIFRE-IXDLUCPKSA-N | C[C@@]12CC(=O)[C@H]3C[C@]1(O)O[C@@H](O2)[C@H]3COC(=O)c1ccccc1 |  |  |  |  |  | 80454-42-8 | 芍药苷元酮 | 其他 |  | Others |  | DS0242 | HPLC≥98% | level2 |
| compound00368 | 4.31\_483.1479m/z | M+Na | C20H28O12 | 42.6 | 0 | 1.22 | Paeonolide |  | 483.1473 | 483.1479 | 4.31 | POS | 3728.376719 | 4945.136047 | 4366.416988 | 0.000498813 | 0.000673361 | 0.000573054 | 0.000581743 | IDZZECHGWAZTIB-NYBIBFQCSA-N | CC(=O)C1=C(C=C(C=C1)OC)OC2C(C(C(C(O2)COC3C(C(C(CO3)O)O)O)O)O)O |  | 68521 |  | C10715 | 442923 | 72520-92-4 | 牡丹酚原甙 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N2156 | HPLC≥98% | level2 |
| compound00369 | 4.37\_507.2081m/z | M+FA-H | C21H34O11 | 55.1 | 67 | -0.52 | patrinoside | 149.0446, 161.0444, 191.0555, 221.0657, 251.0769, 293.0877, 311.0981, 327.1160, 461.2027, 507.2071 | 507.2083 | 507.2081 | 4.37 | NEG | 122292.3317 | 117924.5774 | 117640.5286 | 0.016361278 | 0.016057345 | 0.015439289 | 0.015952637 | BGDMXWQJUGENQP-QPCLWJSESA-N | CC(C)CC(=O)OC1C2C(CC(C2CO)O)C(=CO1)COC3C(C(C(C(O3)CO)O)O)O |  | 69143 |  | C11640 | 162135 | 53962-20-2 |  |  |  |  |  |  |  | level2 |
| compound00370 | 3.39\_155.0341m/z | M+H | C7H6O4 | 45.4 | 26.6 | 1.69 | Patulin | 72.9376, 90.9481, 95.0132, 109.1013, 110.0602, 113.9638, 123.0077, 154.0859, 154.9900, 155.0336 | 155.0339 | 155.0341 | 3.39 | POS | 10083.84064 | 11571.48449 | 11337.23497 | 0.0013491 | 0.001575645 | 0.001487913 | 0.001470886 | ZRWPUFFVAOMMNM-UHFFFAOYSA-N | OC1OCC=C2OC(=O)C=C12 | HMDB0034299 | 71308 |  | C16748 | 4696 | 149-29-1 | 展青霉素 | 其他 |  | Others |  | HY-N6779 | HPLC≥98% | level2 |
| compound00371 | 8.59\_373.1279m/z | M+H | C20H20O7 | 50.5 | 36.3 | -0.86 | Pentamethylquercetin | 312.0976, 333.1087, 343.0811, 355.263, 373.0899, 373.1271 | 373.1282 | 373.1279 | 8.59 | POS | 46094.66123 | 44374.13144 | 46279.00021 | 0.006166925 | 0.006042258 | 0.006073713 | 0.006094299 | ALGDHWVALRSLBT-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=C(OC)C(OC)=CC=3)=C(OC)C(=O)C=2C(OC)=C1 | HMDB0257020 | 44514 | LMPK12112772 |  | 97332 |  | 五甲氧基槲皮素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N7690 | HPLC≥98% | level2 |
| compound00372 | 5.80\_337.1621m/z | M+Na | C16H26O6 | 51.2 | 0 | -0.35 | Perilloside A |  | 337.1622 | 337.1621 | 5.8 | POS | 33377.23218 | 32558.99338 | 31297.61189 | 0.004465482 | 0.004433435 | 0.004107537 | 0.004335485 | YUTAFQVKXLDYFG-YTQIUSBHSA-N | CC(=C)C1CCC(=CC1)COC2C(C(C(C(O2)CO)O)O)O | HMDB0038706 | 93361 |  |  | 3086657 |  |  |  |  |  |  |  |  | level2 |
| compound00373 | 4.94\_263.0920m/z | M-H | C14H16O5 | 40.4 | 5.96 | -1.89 | Peucedanol | 175.1118, 219.102, 263.0924 | 263.0925 | 263.092 | 4.94 | NEG | 8482.76297 | 7923.429251 | 9214.159683 | 0.001134894 | 0.001078903 | 0.001209278 | 0.001141025 | WRTWKAQFZYXAEJ-GFCCVEGCSA-N | CC(C)(O)[C@H](O)Cc1cc2ccc(=O)oc2cc1O |  |  |  |  |  | 20516-23-8 | 白花前胡醇 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DB0150 | HPLC≥98% | level2 |
| compound00374 | 4.95\_251.0556m/z | M+FA-H | C11H10O4 | 56.8 | 61.7 | -2.41 | Phellodenol A | 163.0755, 189.055, 251.0559 | 251.0562 | 251.0556 | 4.95 | NEG | 15553.53888 | 16746.35367 | 16874.51079 | 0.002080881 | 0.002280288 | 0.002214632 | 0.002191933 | UNMQLUGEYMJJSH-UHFFFAOYSA-N | C1=CC(=O)OC2=CC(=C(C=C21)CCO)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00375 | 4.58\_475.1821m/z | M+FA-H | C20H30O10 | 55.7 | 73 | 0.09 | Phenethyl rutinoside | 215.0345, 233.0453, 265.0930, 413.0853, 429.1756, 431.0959, 457.0743, 474.2680, 475.0860, 475.1786 | 475.1821 | 475.1821 | 4.58 | NEG | 73008.96116 | 66000.6595 | 69674.58176 | 0.009767742 | 0.008987061 | 0.009144178 | 0.00929966 | OKUGUNDXBGUFPA-UHFFFAOYSA-N | CC1OC(OCC2OC(OCCC3=CC=CC=C3)C(O)C(O)C2O)C(O)C(O)C1O | HMDB0032622 | 88572 |  |  | 14312558 | 88510-08-1 |  |  |  |  |  |  |  | level2 |
| compound00376 | 4.63\_329.1242m/z | M+FA-H | C14H20O6 | 57.5 | 0 | -0.13 | Phenylethyl b-D-galactopyranoside |  | 329.1242 | 329.1242 | 4.63 | NEG | 10639.98195 | 12227.5175 | 10752.12534 | 0.001423505 | 0.001664975 | 0.001411122 | 0.001499867 | MLRIJUWUQTVDQE-UHFFFAOYSA-N | OCC1OC(OCCC2=CC=CC=C2)C(O)C(O)C1O | HMDB0029819 | 86524 |  |  | 468284 | 18997-54-1 |  |  |  |  |  |  |  | level2 |
| compound00377 | 5.20\_135.0440m/z | M+H | C8H6O2 | 48.4 | 21.1 | -0.51 | Phthalide | 79.0546, 89.0389, 107.0493, 107.0858, 117.0335, 135.0439 | 135.0441 | 135.044 | 5.2 | POS | 22892.78406 | 25364.65842 | 24314.84385 | 0.003062786 | 0.00345381 | 0.00319111 | 0.003235902 | WNZQDUSMALZDQF-UHFFFAOYSA-N | O=C1OCC2=CC=CC=C12 | HMDB0032469 | 328569 |  |  | 6885 | 87-41-2 | 麦冬皂苷 B | 甾体类 | 甾体皂苷类 | Steroids | Steroidal saponins | HY-W015820 | HPLC≥98% | level2 |
| compound00378 | 4.87\_727.2444m/z | M+H-H2O | C33H44O19 | 50.1 | 0 | 0.04 | phyllaemblicin B |  | 727.2444 | 727.2444 | 4.87 | POS | 30076.83243 | 31368.68043 | 25444.80016 | 0.004023927 | 0.004271355 | 0.003339407 | 0.00387823 | RLZZBHBWPWGOSA-WKLGMTJKSA-N | C[C@@H]1CO[C@]2(C[C@@H]1OC(=O)C3=CC=CC=C3)C(=O)[C@]4([C@H](C[C@@H](C[C@H]4O2)C(=O)O[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)CO)O)O)O[C@H]6[C@@H]([C@H]([C@@H]([C@H](O6)CO)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00379 | 8.67\_293.0816m/z | M-H2O-H | C18H16O5 | 57.2 | 0 | -0.94 | Ophiopogonone B |  | 293.0819 | 293.0816 | 8.67 | NEG | 6201.370155 | 6221.659168 | 6670.073153 | 0.000829671 | 0.00084718 | 0.000875389 | 0.000850746 | DVZDRBCAEIJEEA-UHFFFAOYSA-N | CC1=C(C2=C(C=C1O)OC=C(C2=O)CC3=CC=C(C=C3)OC)O |  | 71716 |  | C17472 | 14826840 |  |  |  |  |  |  |  |  | level2 |
| compound00380 | 9.37\_359.1122m/z | M+H | C19H18O7 | 45 | 0 | -0.85 | Ophiopogonanone H |  | 359.1125 | 359.1122 | 9.37 | POS | 7895.453819 | 7370.084712 | 8171.608894 | 0.001056319 | 0.001003557 | 0.001072452 | 0.001044109 | PYWJDXNJXROQEJ-LJQANCHMSA-N | Cc1c(O)c(C)c2c(c1O)C(=O)[C@@](O)(Cc1ccc3c(c1)OCO3)CO2 |  |  |  |  |  | 1427086-65-4 | 麦冬二氢高异黄酮 H | 萜类 | 单萜类 | Terpenes | Monoterpenes | STZ0200105 | HPLC≥98% | level2 |
| compound00381 | 8.49\_302.1017m/z | M+NH4 | C16H12O5 | 41.2 | 0 | -2.24 | Negletein |  | 302.1023 | 302.1017 | 8.49 | POS | 3150.572449 | 2920.569854 | 3047.221551 | 0.00042151 | 0.000397683 | 0.000399921 | 0.000406371 | ZTHLHHDJRXJGRX-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC=CC=3)=CC(=O)C=2C(O)=C1O | HMDB0134889 | 49522 | LMPK12111097 |  | 471719 |  | 黄芩素-7-甲醚 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4285 | HPLC≥98% | level2 |
| compound00382 | 7.51\_297.0766m/z | M-H | C17H14O5 | 53.8 | 0 | -0.77 | Neobavachalcone | 68.9948, 112.9847, 241.0868, 256.9804, 269.0817, 276.9878, 296.997, 297.0776 | 297.0768 | 297.0766 | 7.51 | NEG | 20038.37898 | 19808.05146 | 19854.28478 | 0.0026809 | 0.002697188 | 0.002605701 | 0.002661263 | CMPZYNFZRHFABH-QPJJXVBHSA-N | C1(OC)=C(C=O)C=C(C(=O)/C=C/C2C=CC(O)=CC=2)C(O)=C1 |  | 51879 | LMPK12120073 |  | 5320052 |  |  |  |  |  |  |  |  | level2 |
| compound00383 | 4.95\_777.1979m/z | M+K | C34H42O18 | 53.8 | 0 | -3.22 | neobudofficide |  | 777.2004 | 777.1979 | 4.95 | POS | 11674.91028 | 13066.59265 | 14254.36828 | 0.001561966 | 0.001779229 | 0.001870761 | 0.001737319 | XQQFUXJSLVWQSS-UOMQSTFGSA-N | CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(=C4C(=C3)OC(=CC4=O)C5=CC=C(C=C5)OC)O)OC6C(C(C(C(O6)C)O)O)O)O)O)O)O)O |  | 48894 |  |  | 44257901 |  |  |  |  |  |  |  |  | level2 |
| compound00384 | 3.62\_353.0878m/z | M-H | C16H18O9 | 45.1 | 24.6 | -0.11 | Neochlorogenic acid | 191.0555, 207.0863, 208.0894, 218.0813, 232.1190, 285.0300, 308.1143, 318.0272, 352.1026, 353.0883 | 353.0878 | 353.0878 | 3.62 | NEG | 9713.242702 | 9277.184527 | 10137.22522 | 0.001299518 | 0.001263239 | 0.001330422 | 0.001297726 | CWVRJTMFETXNAD-NXLLHMKUSA-N | [H]\C(=C(\[H])C1=CC(O)=C(O)C=C1)C(=O)O[C@]1([H])C[C@](O)(C[C@@]([H])(O)[C@]1([H])O)C(O)=O | HMDB0240477 |  |  | C17147 | 5280633 |  | 5-咖啡酰奎宁酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N0722 | HPLC≥98% | level2 |
| compound00385 | 4.97\_607.1663m/z | M-H | C28H32O15 | 48 | 41.2 | -0.83 | Neodiosmin | 284.0323, 299.0559, 607.1669 | 607.1668 | 607.1663 | 4.97 | NEG | 103197.3736 | 116218.3842 | 108944.4159 | 0.013806597 | 0.015825019 | 0.014298 | 0.014643205 | VCCNKWWXYVWTLT-CYZBKYQRSA-N | C1(O[C@H]2[C@H](O[C@H]3[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O3)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C2OC(C3C=CC(OC)=C(O)C=3)=CC(=O)C2=C(O)C=1 |  |  | LMPK12113402 |  | 69964214 |  | 新地奥斯明 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N4122 | HPLC≥98% | level2 |
| compound00386 | 4.61\_595.1668m/z | M-H | C27H32O15 | 49.2 | 40.4 | -0.04 | Neoeriocitrin | 135.0441, 151.0028, 287.0559, 595.1672 | 595.1668 | 595.1668 | 4.61 | NEG | 383989.1375 | 381814.4776 | 379778.4622 | 0.051373239 | 0.051990238 | 0.049842595 | 0.051068691 | OBKKEZLIABHSGY-BEDUMGIKSA-N | C[C@@H]1O[C@@H](O[C@H]2[C@H](Oc3cc(O)c4c(c3)OC(c3ccc(O)c(O)c3)CC4=O)O[C@H](CO)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 13241-32-2 | 新北美圣草苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N4119 | HPLC≥98% | level2 |
| compound00387 | 5.01\_610.1889n | M+H, M+Na, M+NH4, M+H-H2O | C28H34O15 | 45.6 | 22.4 | -1.47 | Neohesperidin | 129.0546, 153.0180, 177.0544, 195.0287, 263.0549, 303.0858, 345.0961, 413.1225, 431.1330, 449.1439 | 611.197 | 611.1962 | 5.01 | POS | 24045113.91 | 23858483.66 | 24976149.34 | 3.216953993 | 3.248719786 | 3.277900739 | 3.247858173 | ARGKVCXINMKCAZ-GNKGNJJFSA-N | COc1ccc([C@H]2CC(=O)c3c(O)cc(O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)cc3O2)cc1O |  |  |  |  |  | 13241-33-3 | 新橙皮苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0101 | HPLC≥98% | level2 |
| compound00388 | 5.09\_431.0979m/z | M-H2O-H | C21H22O11 | 52.8 | 0 | -1.04 | Neoisoastilbin |  | 431.0984 | 431.0979 | 5.09 | NEG | 4238.033276 | 3869.803774 | 5125.114698 | 0.000566999 | 0.000526937 | 0.000672626 | 0.000588854 | ZROGCCBNZBKLEL-XEXNSLJOSA-N | C[C@@H]1O[C@@H](O[C@H]2C(=O)c3c(O)cc(O)cc3O[C@H]2c2ccc(O)c(O)c2)[C@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 54141-72-9 | 新异落新妇苷 | 黄酮类 | 二氢黄酮醇类 | Flavonoids | Flavanonols | HY-N5116 | HPLC≥98% | level2 |
| compound00389 | 3.94\_583.1280m/z | M-H | C25H28O16 | 43.2 | 0 | -4.24 | Neomangiferin |  | 583.1305 | 583.128 | 3.94 | NEG | 9483.609604 | 7227.287609 | 7712.573234 | 0.001268796 | 0.000984113 | 0.001012208 | 0.001088372 | VUWOVGXVRYBSGI-IRXABLMPSA-N | O=c1c2cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)c(O)cc2oc2cc(O)c([C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)c(O)c12 |  |  |  |  |  | 64809-67-2 | 新芒果苷 | 苯丙素类 | 氧杂蒽酮 | Phenylpropanoids | Xanthones | HY-N0723 | HPLC≥98% | level2 |
| compound00390 | 5.04\_479.1180m/z | M+H | C22H22O12 | 40.9 | 0 | -0.9 | Nepitrin |  | 479.1184 | 479.118 | 5.04 | POS | 9902.079138 | 8731.458955 | 7610.517436 | 0.001324782 | 0.00118893 | 0.000998814 | 0.001170842 | DMXHXBGUNHLMQO-IWLDQSELSA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=CC2OC(C3C=C(O)C(O)=CC=3)=CC(=O)C=2C(O)=C1OC | HMDB0030548 | 49621 | LMPK12111196 |  | 120742 | 569-90-4 | 假荆芥属苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N5010 | HPLC≥98% | level2 |
| compound00391 | 4.78\_215.0919m/z | M+FA-H | C9H14O3 | 54.3 | 69.7 | -3.53 | ningpogenin | 71.0127, 99.0441, 142.1226, 170.1177, 171.1017, 198.1127, 215.0114, 215.0918 | 215.0927 | 215.0919 | 4.78 | NEG | 15006.70185 | 14501.50834 | 14442.04256 | 0.002007721 | 0.001974616 | 0.001895392 | 0.001959243 | QCZMBBWKHAYATJ-HLTSFMKQSA-N | C1CO[C@@H]2[C@H]1[C@@H](C(=C2)CO)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00392 | 5.98\_383.0773m/z | 2M-H | C10H8O4 | 44.1 | 0 | 0.04 | Noreugenin |  | 383.0772 | 383.0773 | 5.98 | NEG | 7251.000948 | 7270.576101 | 7713.829124 | 0.000970099 | 0.000990007 | 0.001012372 | 0.000990826 | NCUJRUDLFCGVOE-UHFFFAOYSA-N | CC1=CC(=O)C2=C(O1)C=C(O)C=C2O | HMDB0303562 |  |  | C20462 |  |  | 去甲丁香色原酮 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N3029 | HPLC≥98% | level2 |
| compound00393 | 9.95\_377.1353m/z | M+Na | C21H22O5 | 43.2 | 0 | -1.96 | Notopterol |  | 377.136 | 377.1353 | 9.95 | POS | 8907.173355 | 8895.618262 | 9223.942609 | 0.001191675 | 0.001211283 | 0.001210562 | 0.001204507 | BKIACVAZUKISOR-MKMNVTDBSA-N | CC(=CC(CC(=CCOC1=C2C=CC(=O)OC2=CC3=C1C=CO3)C)O)C |  | 71739 |  | C17499 | 5320227 | 88206-46-6 | 羌活醇 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0564 | HPLC≥98% | level2 |
| compound00394 | 5.31\_718.1522n | M+Na, M+K, M+H, M+NH4 | C36H30O16 | 64.5 | 85.2 | -1.71 | np02140176-40 | 319.0570, 323.0538, 337.0673, 345.0361, 362.0388, 363.0452, 381.0569, 543.0891, 561.0997, 741.1405 | 736.1872 | 736.186 | 5.31 | POS | 27718809.41 | 26534239.23 | 27060123.87 | 3.708451328 | 3.613067334 | 3.551404135 | 3.624307599 | VKWZFIDWHLCPHJ-UHFFFAOYSA-N | C1=CC(=C(C=C1CC(C(=O)O)OC(=O)C2C(C3=CC(=C(C=C3C=C2C(=O)OC(CC4=CC(=C(C=C4)O)O)C(=O)O)O)O)C5=CC(=C(C=C5)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00395 | 4.89\_478.2414n | M-H2O-H, M+FA-H | C22H38O11 | 50 | 0 | -0.09 | Nuciferoside |  | 459.2236 | 459.2235 | 4.89 | NEG | 38630.68595 | 42194.90648 | 38402.47648 | 0.005168332 | 0.005745521 | 0.005039989 | 0.005317947 | WFJDTYSQBHCNGC-LWZURRPWSA-N | CC1=C(C(CCC1)(C)C)CO[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00396 | 7.85\_517.2075m/z | M+FA-H | C26H32O8 | 56.6 | 73.7 | -0.82 | Obacunoic acid | 429.1912, 453.1893, 471.2044, 517.0168, 517.2064 | 517.208 | 517.2075 | 7.85 | NEG | 44469.30494 | 47415.03349 | 46304.72973 | 0.005949471 | 0.006456326 | 0.00607709 | 0.006160962 | GUIYORVNNIUEBH-SXMAHZFBSA-N | C[C@@]12CC[C@@H]3[C@@]([C@@H](CC(=O)[C@]3([C@@]14[C@H](O4)C(=O)O[C@H]2C5=COC=C5)C)C(C)(C)O)(C)/C=C\C(=O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00397 | 1.03\_255.0743n | M+H-H2O, M+H | C11H13NO6 | 41.7 | 2.44 | -0.13 | Nicotinic acid riboside | 97.0287, 109.0286, 114.0551, 142.0498, 154.0497, 164.0704, 192.0652, 210.0759, 238.0707 | 256.0816 | 256.0815 | 1.03 | POS | 825145.0633 | 802962.6473 | 768935.8066 | 0.110394724 | 0.109336397 | 0.100916087 | 0.106882402 | PUEDDPCUCPRQNY-ZYUZMQFOSA-N | O=C([O-])c1ccc[n+]([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c1 |  |  |  |  |  | 17720-18-2 | 烟酸核糖 | 生物碱 |  | Alkaloids |  | HY-W104368 | HPLC≥98% | level2 |
| compound00398 | 6.75\_271.0611m/z | M-H | C15H12O5 | 54.8 | 25.7 | -0.4 | Naringenin chalcone | 119.0492, 151.0029, 271.0612 | 271.0612 | 271.0611 | 6.75 | NEG | 66642.90834 | 63754.87039 | 70658.23109 | 0.008916039 | 0.00868126 | 0.009273274 | 0.008956858 | YQHMWTPYORBCMF-ZZXKWVIFSA-N | C1(O)=CC(O)=C(C(=O)/C=C/C2C=CC(O)=CC=2)C(O)=C1 | HMDB0029631 | 3402 | LMPK12120264 | C06561 | 5280960 | 5071-40-9 | 柚皮素查耳酮 | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | HY-N3007 | HPLC≥98% | level2 |
| compound00399 | 10.17\_497.3273m/z | M-H2O-H | C31H48O6 | 54.9 | 0 | 0.06 | Phytolaccinic acid | 467.3163, 496.9983, 497.3272 | 497.3272 | 497.3273 | 10.17 | NEG | 19209.97397 | 20750.92627 | 19632.95178 | 0.002570069 | 0.002825575 | 0.002576653 | 0.002657432 | YAGYBNOEVSEGSL-UHFFFAOYSA-N | COC(=O)C1(C)CCC2(CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(CO)C5CCC34C)C2C1)C(O)=O | HMDB0034640 | 90102 |  |  | 13878339 | 54928-05-1 |  |  |  |  |  |  |  | level2 |
| compound00400 | 4.58\_391.1611m/z | M+FA-H | C16H26O8 | 53.6 | 59.1 | 0.35 | picrocrocinicacido-β-d-glucopyrinoside | 161.0448, 164.0699, 183.1020, 197.0453, 207.0507, 225.1124, 271.0836, 289.1259, 345.1553, 391.1566 | 391.161 | 391.1611 | 4.58 | NEG | 34901.14883 | 34271.92646 | 35687.29097 | 0.004669364 | 0.004666679 | 0.004683644 | 0.004673229 | LBTAFDHXNSPZSZ-UHFFFAOYSA-N | CC1=C(C(CC(C1)OC2C(C(C(C(O2)CO)O)O)O)(C)C)C(=O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00401 | 10.77\_497.3270m/z | M-H2O-H | C31H48O6 | 57.4 | 71.7 | -0.56 | pseudolarolide c | 423.2906, 497.327 | 497.3272 | 497.327 | 10.77 | NEG | 64251.28605 | 62327.41603 | 64113.51482 | 0.008596068 | 0.008486889 | 0.008414337 | 0.008499098 | YBQWVVDWBNHYPN-TZXWZJMFSA-N | CC1C[C@]2(CC(C(=O)O2)C)OC3C1[C@]4(CC[C@@]56C[C@@]5(C(CCC6C4(C3)C)C(C)(C)O)CCC(=O)OC)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00402 | 4.93\_397.1855m/z | M+H | C20H28O8 | 52 | 0 | -0.59 | pterosin c-3-o-glucoside |  | 397.1857 | 397.1855 | 4.93 | POS | 14016.72594 | 15532.65879 | 16065.20375 | 0.001875273 | 0.002115024 | 0.002108417 | 0.002032905 | VKDMMOFAMUXTQZ-VTNBQNSRSA-N | C[C@H]1[C@@H](C2=C(C1=O)C(=C(C(=C2)C)CCO[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00403 | 4.50\_577.1205m/z | M-H2O-H | C26H28O16 | 58.2 | 0 | 0.95 | Quercetin 3-sambubioside |  | 577.1199 | 577.1205 | 4.5 | NEG | 16592.68591 | 18158.89875 | 16622.52055 | 0.002219907 | 0.002472629 | 0.00218156 | 0.002291365 | NKFZLEYLWAFYEH-CJNLAGEVSA-N | C1C(C(C(C(O1)OC2C(C(C(OC2OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)CO)O)O)O)O)O |  | 50506 |  | C12637 | 5487635 |  | 槲皮素-3-O-木糖（1-2）葡萄糖 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DH0382 | HPLC≥98% | level2 |
| compound00404 | 4.41\_327.1424m/z | M+H | C16H22O7 | 40.9 | 0 | -4.35 | Raspberry ketone glucoside |  | 327.1438 | 327.1424 | 4.41 | POS | 2425.531437 | 2679.946943 | 2867.852538 | 0.000324508 | 0.000364918 | 0.000376381 | 0.000355269 | IDONYWHRKBUDOR-IBEHDNSVSA-N | CC(=O)CCc1ccc(O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)cc1 |  |  |  |  |  | 38963-94-9 | 覆盆子酮葡萄糖甙 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N6069 | HPLC≥98% | level2 |
| compound00405 | 4.37\_400.1366n | M-H, M+FA-H | C18H24O10 | 50.5 | 37.8 | -0.82 | Regaloside A | 129.0183, 135.0441, 145.0285, 163.0391, 179.0341, 205.0346, 219.0269, 223.0453, 381.0584, 399.1300 | 399.1297 | 399.1293 | 4.37 | NEG | 104142.6721 | 103056.2675 | 101590.5743 | 0.013933067 | 0.014032783 | 0.013332873 | 0.013766241 | PADHSFRQMFRWLS-MUWVXHEGSA-N | C1=CC(=CC=C1/C=C/C(=O)OC[C@H](COC2C(C(C(C(O2)CO)O)O)O)O)O |  |  |  |  |  | 114420-66-5 | 王百合苷 A | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DW0107-0020 | HPLC≥98% | level2 |
| compound00406 | 5.06\_441.1398m/z | M-H | C20H26O11 | 46.4 | 0 | -0.95 | Regaloside B |  | 441.1402 | 441.1398 | 5.06 | NEG | 17933.46219 | 18491.67715 | 18853.48787 | 0.002399287 | 0.002517942 | 0.002474355 | 0.002463861 | YQKQOLPNKNHLBO-KRJCNZRASA-N | CC(=O)OC[C@@H](COC(=O)/C=C/c1ccc(O)cc1)OC1OC(CO)C(O)C(O)C1O |  |  |  |  |  | 114420-67-6 | 王百合苷B | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DW0072-0020 | HPLC≥98% | level2 |
| compound00407 | 4.47\_429.1402m/z | M-H | C19H26O11 | 50.4 | 45.8 | -0.02 | regaloside F | 134.0363, 149.0599, 175.0392, 193.0499, 429.1394 | 429.1402 | 429.1402 | 4.47 | NEG | 31186.44402 | 30521.01321 | 29727.17968 | 0.00417238 | 0.004155931 | 0.003901432 | 0.004076581 | ZGENOXMVMATRDW-FSTLHUPISA-N | COC1=C(C=CC(=C1)/C=C/C(=O)OC[C@H](CO[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00408 | 4.20\_399.1291m/z | M-H | C18H24O10 | 48.1 | 28 | -1.4 | Regaloside H | 125.0234, 145.0285, 163.0391, 205.0346, 223.0453, 399.1302 | 399.1297 | 399.1291 | 4.2 | NEG | 25958.88071 | 25647.19329 | 26272.86964 | 0.003472994 | 0.003492282 | 0.003448084 | 0.00347112 | WYSRAMKKFNDRPR-BFQBLSCMSA-N | O=C(/C=C/c1ccc(O)cc1)O[C@H](CO)CO[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 126239-77-8 | 王百合苷 H | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DW0114-0010 | HPLC≥98% | level2 |
| compound00409 | 5.66\_267.0415m/z | M+K | C14H12O3 | 43.5 | 0 | -1.33 | Resveratrol |  | 267.0419 | 267.0415 | 5.66 | POS | 2575.161292 | 2800.829637 | 2789.970558 | 0.000344526 | 0.000381378 | 0.000366159 | 0.000364021 | LUKBXSAWLPMMSZ-OWOJBTEDSA-N | C1=C(O)C=C(/C=C/C2=CC=C(O)C=C2)C=C1O | HMDB0003747 | 6979 | LMPK13090005 | C03582 | 445154 | 501-36-0 | 白藜芦醇 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-16561 | HPLC≥98% | level2 |
| compound00410 | 4.92\_415.0674m/z | M-H2O-H | C20H18O11 | 43.6 | 0.135 | 0.77 | Reynoutrin | 175.0392, 179.0338, 179.0549, 193.0500, 197.0446, 237.0394, 283.0968, 327.0870, 371.0764, 415.0644 | 415.0671 | 415.0674 | 4.92 | NEG | 29565.39412 | 27401.46731 | 27323.25141 | 0.003955503 | 0.003731155 | 0.003585937 | 0.003757532 | PZZRDJXEMZMZFD-BWYUNELBSA-N | O=C1C(OC2OCC(O)C(O)C2O)=C(OC=3C=C(O)C=C(O)C13)C=4C=CC(O)=C(O)C4 |  |  |  |  | 5320863 | 549-32-6 | 槲皮素-3-O-β-D-木糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N1354 | HPLC≥98% | level2 |
| compound00411 | 5.24\_443.1310m/z | M+Na | C21H24O9 | 40.6 | 0 | -0.54 | Rhapontin |  | 443.1313 | 443.131 | 5.24 | POS | 6902.702353 | 7395.580481 | 6837.057789 | 0.000923501 | 0.001007028 | 0.000897304 | 0.000942611 | GKAJCVFOJGXVIA-DXKBKAGUSA-N | C1=C(O)C=C(/C=C/C2=CC(O)=C(OC)C=C2)C=C1O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO | HMDB0304731 | 44320 | LMPK13090002 | C10288 | 637213 | 155-58-8 | 勒胖停 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N0671 | HPLC≥98% | level2 |
| compound00412 | 4.07\_610.1538n | M+H, M+Na | C27H30O16 | 57.1 | 0 | 0.68 | Rheinoside A | 377.0636, 395.0758, 407.0764, 419.0758, 425.0849, 473.1076, 592.3833, 593.1528, 610.3941, 611.1599 | 611.1607 | 611.1611 | 4.07 | POS | 147737.5824 | 143903.3051 | 146585.1221 | 0.019765554 | 0.019594771 | 0.019238013 | 0.019532779 | OJZWDOKDQBCANR-UHFFFAOYSA-N | OCC1OC(OC2=CC=CC3=C2C(=O)C2=C(C=C(C=C2O)C(O)=O)C3(O)C2OC(CO)C(O)C(O)C2O)C(O)C(O)C1O | HMDB0040715 | 95189 |  |  | 13888123 | 111545-28-9 |  |  |  |  |  |  |  | level2 |
| compound00413 | 4.65\_303.0501m/z | M+H | C15H10O7 | 45 | 23 | 0.61 | Robinetin | 86.0969, 132.102, 143.1178, 171.1127, 284.1101, 303.0496 | 303.0499 | 303.0501 | 4.65 | POS | 15536.90024 | 14551.80292 | 15502.24631 | 0.002078655 | 0.001981464 | 0.002034534 | 0.002031551 | SOEDEYVDCDYMMH-UHFFFAOYSA-N | C1(O)=CC2OC(C3C=C(O)C(O)=C(O)C=3)=C(O)C(=O)C=2C=C1 |  | 49995 | LMPK12111577 | C10177 | 5281692 |  | 洋槐黄素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N1347 | HPLC≥98% | level2 |
| compound00414 | 4.51\_739.2090m/z | M-H | C33H40O19 | 46.1 | 0 | -0.2 | Robinin |  | 739.2091 | 739.209 | 4.51 | NEG | 17243.00253 | 18418.49602 | 15101.44009 | 0.002306911 | 0.002507977 | 0.001981932 | 0.002265607 | PEFASEPMJYRQBW-HKWQTAEVSA-N | C1(O[C@H]2[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O2)=CC2OC(C3C=CC(O)=CC=3)=C(O[C@H]3[C@H](O)[C@@H](O)[C@@H](O)[C@@H](CO[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)O3)C(=O)C=2C(O)=C1 | HMDB0302847 |  | LMPK12111685 | C10178 | 5281693 |  | 刺槐素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N1346 | HPLC≥98% | level2 |
| compound00415 | 4.34\_386.1942n | M+H, M+NH4, M+Na, M+H-H2O | C19H30O8 | 44.6 | 14.9 | 0.26 | Roseoside | 163.1115, 165.0909, 177.0547, 189.1270, 207.0658, 207.1040, 207.1378, 225.1112, 225.1480, 387.1593 | 409.1833 | 409.1834 | 4.34 | POS | 477118.1435 | 486244.3386 | 500519.9984 | 0.063832807 | 0.066210059 | 0.065688864 | 0.06524391 | SWYRVCGNMNAFEK-MHXFFUGFSA-N | CC1=CC(=O)CC(C)(C)[C@@]1(O)/C=C/[C@@H](C)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 54835-70-0 | 长寿花糖甙 | 萜类 | 胡萝卜素 | Terpenes | Carotenoids | STC6030205 | HPLC≥95% | level2 |
| compound00416 | 5.11\_332.1831n | M+Na, M+K, M+H | C16H28O7 | 44.7 | 5.61 | -1.31 | Rosiridin | 355.172 | 355.1728 | 355.1723 | 5.11 | POS | 130378.8708 | 132706.1718 | 129981.2919 | 0.017443162 | 0.018070099 | 0.017058906 | 0.017524056 | PBPYEEMQIFDGSQ-MIYBPCGNSA-N | OCC1OC(OCC=C(C)C(O)CC=C(C)C)C(O)C(O)C1O |  |  |  |  |  |  | 络塞定 | 萜类 | 单萜类 | Terpenes | Monoterpenes | B20807-10mg | HPLC≥97% | level2 |
| compound00417 | 9.64\_471.3466m/z | M+H-H2O | C30H48O5 | 54.3 | 0 | -0.67 | Rotundic acid |  | 471.3469 | 471.3466 | 9.64 | POS | 43048.95098 | 44612.77843 | 45321.38066 | 0.005759444 | 0.006074754 | 0.005948034 | 0.005927411 | YLHQFGOOMKJFLP-LTFXOGOQSA-N | CC1CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)O)C)C)C2C1(C)O)C)C(=O)O |  | 449467 |  |  | 12315075 |  | 铁冬青酸 | 萜类 | 三萜类 | Terpenes | Triterpenes | HY-N2217 | HPLC≥98% | level2 |
| compound00418 | 5.49\_245.0806m/z | M+H-H2O | C14H14O5 | 43.5 | 4.56 | -1.05 | Rutaretin | 245.0804 | 245.0808 | 245.0806 | 5.49 | POS | 17758.29293 | 19060.00726 | 17623.31391 | 0.002375851 | 0.002595329 | 0.002312906 | 0.002428029 | FVFQELHSZVFPDZ-VIFPVBQESA-N | CC(C)(O)[C@@H]1Cc2cc3ccc(=O)oc3c(O)c2O1 |  |  |  |  |  | 13895-92-6 | 芸香霉素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DY0516 | HPLC≥98% | level2 |
| compound00419 | 4.66\_469.1350m/z | M+FA-H | C20H24O10 | 50.2 | 1.24 | -0.24 | Rutarin | 145.0284, 163.0393, 205.0501, 235.0594, 265.0711, 325.0929, 357.0370, 401.0260, 425.0249, 469.1383 | 469.1352 | 469.135 | 4.66 | NEG | 27128.82647 | 28122.25365 | 25140.98421 | 0.003629519 | 0.003829301 | 0.003299534 | 0.003586118 | JWWFVRMFYKPZNE-VVIWCBLHSA-N | CC(C)(C1CC2=C(O1)C(=C3C(=C2)C=CC(=O)O3)OC4C(C(C(C(O4)CO)O)O)O)O |  | 67593 |  | C09309 | 442149 | 20320-81-4 |  | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DR0139-0005 | HPLC≥98% | level2 |
| compound00420 | 8.21\_531.2234m/z | M-H2O-H | C28H38O11 | 40.8 | 0.0449 | -0.34 | Pseudolaric Acid A-O-beta-D-glucopyranoside | 59.0127, 61.9873, 112.9846, 137.0957, 395.205, 427.2108, 471.1987, 471.2072, 531.0137, 531.2216 | 531.2236 | 531.2234 | 8.21 | NEG | 52815.59357 | 54105.26988 | 48502.88502 | 0.007066106 | 0.007367311 | 0.006365579 | 0.006932999 | IVYWRYGMQNKDQB-KNPVXXFYSA-N | CC(=O)O[C@]12CCC(C)=CC[C@]13CC[C@H]2[C@@](C)(/C=C/C=C(\C)C(=O)O[C@H]1OC(CO)C(O)C(O)C1O)OC3=O |  |  |  |  |  | 98891-44-2 | 土槿皮甲酸苷 | 萜类 | 二萜类 | Terpenes | Diterpenes | DT0051 | HPLC≥98% | level2 |
| compound00421 | 4.70\_570.3433m/z | M+H-H2O | C33H49NO8 | 40.9 | 0 | 1.33 | Pseudojervine |  | 570.3426 | 570.3433 | 4.7 | POS | 18066.42848 | 18087.53981 | 17715.24993 | 0.002417076 | 0.002462912 | 0.002324971 | 0.002401653 | HYDDDNUKNMMWBD-VPLHBGEQSA-N | CC1=C2C(=O)[C@H]3[C@@H](CC=C4C[C@@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O)[C@H]5O)CC[C@@]43C)[C@@H]2CC[C@]12O[C@@H]1C[C@H](C)CN[C@H]1[C@H]2C |  |  |  |  |  | 36069-05-3 | 假白藜芦碱 | 生物碱 |  | Alkaloids |  | DJ0249 | HPLC≥95% | level2 |
| compound00422 | 9.92\_310.1201n | M+Na, M+K, M+H-H2O | C19H18O4 | 46.7 | 25.9 | -1.18 | Przewaquinone A | 245.1171, 253.1584, 297.1484, 315.1575, 332.0968, 333.1092 | 333.1098 | 333.1094 | 9.92 | POS | 206584.2109 | 209432.3089 | 209348.744 | 0.027638542 | 0.028517608 | 0.027475188 | 0.027877113 | CEHVTERMWMYLCP-UHFFFAOYSA-N | O=C1C(=O)C2=C(C=CC3=C2CCCC3(C)C)C=4OC=C(C14)CO |  |  |  |  |  | 76843-23-7 | 紫丹参甲素 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | DZ0115 | HPLC≥98% | level2 |
| compound00423 | 4.66\_403.0670m/z | M+FA-H | C18H14O8 | 55.6 | 0 | -0.26 | Przewalskinic acid A |  | 403.0671 | 403.067 | 4.66 | NEG | 9614.401112 | 9148.49051 | 8894.485783 | 0.001286294 | 0.001245715 | 0.001167323 | 0.001233111 | GJHXGOBGPWPCCK-DBLORFJXSA-N | O=C(O)/C=C/c1ccc(O)c2c1[C@@H](C(=O)O)[C@H](c1ccc(O)c(O)c1)O2 |  |  |  |  |  | 136112-75-9 | 甘西鼠尾草酸甲 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DG0050 | HPLC≥98% | level2 |
| compound00424 | 5.12\_291.0872m/z | M-H2O-H | C15H18O7 | 40.5 | 0 | -0.81 | Picrotin |  | 291.0874 | 291.0872 | 5.12 | NEG | 7626.296323 | 7841.5404 | 8925.705641 | 0.001020309 | 0.001067753 | 0.001171421 | 0.001086494 | RYEFFICCPKWYML-QCGISDTRSA-N | CC12C3C4C(C(C1(CC5C2(O5)C(=O)O3)O)C(=O)O4)C(C)(C)O |  | 43703 |  | C09528 | 442291 | 21416-53-5 | 苦亭 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-107782 | HPLC≥98% | level2 |
| compound00425 | 6.05\_291.0878m/z | M-H | C15H16O6 | 43.1 | 0 | 1.16 | Picrotoxinin |  | 291.0874 | 291.0878 | 6.05 | NEG | 5738.017742 | 5927.422246 | 5868.59075 | 0.000767679 | 0.000807115 | 0.000770201 | 0.000781665 | PIMZUZSSNYHVCU-WHHVQDKOSA-N | C=C(C)[C@@H]1[C@@H]2OC(=O)[C@@H]1[C@]1(O)C[C@H]3O[C@]34C(=O)O[C@H]2[C@@]41C |  |  |  |  |  | 17617-45-7 | 木防己苦毒宁 | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | HY-B1494 | HPLC≥98% | level2 |
| compound00426 | 8.98\_315.0854m/z | M+H | C17H14O6 | 41.7 | 0 | -2.83 | Pinobanksin 3-acetate |  | 315.0863 | 315.0854 | 8.98 | POS | 3353.688419 | 3246.467769 | 3627.62724 | 0.000448684 | 0.000442059 | 0.000476094 | 0.000455613 | BJYHZSNSMVEQEH-SJORKVTESA-N | CC(=O)OC1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=CC=C3 |  | 64204 |  | C16418 | 148556 | 52117-69-8 | 3-O-乙酰短叶松素 | 黄酮类 | 二氢黄酮醇类 | Flavonoids | Flavanonols | HY-N1854 | HPLC≥98% | level2 |
| compound00427 | 6.39\_419.1334m/z | M+H | C21H22O9 | 47.4 | 0 | -0.56 | Pinocembrin-7-O-beta-D-glucopyranoside |  | 419.1337 | 419.1334 | 6.39 | POS | 25229.13344 | 23889.80432 | 23003.87625 | 0.003375362 | 0.003252985 | 0.003019057 | 0.003215801 | GPGFGFUBECSNTG-UHFFFAOYSA-N | O=C1CC(c2ccccc2)Oc2cc(OC3OC(CO)C(O)C(O)C3O)cc(O)c21 |  |  |  |  |  | 75829-43-5 | 乔松素7-O-Β-D葡萄糖苷,乔松苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N6616 | HPLC≥98% | level2 |
| compound00428 | 4.86\_449.1080m/z | M+H-H2O | C21H22O12 | 43.4 | 0 | 0.41 | Plantagoside |  | 449.1078 | 449.108 | 4.86 | POS | 10441.39507 | 10656.40922 | 8990.210878 | 0.001396936 | 0.001451043 | 0.001179886 | 0.001342622 | SNFFBROYEDWRGB-NHXQFOETSA-N | C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC(=C(C(=C3)OC4C(C(C(C(O4)CO)O)O)O)O)O |  | 52936 |  | C17531 | 174157 |  | 车前子苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N1470 | HPLC≥98% | level2 |
| compound00429 | 4.89\_389.1242m/z | M-H | C20H22O8 | 43.3 | 0 | 0 | Polydatin |  | 389.1242 | 389.1242 | 4.89 | NEG | 29619.22438 | 29706.19504 | 29082.88784 | 0.003962705 | 0.004044981 | 0.003816874 | 0.00394152 | HSTZMXCBWJGKHG-CUYWLFDKSA-N | C1=C(O)C=C(/C=C/C2=CC=C(O)C=C2)C=C1O[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 | HMDB0030564 | 53240 | LMPK13090012 | C10275 | 5281718 | 27208-80-6 | 虎杖苷 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N0120A | HPLC≥98% | level2 |
| compound00430 | 6.75\_369.1310m/z | M+Na | C19H22O6 | 54.2 | 0 | 0.54 | ponalactone a |  | 369.1308 | 369.131 | 6.75 | POS | 8278.448932 | 8350.332044 | 8699.494912 | 0.001107559 | 0.001137033 | 0.001141732 | 0.001128775 | KDORDIOOUCRJPK-PAFIYYKWSA-N | CC(C)C1C2=CC3C4C(C(C5C(C4(C2=CC(=O)O1)C)O5)O)(C(=O)O3)C |  | 67487 |  | C09174 | 442079 | 33722-77-9 |  |  |  |  |  |  |  | level2 |
| compound00431 | 10.77\_499.3410m/z | M+H | C31H46O5 | 40.4 | 0 | -1.57 | Poricoic acid A |  | 499.3418 | 499.341 | 10.77 | POS | 16804.93284 | 18477.98747 | 18721.96708 | 0.002248303 | 0.002516078 | 0.002457094 | 0.002407158 | KVAQLXUMUVEKGR-SMFZDKLCSA-N | C=C(CC[C@@H](C(=O)O)[C@H]1[C@H](O)C[C@@]2(C)C3=CC[C@@H](C(=C)C)[C@](C)(CCC(=O)O)C3=CC[C@]12C)C(C)C |  |  |  |  |  | 137551-38-3 | 茯苓酸 A | 萜类 | 三萜类 | Terpenes | Triterpenes | HY-N2995 | HPLC≥98% | level2 |
| compound00432 | 11.06\_481.3319m/z | M-H2O-H | C31H48O5 | 54.6 | 0 | -0.79 | poricoicacid h | 481.3314 | 481.3323 | 481.3319 | 11.06 | NEG | 26249.57335 | 29276.83 | 24313.38007 | 0.003511885 | 0.003986516 | 0.003190918 | 0.003563106 | GKXXWKRLARTIQL-UHFFFAOYSA-N | CC(C)C(=C)CCC(C1C(CC2(C1(CCC3=C2CCC(C3(C)CCC(=O)O)C(=C)C)C)C)O)C(=O)O |  |  |  |  | 10918099 |  |  |  |  |  |  |  |  | level2 |
| compound00433 | 5.14\_463.1228m/z | M+H | C22H22O11 | 45.1 | 0 | -1.59 | Pratensein 7-O-glucopyranoside |  | 463.1235 | 463.1228 | 5.14 | POS | 13514.55152 | 14538.15989 | 14232.44408 | 0.001808088 | 0.001979606 | 0.001867884 | 0.001885193 | FGAAKLDKKBMYCB-RECXWPGBSA-N | O([C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1)C1C=C(O)C2C(=O)C(C3C=C(O)C(OC)=CC=3)=COC=2C=1 |  |  | LMPK12050259 |  | 16202157 |  | 红车轴草素-7-O-β-D-吡喃葡萄糖苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | ST20300210 | HPLC≥95% | level2 |
| compound00434 | 4.75\_557.1076m/z | M-H2O-H | C30H24O12 | 47.5 | 0 | -2.33 | Procyanidin A1 |  | 557.1089 | 557.1076 | 4.75 | NEG | 13547.10667 | 14493.91061 | 14926.23677 | 0.001812444 | 0.001973581 | 0.001958938 | 0.001914988 | NSEWTSAADLNHNH-LQBIBLAPSA-N | Oc1cc(O)c2c(c1)O[C@@]1(c3ccc(O)c(O)c3)Oc3cc(O)c4c(c3[C@@H]2[C@@H]1O)O[C@H](c1ccc(O)c(O)c1)[C@@H](O)C4 |  |  |  |  |  | 103883-03-0 | 原花青素 A1 | 黄酮类 | 原花青素类 | Flavonoids | Procyanidins | HY-N2344 | HPLC≥98% | level2 |
| compound00435 | 4.92\_621.1233m/z | M+FA-H | C30H24O12 | 52.1 | 0 | -2.88 | Procyanidin A2 |  | 621.1251 | 621.1233 | 4.92 | NEG | 18293.63888 | 20963.0423 | 17751.3222 | 0.002447474 | 0.002854458 | 0.002329705 | 0.002543879 | NSEWTSAADLNHNH-LSBOWGMISA-N | O[C@@H]1CC2=C(O[C@@H]1C1=CC=C(O)C(O)=C1)C1=C(O[C@@]3(OC4=C([C@H]1[C@H]3O)C(O)=CC(O)=C4)C1=CC(O)=C(O)C=C1)C=C2O | HMDB0037655 | 68190 |  | C10237 | 124025 | 41743-41-3 | 原花青素 A2 | 黄酮类 | 原花青素类 | Flavonoids | Procyanidins | HY-N2343 | HPLC≥98% | level2 |
| compound00436 | 4.89\_459.0929m/z | M+FA-H | C21H18O9 | 55.1 | 0 | -0.84 | Prodelphinidin B6 | 135.0443, 151.0020, 173.0599, 179.0344, 197.0449, 217.0496, 235.0600, 397.0926, 413.2187, 459.0911 | 459.0933 | 459.0929 | 4.89 | NEG | 68308.4203 | 74193.70038 | 72452.60262 | 0.009138865 | 0.010102677 | 0.009508769 | 0.009583437 | OKJJBTUOKCQSPH-PWRODBHTSA-N | C1C2O[C@H](C3C=C(O)C(O)=CC=3)[C@H](O)[C@@H](C3C(O)=CC(O)=CC=3O)C=2C(O)=CC=1O |  | 47290 | LMPK12020074 |  | 14009028 |  |  |  |  |  |  |  |  | level2 |
| compound00437 | 5.70\_193.0496m/z | M-H2O-H | C10H12O5 | 45.9 | 23 | -4.73 | Propyl gallate | 135.0443, 137.0233, 147.0293, 149.0598, 152.9963, 173.0025, 178.0264, 192.9892, 193.0087, 193.0500 | 193.0505 | 193.0496 | 5.7 | NEG | 14386.28855 | 14667.68481 | 14850.39906 | 0.001924717 | 0.001997243 | 0.001948985 | 0.001956982 | ZTHYODDOHIVTJV-UHFFFAOYSA-N | CCCOC(=O)C1=CC(O)=C(O)C(O)=C1 | HMDB0033835 | 68880 |  | C11155 | 4947 | 121-79-9 | 没食子酸丙酯 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0524 | HPLC≥98% | level2 |
| compound00438 | 7.56\_1089.5487m/z | M+FA-H | C52H84O21 | 61.1 | 94.8 | 0.01 | prosapogenin cp8a | 911.5005, 1043.543, 1089.5479 | 1089.5487 | 1089.5487 | 7.56 | NEG | 189844.2257 | 180384.7979 | 186799.2348 | 0.025398929 | 0.024562318 | 0.024515763 | 0.02482567 | BECKQSNYULYJHB-UHFFFAOYSA-N | CC1C(C(C(C(O1)OC2C(C(COC2OC3CCC4(C(C3(C)CO)CCC5(C4CC=C6C5(CCC7(C6CC(CC7)(C)C)C(=O)O)C)C)C)O)O)O)OC8C(C(C(CO8)OC9C(C(C(C(O9)CO)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00439 | 5.13\_273.0754m/z | M+H | C15H12O5 | 46.8 | 0 | -1.19 | Protosappanin A |  | 273.0758 | 273.0754 | 5.13 | POS | 9306.879738 | 9401.459025 | 8967.628917 | 0.001245151 | 0.001280161 | 0.001176923 | 0.001234078 | MUKYVRVYBBYJSI-UHFFFAOYSA-N | OC1=CC=C2C(OCC(=O)CC3=CC(O)=C(O)C=C23)=C1 | HMDB0256874 |  |  |  |  |  | 原苏木素 A | 酚类 | 多酚类 | Phenols | Polyphenols | HY-113573 | HPLC≥98% | level2 |
| compound00440 | 4.48\_285.0768m/z | M-H2O-H | C16H16O6 | 41.6 | 2.44 | -0.18 | Protosappanin B | 109.0284, 175.0392, 285.0766 | 285.0768 | 285.0768 | 4.48 | NEG | 11173.77945 | 10385.28791 | 10554.41632 | 0.001494921 | 0.001414126 | 0.001385175 | 0.001431407 | QRTYTQTVJQUCEP-INIZCTEOSA-N | OC[C@]1(O)COc2cc(O)ccc2-c2cc(O)c(O)cc2C1 |  |  |  |  |  | 102036-29-3 | 原苏木素 B | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0800 | HPLC≥98% | level2 |
| compound00441 | 9.24\_317.1756m/z | M+FA-H | C18H24O2 | 55.6 | 0 | -0.7 | Przewalskin | 112.9845, 180.9724, 248.9601, 273.1857, 317.174 | 317.1759 | 317.1756 | 9.24 | NEG | 30240.58464 | 28767.14147 | 29555.51785 | 0.004045835 | 0.003917113 | 0.003878903 | 0.003947284 | RHXIVZRYHFCBDN-UHFFFAOYSA-N | CC1=CC2=C(C=C1O)C34CCCC(C3CC2OC4)(C)C |  |  |  |  | 138113846 | 119400-87-2 |  |  |  |  |  |  |  | level2 |
| compound00442 | 9.66\_331.1913m/z | M-H | C20H28O4 | 58.5 | 0 | -0.52 | premarrubiin | 287.1655, 301.1804, 331.1521, 331.1914 | 331.1915 | 331.1913 | 9.66 | NEG | 122129.6048 | 124278.9997 | 126943.6177 | 0.016339508 | 0.016922603 | 0.016660237 | 0.016640783 | OQLCWZJEAYGVQE-UHFFFAOYSA-N | CC1CC2C3C(CCCC3(C14CCC5(O4)COC=C5)C)(C(=O)O2)C |  |  |  |  | 168199 |  |  |  |  |  |  |  |  | level2 |
| compound00443 | 5.52\_295.1880m/z | M+Na | C15H28O4 | 52.4 | 0 | -0.04 | Homalomentetraol |  | 295.188 | 295.188 | 5.52 | POS | 39326.65491 | 40334.34382 | 39956.83732 | 0.005261445 | 0.005492176 | 0.005243985 | 0.005332535 | OOVYFGQDUNZBAS-QANKYFMGSA-N | C[C@@]12CC[C@@H]([C@@H]1[C@@](C[C@@H]([C@H]2O)O)(C)O)CC(C)(C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00444 | 4.09\_412.1945n | M-H2O-H, M+FA-H | C17H32O11 | 55.5 | 75.2 | 0.02 | Grandoside | 161.0446, 179.0555, 247.1184, 325.1270, 331.0818, 331.0870, 347.1709, 350.1701, 393.0825, 393.1803 | 393.1766 | 393.1766 | 4.09 | NEG | 173707.7155 | 174666.2883 | 171040.7124 | 0.023240053 | 0.02378365 | 0.022447595 | 0.023157099 | VLRGBWXSYFMTKJ-VGNHIMHRSA-N | CC(C)CCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00445 | 3.85\_272.1282m/z | M+H | C16H17NO3 | 46.7 | 0 | 0.32 | Higenamine |  | 272.1281 | 272.1282 | 3.85 | POS | 3506.369782 | 3304.202566 | 3793.693189 | 0.000469111 | 0.000449921 | 0.000497889 | 0.000472307 | WZRCQWQRFZITDX-UHFFFAOYSA-N | OC1=CC=C(CC2NCCC3=C2C=C(O)C(O)=C3)C=C1 | HMDB0033103 | 88994 |  | C06346 | 114840 | 106032-53-5 | 盐酸去甲乌头碱 | 生物碱 |  | Alkaloids |  | HY-N2037A | HPLC≥98% | level2 |
| compound00446 | 4.70\_177.0185m/z | M-H | C9H6O4 | 42.8 | 0 | -4.44 | 5,7-Dihydroxycoumarin |  | 177.0193 | 177.0185 | 4.7 | NEG | 2621.584712 | 2970.655872 | 2545.070339 | 0.000350737 | 0.000404503 | 0.000334018 | 0.000363086 | KIQQFVJHWNCGAU-UHFFFAOYSA-N | O=c1ccc2c(O)cc(O)cc2o1 |  |  |  |  |  | 2732-18-5 | 5,7-二羟基香豆素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-W072009 | HPLC≥98% | level2 |
| compound00447 | 5.62\_343.0819m/z | M+FA-H | C17H14O5 | 52.5 | 28.3 | -1.33 | 5,9-dihydroxy-4-(4-hydroxyphenyl)-5,6-dihydro-1-benzoxocin-2-one | 181.0501, 197.0449, 201.1125, 209.1161, 229.1438, 237.0921, 255.1026, 281.0821, 299.0924, 343.0821 | 343.0824 | 343.0819 | 5.62 | NEG | 105322.5569 | 97562.30707 | 99335.61947 | 0.014090922 | 0.013284692 | 0.01303693 | 0.013470848 | WRIXGOHFTHKWMM-UHFFFAOYSA-N | C1C(C(=CC(=O)OC2=C1C=CC(=C2)O)C3=CC=C(C=C3)O)O |  |  |  |  | 371598 | 126617-61-6 |  |  |  |  |  |  |  | level2 |
| compound00448 | 9.51\_298.1567n | M+H, M+Na | C19H22O3 | 58.8 | 0 | -0.56 | 5-(1-methoxyethyl)-1,7-dimethyl-9,10-dihydrophenanthrene-2,6-diol | 241.1220, 253.1564, 262.0941, 263.1424, 280.1049, 281.1521, 298.1130, 298.1434, 299.1228, 299.1611 | 321.1461 | 321.1459 | 9.51 | POS | 97450.2691 | 106685.7438 | 107739.3268 | 0.013037702 | 0.014526996 | 0.014139843 | 0.013901513 | QJSIPUGXYKUMHM-UHFFFAOYSA-N | CC1=C(C(=C2C(=C1)CCC3=C2C=CC(=C3C)O)C(C)OC)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00449 | 5.18\_180.0421n | M-H2O-H, 2M-H, M-H | C9H8O4 | 43.1 | 16.9 | -0.9 | 5-Acetylsalicylic acid | 59.0128, 73.0285, 85.0284, 131.034, 133.0285, 161.0236 | 359.0772 | 359.0769 | 5.18 | NEG | 11399604.14 | 11226822.86 | 11687738.93 | 1.525133223 | 1.528714149 | 1.533913317 | 1.529253563 | NZRDKNBIPVLNHA-UHFFFAOYSA-N | CC(=O)C1=CC(=C(C=C1)O)C(=O)O |  | 417632 |  |  | 83151 |  | 5-乙酰基水杨酸 | 酚类 | 单酚类 | Phenols | Monophenols | HY-107831 | HPLC≥98% | level2 |
| compound00450 | 1.08\_171.0765m/z | M+NH4 | C7H7NO3 | 40.1 | 0 | 0.57 | 5-Aminosalicylic Acid |  | 171.0764 | 171.0765 | 1.08 | POS | 2153.034629 | 2306.192148 | 1833.162671 | 0.000288051 | 0.000314025 | 0.000240587 | 0.000280888 | KBOPZPXVLCULAV-UHFFFAOYSA-N | NC1=CC(C(O)=O)=C(O)C=C1 | HMDB0014389 | 1145 |  | C07138 | 4075 | 89-57-6 | 5-氨基水杨酸 | 酚类 | 单酚类 | Phenols | Monophenols | HY-15027 | HPLC≥98% | level2 |
| compound00451 | 3.78\_363.0722m/z | M-H2O-H | C17H18O10 | 52 | 60.8 | 0.2 | 5-carboxy-7-glucosyloxy-2-methyl-benzopyran-gamma-one | 97.0285, 176.0466, 177.0549, 301.0718, 345.0614, 363.072 | 363.0722 | 363.0722 | 3.78 | NEG | 22511.80751 | 23138.80162 | 23176.49922 | 0.003011816 | 0.003150723 | 0.003041712 | 0.003068084 | YXPDWQIPHUQHKB-UHFFFAOYSA-N | CC1=CC(=O)C2=C(C=C(OC3OC(CO)C(O)C(O)C3O)C=C2O1)C(O)=O | HMDB0036377 | 91520 |  |  | 73981794 |  |  |  |  |  |  |  |  | level2 |
| compound00452 | 4.14\_367.1033m/z | M-H | C17H20O9 | 49.1 | 40.6 | -0.42 | 5-Feruloylquinic acid | 61.9874, 125.0236, 134.0364, 179.0346, 193.05, 197.0448, 366.1173, 367.1028 | 367.1035 | 367.1033 | 4.14 | NEG | 8036.042283 | 9128.843515 | 8287.344637 | 0.001075128 | 0.00124304 | 0.001087641 | 0.00113527 | RAGZUCNPTLULOL-KQJPBSFVSA-N | COC1=CC(\C=C\C(=O)O[C@@H]2C[C@](O)(C[C@@H](O)[C@@H]2O)C(O)=O)=CC=C1O | HMDB0240478 |  |  |  |  | 87099-72-7 | 5-O-阿魏酰奎尼酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N7929 | HPLC≥98% | level2 |
| compound00453 | 1.03\_102.0554m/z | M+H | C4H7NO2 | 57.7 | 95.9 | 4.08 | 5-Hydroxy-2-pyrrolidone | 57.0341, 60.045, 84.0448, 85.0288, 102.0552 | 102.055 | 102.0554 | 1.03 | POS | 109095.1171 | 110056.2309 | 113145.6074 | 0.014595646 | 0.014985942 | 0.014849369 | 0.014810319 | WBGWUCXEMSSZJL-UHFFFAOYSA-N | C1CC(=O)NC1O |  |  |  |  | 194148 |  |  |  |  |  |  |  |  | level2 |
| compound00454 | 6.40\_213.1126m/z | M+FA-H | C10H16O2 | 57.5 | 74.9 | -3.62 | 5-hydroxy-p-menth-6-en-2-one | 151.1118, 169.1225, 192.9895, 212.997, 213.112 | 213.1134 | 213.1126 | 6.4 | NEG | 8887.186319 | 9056.292857 | 9551.143084 | 0.001189001 | 0.001233161 | 0.001253504 | 0.001225222 | ZFUJCNJIGDBFEP-UHFFFAOYSA-N | CC1=CC(C(CC1=O)C(C)C)O |  |  |  |  | 6429208 |  |  |  |  |  |  |  |  | level2 |
| compound00455 | 5.10\_207.0292m/z | M+FA-H | C9H6O3 | 57.7 | 84.4 | -4.14 | 5-Hydroxycoumarin | 135.0441, 137.0234, 161.0447, 163.0392, 166.9923, 179.0344, 186.9987, 206.9872, 207.0056, 207.0289 | 207.0301 | 207.0292 | 5.1 | NEG | 8789.341165 | 9395.325572 | 8993.321964 | 0.001175911 | 0.001279326 | 0.001180295 | 0.001211844 | CDHSCTCRBLLCBJ-UHFFFAOYSA-N | C1=CC(=C2C=CC(=O)OC2=C1)O |  | 325483 |  |  | 5318179 |  |  |  |  |  |  |  |  | level2 |
| compound00456 | 4.50\_209.0450m/z | M-H | C10H10O5 | 57.1 | 0 | -2.74 | 5-Hydroxyferulic acid |  | 209.0455 | 209.045 | 4.5 | NEG | 6095.423128 | 6257.600754 | 6157.494087 | 0.000815496 | 0.000852074 | 0.000808117 | 0.000825229 | YFXWTVLDSKSYLW-NSCUHMNNSA-N | COC1=C(O)C(O)=CC(\C=C\C(O)=O)=C1 | HMDB0035484 |  |  | C05619 | 446834 | 110642-42-7 | 5-羟基阿魏酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-133068 | HPLC≥98% | level2 |
| compound00457 | 1.03\_275.1347m/z | M+NH4 | C10H15N3O5 | 40.3 | 2.5 | -0.97 | 5-Hydroxymethyldeoxycytidine monophosphate | 164.0704, 175.1189, 192.0652, 226.0708, 238.0708, 256.0814, 256.1265, 274.0916, 274.1385, 275.1344 | 275.135 | 275.1347 | 1.03 | POS | 239156.134 | 231282.6387 | 231430.0517 | 0.031996283 | 0.031492885 | 0.030373166 | 0.031287445 | HMUOMFLFUUHUPE-XLPZGREQSA-N | OC[C@@H]1[C@H](C[C@H](N2C(N=C(C(CO)=C2)N)=O)O1)O |  |  |  |  |  | 7226-77-9 | 5-羟甲基-2'-脱氧胞苷 | 其他 |  | Others |  | HY-131394 | HPLC≥98% | level2 |
| compound00458 | 2.41\_109.0288m/z | M+H-H2O | C6H6O3 | 49.8 | 46.9 | 3.51 | 5-Hydroxymethylfurfural | 80.0500, 81.0339, 81.0703, 82.0656, 89.5070, 91.0546, 98.5124, 108.0447, 108.0810, 109.0286 | 109.0285 | 109.0288 | 2.41 | POS | 34347.94031 | 35897.57851 | 38359.50428 | 0.004595351 | 0.004888038 | 0.005034349 | 0.004839246 | NOEGNKMFWQHSLB-UHFFFAOYSA-N | OCC1=CC=C(O1)C=O | HMDB0034355 | 68842 |  | C11101 | 237332 | 67-47-0 | 5-羟甲基糠醛 | 其他 |  | Others |  | HY-Y0051 | HPLC≥98% | level2 |
| compound00459 | 4.55\_381.0829m/z | M+FA-H | C16H16O8 | 47 | 1.9 | 0.39 | 5-O-Caffeoylshikimic acid | 169.0133, 187.0239, 193.0501, 205.0346, 207.9772, 314.2079, 336.1906, 337.2013, 380.1793, 381.0819 | 381.0827 | 381.0829 | 4.55 | NEG | 12992.88378 | 13340.28482 | 12816.39287 | 0.001738295 | 0.001816496 | 0.001682039 | 0.00174561 | QMPHZIPNNJOWQI-GDDAOPKQSA-N | O[C@@H]1C=C(C[C@@H](OC(=O)\C=C\C2=CC(O)=C(O)C=C2)[C@@H]1O)C(O)=O | HMDB0033999 | 64172 |  | C10434 | 5281762 | 73263-62-4 | 5-O-咖啡酰莽草酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N8321 | HPLC≥98% | level2 |
| compound00460 | 4.05\_541.1532m/z | M+Na | C22H30O14 | 41.5 | 0 | 0.73 | 6'-O-beta-D-Glucosylgentiopicroside |  | 541.1528 | 541.1532 | 4.05 | POS | 18662.23249 | 19425.96582 | 18389.67514 | 0.002496788 | 0.002645161 | 0.002413484 | 0.002518477 | BERNCPGDRADLCG-KEXDUYRESA-N | C=C[C@@H]1C2=CCOC(=O)C2=CO[C@H]1O[C@@H]1O[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 115713-06-9 | 6’-O-β-D-葡萄糖基龙胆苦苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N2100 | HPLC≥98% | level2 |
| compound00461 | 4.83\_729.2023m/z | M+H | C35H36O17 | 50.4 | 0 | -0.34 | 6'-p-hydroxybenzoylspinosin |  | 729.2025 | 729.2023 | 4.83 | POS | 41975.62972 | 42385.41088 | 40150.49585 | 0.005615847 | 0.005771462 | 0.005269401 | 0.005552236 | UEJBQAKFBPGCJC-YGGCYOLSSA-N | COC1=C(C(=C2C(=C1)OC(=CC2=O)C3=CC=C(C=C3)O)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)COC(=O)C6=CC=C(C=C6)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00462 | 5.40\_271.0593m/z | M+H | C15H10O5 | 50.6 | 0 | -3.09 | 6,7,4'-Trihydroxyisoflavone |  | 271.0601 | 271.0593 | 5.4 | POS | 10474.10268 | 10792.72343 | 10331.57841 | 0.001401312 | 0.001469604 | 0.001355929 | 0.001408949 | GYLUFQJZYAJQDI-UHFFFAOYSA-N | C1(O)=CC2OC=C(C3C=CC(O)=CC=3)C(=O)C=2C=C1O | HMDB0031715 | 47619 | LMPK12050102 | C14314 | 5284649 | 17817-31-1 | 4',6,7-三羟异黄酮 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | DH0120 | HPLC≥98% | level2 |
| compound00463 | 4.74\_201.1126m/z | M-H | C10H18O4 | 54.9 | 76.4 | -3.37 | 6,7-dihydroxy-3,7-dimethyloct-2-enoic acid | 72.9915, 155.1066, 183.102, 200.9975, 201.1125 | 201.1132 | 201.1126 | 4.74 | NEG | 6640.409428 | 6649.539679 | 6586.604764 | 0.000888409 | 0.000905443 | 0.000864434 | 0.000886095 | MUEMUGYSVXBBRL-UHFFFAOYSA-N | CC(=CC(=O)O)CCC(C(C)(C)O)O |  |  |  |  | 54091496 |  |  |  |  |  |  |  |  | level2 |
| compound00464 | 9.86\_315.1941m/z | M+H-H2O | C20H28O4 | 55.3 | 0 | -4.09 | 6-angeloylfuranofukinol |  | 315.1954 | 315.1941 | 9.86 | POS | 9239.024223 | 9470.149843 | 11012.59447 | 0.001236073 | 0.001289515 | 0.001445307 | 0.001323631 | QSXNOUPYXMWUKT-IZZDOVSWSA-N | C\C=C(/C)C(=O)OC1C2=C(CC3CCC(O)C(C)C13C)OC=C2C | HMDB0036146 | 91301 |  |  | 6374435 |  |  |  |  |  |  |  |  | level2 |
| compound00465 | 6.19\_302.0790n | M-H2O-H, M-H | C16H14O6 | 63.8 | 55.1 | -0.04 | 5,7,4'-Trihydroxy-8-methoxyflavanone | 197.0027, 271.1337, 285.0394, 286.0476, 300.1819, 300.9926, 301.0348, 301.0714 | 301.0718 | 301.0718 | 6.19 | NEG | 13112.68224 | 13063.02487 | 13527.18699 | 0.001754323 | 0.001778743 | 0.001775325 | 0.001769464 | OJCCBPWPNVUJFG-UHFFFAOYSA-N | C1C(O)=C(OC)C2OC(C3C=CC(O)=CC=3)CC(=O)C=2C=1O |  | 53147 | LMPK12140670 |  | 42608119 |  |  |  |  |  |  |  |  | level2 |
| compound00466 | 7.99\_360.1435m/z | M+NH4 | C19H18O6 | 48.8 | 0 | -1.91 | 5,7,3',4'-Tetramethoxyflavone |  | 360.1442 | 360.1435 | 7.99 | POS | 24256.70879 | 24099.18513 | 24462.70972 | 0.003245263 | 0.003281495 | 0.003210516 | 0.003245758 | CLXVBVLQKLQNRQ-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=C(OC)C(OC)=CC=3)=CC(=O)C=2C(OC)=C1 | HMDB0301862 | 49500 | LMPK12111074 |  | 631170 |  | 木犀草素四甲醚 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N7030 | HPLC≥98% | level2 |
| compound00467 | 9.03\_293.0818m/z | M-H2O-H | C18H16O5 | 48.3 | 0 | -0.56 | 5,6,7-Trimethoxyflavone |  | 293.0819 | 293.0818 | 9.03 | NEG | 7777.422867 | 7082.459262 | 7004.107116 | 0.001040528 | 0.000964392 | 0.000919228 | 0.000974716 | HJNJAUYFFFOFBW-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC=CC=3)=CC(=O)C=2C(OC)=C1OC | HMDB0128592 | 49525 | LMPK12111100 | C10024 | 442583 |  | 黄岑素-5,6,7-三甲醚 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-110398 | HPLC≥98% | level2 |
| compound00468 | 1.15\_314.0918m/z | M+H | C10H17ClFN3O5 | 50.3 | 71.4 | 1.28 | 5,4'-dihydroxyl-6,7-dimethoxyl-8-c-[β-d-xylo-copyranosyl-(1→2)]-β-d-glucopyranosylflavone | 97.0287, 136.0617, 296.0761, 313.1462, 314.0862 | 314.0914 | 314.0918 | 1.15 | POS | 133390.292 | 104501.7591 | 114489.3535 | 0.017846055 | 0.014229611 | 0.015025724 | 0.015700463 | CBBGXPAZNJYNHO-UHFFFAOYSA-N | CC(C(=O)O)NC(=O)C(CCC(C(C(=O)O)N)(F)Cl)N |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00469 | 5.01\_413.1217m/z | M+H-H2O | C22H22O9 | 51.9 | 57.4 | -3.16 | 4'-O-Methylpuerarin | 165.0182, 177.0544, 203.0337, 217.0493, 219.0286, 245.0443, 263.0548, 315.0855, 395.1121, 413.1227 | 413.123 | 413.1217 | 5.01 | POS | 105323.4527 | 107128.7092 | 109388.2797 | 0.014091042 | 0.014587313 | 0.014356253 | 0.014344869 | UWRLUNPRLSNXRR-UHFFFAOYSA-N | COC1=CC=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3C4C(C(C(C(O4)CO)O)O)O)O |  |  |  |  | 5319486 |  |  |  |  |  |  |  |  | level2 |
| compound00470 | 5.30\_553.1336m/z | M+Na | C26H26O12 | 41.8 | 0 | 3.7 | 4,5-Di-O-caffeoylquinic acid methyl ester |  | 553.1316 | 553.1336 | 5.3 | POS | 57102.84439 | 53690.26806 | 53483.75448 | 0.00763969 | 0.007310801 | 0.007019274 | 0.007323255 | PKJBSZTYNDRXEQ-GMGOHGFSSA-N | COC(=O)[C@@]1(O)C[C@@H](O)[C@H](OC(=O)/C=C/c2ccc(O)c(O)c2)[C@H](OC(=O)/C=C/c2ccc(O)c(O)c2)C1 |  |  |  |  |  | 188742-80-5 | 4,5-O-二咖啡酰基奎宁酸甲酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | B33146-5mg | HPLC≥97% | level2 |
| compound00471 | 0.92\_217.0347m/z | M+FA-H | C7H8O5 | 55.3 | 84.1 | -4.08 | 4,5-dihydroxy-3-oxocyclohexene-1-carboxylic acid | 111.0439, 115.0388, 127.0390, 128.0342, 129.0546, 133.0132, 155.0341, 199.0241, 217.0146, 217.0345 | 217.0356 | 217.0347 | 0.92 | NEG | 15356.81956 | 13748.11526 | 15062.88153 | 0.002054562 | 0.001872029 | 0.001976871 | 0.001967821 | SLWWJZMPHJJOPH-UHFFFAOYSA-N | C1C(C(C(=O)C=C1C(=O)O)O)O |  |  |  |  | 439774 | 2922-42-1 |  |  |  |  |  |  |  | level2 |
| compound00472 | 5.11\_252.1569m/z | M+Na | C12H23NO3 | 51.9 | 0 | -0.37 | 4,5-dihydroxy-N-(2-methylpropyl)oct-2-enamide |  | 252.157 | 252.1569 | 5.11 | POS | 2023.225232 | 2314.200532 | 2301.986704 | 0.000270684 | 0.000315116 | 0.000302116 | 0.000295972 | DVFBBRGYRFXMCJ-UHFFFAOYSA-N | CCCC(C(C=CC(=O)NCC(C)C)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00473 | 8.66\_337.1042m/z | M+Na | C18H18O5 | 55.8 | 0 | -1.55 | 4,7-Dihydroxy-5-methoxy-6-methyl-8-formylflavan |  | 337.1047 | 337.1042 | 8.66 | POS | 4345.047527 | 4951.441212 | 5108.604856 | 0.000581316 | 0.000674219 | 0.00067046 | 0.000641998 | DAAVAQORZATFQC-UHFFFAOYSA-N | CC1=C(C(=C2C(=C1OC)C(CC(O2)C3=CC=CC=C3)O)C=O)O |  |  |  |  | 129394 |  |  |  |  |  |  |  |  | level2 |
| compound00474 | 6.30\_299.1288m/z | 2M-H | C9H10O2 | 41.5 | 0 | -0.12 | 4-Allylcatechol |  | 299.1289 | 299.1288 | 6.3 | NEG | 3913.993534 | 3765.330337 | 3579.409564 | 0.000523646 | 0.000512711 | 0.000469766 | 0.000502041 | FHEHIXJLCWUPCZ-UHFFFAOYSA-N | C=CCC1=CC(=C(C=C1)O)O |  | 404919 |  |  | 70775 |  | 4-烯丙基邻苯二酚 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1887 | HPLC≥98% | level2 |
| compound00475 | 4.34\_181.0972m/z | M+NH4 | C9H9NO2 | 41 | 0 | 0.47 | 4-Aminocinnamic Acid |  | 181.0971 | 181.0972 | 4.34 | POS | 5884.876986 | 5975.855264 | 6264.707053 | 0.000787327 | 0.00081371 | 0.000822188 | 0.000807742 | JOLPMPPNHIACPD-ZZXKWVIFSA-N | Nc1ccc(/C=C/C(=O)O)cc1 |  |  |  |  |  | 2393-18-2 | 氨桂皮酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | ST08190120 | HPLC≥98% | level2 |
| compound00476 | 3.90\_190.0502m/z | M+H | C10H7NO3 | 52.6 | 0 | 1.71 | 4-Carboxycarbostyril |  | 190.0499 | 190.0502 | 3.9 | POS | 3096.7161 | 3357.571425 | 3534.81923 | 0.000414304 | 0.000457188 | 0.000463914 | 0.000445135 | MFSHNFBQNVGXJX-UHFFFAOYSA-N | C1=CC=C2C(=C1)C(=CC(=O)N2)C(=O)O |  | 434921 |  |  | 85076 |  |  |  |  |  |  |  |  | level2 |
| compound00477 | 4.92\_119.0493m/z | M+H-H2O | C8H8O2 | 41.6 | 0 | 1.23 | 4-Hydroxyacetophenone |  | 119.0492 | 119.0493 | 4.92 | POS | 1234.668117 | 1181.862932 | 1517.874877 | 0.000165184 | 0.00016093 | 0.000199208 | 0.000175107 | TXFPEBPIARQUIG-UHFFFAOYSA-N | CC(=O)C1=CC=C(C=C1)O |  | 68507 |  | C10700 | 7469 | 99-93-4 | 对羟基苯乙酮 | 其他 |  | Others |  | HY-Y0073 | HPLC≥98% | level2 |
| compound00478 | 2.12\_213.0400m/z | M+FA-H | C8H8O4 | 50.2 | 51.5 | -2.63 | 4-hydroxyacetyl-catechol | 72.9920, 85.0284, 87.0077, 129.0183, 151.0392, 167.0341, 169.0506, 186.9918, 195.0289, 213.0399 | 213.0406 | 213.04 | 2.12 | NEG | 4835.198597 | 5229.6215 | 5023.66157 | 0.000646893 | 0.000712098 | 0.000659312 | 0.000672767 | LNZSKFZHPHBUDI-UHFFFAOYSA-N | C1=CC(=C(C=C1C(=O)CO)O)O |  |  |  |  | 22134444 |  |  |  |  |  |  |  |  | level2 |
| compound00479 | 8.88\_309.0766m/z | M-H | C18H14O5 | 63.8 | 82.6 | -0.79 | 6-Deoxyjacareubin | 104.9531, 185.1171, 204.9888, 209.1175, 237.0917, 265.0869, 291.1961, 308.9978, 309.0763 | 309.0768 | 309.0766 | 8.88 | NEG | 60409.67653 | 63165.99715 | 62621.54692 | 0.008082106 | 0.008601076 | 0.008218529 | 0.00830057 | NHNIESSJWQBRJW-UHFFFAOYSA-N | CC1(C=CC2=C(O1)C=C3C(=C2O)C(=O)C4=C(O3)C(=CC=C4)O)C |  | 68101 |  | C10059 | 5281629 | 16265-56-8 |  |  |  |  |  |  |  | level2 |
| compound00480 | 4.84\_134.0601m/z | M+H | C8H7NO | 41.1 | 0 | 0.38 | 4-Hydroxybenzyl cyanide |  | 134.06 | 134.0601 | 4.84 | POS | 3485.97824 | 3413.452679 | 3365.020898 | 0.000466383 | 0.000464797 | 0.00044163 | 0.000457603 | AYKYOOPFBCOXSL-UHFFFAOYSA-N | OC1=CC=C(CC#N)C=C1 | HMDB0029757 | 34513 |  | C03766 | 26548 | 14191-95-8 | 对羟基苯乙腈 | 生物碱 |  | Alkaloids |  | HY-W015823 | HPLC≥98% | level2 |
| compound00481 | 6.97\_299.0923m/z | M-H | C17H16O5 | 60.9 | 94.9 | -0.54 | 4-Methoxymedicarpin | 269.0818, 299.0924 | 299.0925 | 299.0923 | 6.97 | NEG | 727913.151 | 719456.5346 | 732255.0121 | 0.097386235 | 0.097965684 | 0.096102054 | 0.097151324 | IPDALSAPRYQWGQ-UHFFFAOYSA-N | C1(O)C=CC2C3OC4=CC(OC)=CC=C4C3COC=2C=1OC | HMDB0034001 | 48163 | LMPK12070075 |  | 14077265 |  |  |  |  |  |  |  |  | level2 |
| compound00482 | 5.66\_159.0440m/z | M+H-H2O | C10H8O3 | 43.2 | 0 | -0.09 | 4-Methylumbelliferone |  | 159.0441 | 159.044 | 5.66 | POS | 3026.027621 | 3112.960692 | 3515.601363 | 0.000404847 | 0.00042388 | 0.000461392 | 0.00043004 | HSHNITRMYYLLCV-UHFFFAOYSA-N | CC1=CC(=O)OC2=C1C=CC(O)=C2 | HMDB0059622 | 65904 |  | C03081 | 5280567 | 90-33-5 | 7-羟基-4-甲基香豆素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0187 | HPLC≥98% | level2 |
| compound00483 | 11.32\_280.1459n | M+H, M+Na | C19H20O2 | 44.9 | 9.07 | -1.41 | 4-O-Methyl honokiol | 149.0233, 221.0962, 253.1585, 281.1529 | 281.1536 | 281.1532 | 11.32 | POS | 149999.0354 | 164849.039 | 164850.4372 | 0.02006811 | 0.022446872 | 0.021635175 | 0.021383386 | OQFHJKZVOALSPV-UHFFFAOYSA-N | COC1=CC=C(C=C1CC=C)C1=CC(CC=C)=CC=C1O | HMDB0246556 |  |  |  | 155160 |  | 4'-甲氧基-3',5-二-2-丙烯基-(1,1'-联苯)-2-醇 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | HY-U00450 | HPLC≥98% | level2 |
| compound00484 | 8.77\_285.1125m/z | M+H | C17H16O4 | 42.7 | 0 | 1.12 | 4-O-Methylechinatin |  | 285.1121 | 285.1125 | 8.77 | POS | 3054.545083 | 3130.52744 | 3597.967521 | 0.000408662 | 0.000426272 | 0.000472202 | 0.000435712 | LNEYYODFMSUKGY-UXBLZVDNSA-N | COC1=CC(=C(C=C1)/C=C/C(=O)C2=CC=C(C=C2)O)OC |  |  |  |  |  | 151135-64-7 | 4-O-甲基刺甘草查尔酮 | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | DJ0356 | HPLC≥98% | level2 |
| compound00485 | 4.66\_593.1515m/z | M-H | C27H30O15 | 51.7 | 15.3 | 0.55 | 4”-O-Glucosylvitexin | 285.0402, 308.0324, 323.0559, 443.0981, 593.1503 | 593.1512 | 593.1515 | 4.66 | NEG | 264486.9542 | 275312.6113 | 259869.5843 | 0.03538525 | 0.03748828 | 0.034105606 | 0.035659712 | NDSUKTASTPEKBX-YGBVHABKSA-N | O=c1cc(-c2ccc(O)cc2)oc2c(C3O[C@H](CO)[C@@H](O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)c(O)cc(O)c12 |  |  |  |  |  | 76135-82-5 | 牡荆素葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0533 | HPLC≥98% | level2 |
| compound00486 | 1.13\_362.0507m/z | M-H | C10H14N5O8P | 53.5 | 69.4 | 0.03 | 5'-GMP;5'-guanosine monophosphate | 78.958, 128.0346, 150.0413, 191.0186, 211.0006, 362.0504 | 362.0507 | 362.0507 | 1.13 | NEG | 19231.66054 | 18885.8129 | 19393.66076 | 0.00257297 | 0.00257161 | 0.002545248 | 0.002563276 | RQFCJASXJCIDSX-UHFFFAOYSA-N | OC1C(COP(O)(O)=O)OC(C1O)N1C=NC2=C1NC(=N)N=C2O | HMDB0257693 |  |  |  | 135400774 |  |  |  |  |  |  |  |  | level2 |
| compound00487 | 10.64\_283.0960m/z | M+H-H2O | C17H16O5 | 42.1 | 0 | -1.54 | 4',7-Di-O-methylnaringenin |  | 283.0965 | 283.096 | 10.64 | POS | 10662.10587 | 10816.39879 | 11290.61114 | 0.001426465 | 0.001472828 | 0.001481794 | 0.001460362 | CKEXCBVNKRHAMX-HNNXBMFYSA-N | COC1=CC=C(C=C1)C2CC(=O)C3=C(C=C(C=C3O2)OC)O |  | 709756 |  |  | 14057196 |  | 4',7-二甲基柚皮素 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N1884 | HPLC≥98% | level2 |
| compound00488 | 5.17\_253.0491m/z | M+H-H2O | C15H10O5 | 45.1 | 0 | -1.49 | 7,3',4'-trihydroxyflavone |  | 253.0495 | 253.0491 | 5.17 | POS | 12899.45407 | 12897.62082 | 12433.89346 | 0.001725796 | 0.00175622 | 0.00163184 | 0.001704619 | PVFGJHYLIHMCQD-UHFFFAOYSA-N | C1(O)=CC2OC(C3C=C(O)C(O)=CC=3)=CC(=O)C=2C=C1 | HMDB0133311 | 48478 | LMPK12110042 |  | 5322065 |  | 3’,4’,7-三羟基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | B29083-10mg | HPLC≥98% | level2 |
| compound00489 | 2.54\_203.1393m/z | M+H | C9H18N2O3 | 45.5 | 30.5 | 1.2 | Alanyleucine | 128.9507, 129.1385, 130.9664, 132.1019, 157.1334, 184.1333, 186.1124, 202.1790, 203.0523, 203.1390 | 203.139 | 203.1393 | 2.54 | POS | 27264.13795 | 26975.29879 | 28077.73356 | 0.003647622 | 0.003673125 | 0.003684956 | 0.003668568 | RDIKFPRVLJLMER-BQBZGAKWSA-N | CC(C)C[C@H](NC(=O)[C@H](C)N)C(O)=O | HMDB0028691 | 44268 |  |  | 96801 | 3303-34-2 | L-丙氨酰-L-亮氨酸 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-W040088 | HPLC≥98% | level2 |
| compound00490 | 4.39\_757.2192m/z | M+H | C33H40O20 | 43.3 | 0 | 0.86 | Alcesefoliside |  | 757.2186 | 757.2192 | 4.39 | POS | 10444.00216 | 9731.320285 | 8900.061266 | 0.001397285 | 0.001325077 | 0.001168055 | 0.001296806 | HKNBJSRIYRDSLB-MIORVHIISA-N | C1(O)=CC2OC(C3C=C(O)C(O)=CC=3)=C(O[C@H]3[C@H](O[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)[C@@H](O)[C@@H](O)[C@@H](CO[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)O3)C(=O)C=2C(O)=C1 |  |  | LMPK12112060 |  | 11828754 |  | 粗叶悬钩子甙 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DC0090-0005 | HPLC≥98% | level2 |
| compound00491 | 10.55\_471.3477m/z | M-H | C30H48O4 | 51.3 | 0 | -0.63 | alnigenic acid | 470.9955, 471.3475 | 471.348 | 471.3477 | 10.55 | NEG | 18358.3026 | 20415.99037 | 16401.16595 | 0.002456125 | 0.002779968 | 0.002152509 | 0.002462868 | NOHMTCLUYAVQEY-UHFFFAOYSA-N | CC1(CCC2(C(CC3(C(=C2C1)CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C)O)C(=O)O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00492 | 6.97\_315.0873m/z | M+FA-H | C16H14O4 | 41.8 | 0 | -0.51 | Alpinetin |  | 315.0874 | 315.0873 | 6.97 | NEG | 6561.962959 | 5949.569388 | 6057.141299 | 0.000877914 | 0.00081013 | 0.000794947 | 0.000827664 | QQQCWVDPMPFUGF-ZDUSSCGKSA-N | COC1=CC(=CC2=C1C(=O)CC(O2)C3=CC=CC=C3)O |  | 52704 |  |  | 154279 |  | 山姜素 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0625A | HPLC≥98% | level2 |
| compound00493 | 7.02\_301.0716m/z | M-H | C16H14O6 | 52 | 21.4 | -0.58 | Alysifolinone | 164.0107, 286.0479, 301.07 | 301.0718 | 301.0716 | 7.02 | NEG | 110058.6234 | 106942.6048 | 107609.0136 | 0.014724552 | 0.014561971 | 0.01412274 | 0.014469754 | YNYGAMJOLICYES-AWEZNQCLSA-N | C1(O)C=C2O[C@H](C3C=C(OC)C=C(O)C=3)CC(=O)C2=C(O)C=1 |  | 52710 | LMPK12140222 |  | 42607889 |  |  |  |  |  |  |  |  | level2 |
| compound00494 | 5.53\_585.1606m/z | M-H | C29H30O13 | 42.6 | 0 | -1.39 | Amarogentin |  | 585.1614 | 585.1606 | 5.53 | NEG | 9936.690216 | 9907.538744 | 8219.210896 | 0.001329413 | 0.001349072 | 0.001078699 | 0.001252395 | DBOVHQOUSDWAPQ-WTONXPSSSA-N | C=CC1C2CCOC(=O)C2=COC1OC3C(C(C(C(O3)CO)O)O)OC(=O)C4=C(C=C(C=C4O)O)C5=CC(=CC=C5)O |  | 73556 |  | C09767 | 115149 | 21018-84-8 | 苦杏苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N2447 | HPLC≥98% | level2 |
| compound00495 | 6.37\_331.1914m/z | M-H2O-H | C20H30O5 | 47.7 | 3.92 | -0.15 | Andropanolide | 331.1169, 331.1223, 331.1541, 331.1914 | 331.1915 | 331.1914 | 6.37 | NEG | 34914.54814 | 35546.80841 | 37283.591 | 0.004671157 | 0.004840275 | 0.004893145 | 0.004801525 | BOJKULTULYSRAS-QPSYGYIJSA-N | C=C1CC[C@H]2[C@@](C)(CC[C@@H](O)[C@@]2(C)CO)[C@@H]1C/C=C1\C(=O)OC[C@H]1O |  |  |  |  |  | 869807-57-8 | 穿心莲内酯 | 萜类 | 二萜类 | Terpenes | Diterpenes | DY0599 | HPLC≥98% | level2 |
| compound00496 | 5.70\_291.0871m/z | M-H | C15H16O6 | 42.9 | 0 | -1.21 | Angelicain |  | 291.0874 | 291.0871 | 5.7 | NEG | 5960.349399 | 5942.200105 | 5751.918781 | 0.000797425 | 0.000809127 | 0.000754889 | 0.000787147 | FHCHSXPHLRBEBR-UHFFFAOYSA-N | CC(C)(O)C1CC2=C(O)C3=C(OC(CO)=CC3=O)C=C2O1 | HMDB0030120 | 86735 |  |  | 11022681 | 49624-66-0 | 去甲升麻素 | 酚类 | 单酚类 | Phenols | Monophenols | HY-N6941 | HPLC≥98% | level2 |
| compound00497 | 10.34\_402.1310m/z | M+Na | C22H21NO5 | 43.5 | 0 | -0.54 | Angoline |  | 402.1312 | 402.131 | 10.34 | POS | 21462.08955 | 19815.39252 | 24678.92367 | 0.002871376 | 0.002698187 | 0.003238892 | 0.002936152 | LVWAKZBZWYHYCJ-UHFFFAOYSA-N | CN1C(C2=C(C=CC(=C2OC)OC)C3=C1C4=CC5=C(C=C4C=C3)OCO5)OC |  | 67611 |  | C09336 | 189060 | 21080-31-9 | 6-甲氧基二氢白屈菜红碱 | 生物碱 |  | Alkaloids |  | HY-N7674 | HPLC≥98% | level2 |
| compound00498 | 7.07\_347.1862m/z | M-H2O-H | C20H30O6 | 60.6 | 17.1 | -0.64 | Anhydrocinnzeylanol | 245.1544, 255.1389, 273.15, 285.1494, 299.1651, 303.1603, 347.1485, 347.1879 | 347.1864 | 347.1862 | 7.07 | NEG | 64311.61433 | 66809.45108 | 66394.46644 | 0.008604139 | 0.009097191 | 0.008713692 | 0.008805007 | JFDHTDLZWVKRQT-UHFFFAOYSA-N | CC(C)C1=C(C)C2(O)C(O)(C1)C1(C)CC(=O)OC22C(O)C(C)CCC12O | HMDB0036863 | 91866 |  |  | 73099741 | 65230-04-8 |  |  |  |  |  |  |  | level2 |
| compound00499 | 9.67\_314.1518n | M-H, M+FA-H, 2M-H | C19H22O4 | 45.1 | 6.84 | -0.01 | Anisocoumarin H | 187.0756, 213.0912, 213.1276, 269.1544, 313.1445 | 313.1445 | 313.1445 | 9.67 | NEG | 4915939.696 | 4870304.672 | 4897240.196 | 0.657695027 | 0.663171029 | 0.642719862 | 0.654528639 | VNADFOGBKXRWGC-RIYZIHGNSA-N | CC(=CC(CC(=CCOC1=CC2=C(C=C1)C=CC(=O)O2)C)O)C |  | 985372 |  |  | 14376449 |  | 5’-羟基葡萄内酯 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DQ0473-0005 | HPLC≥98% | level2 |
| compound00500 | 4.85\_477.1034m/z | M+FA-H | C21H20O10 | 48.2 | 0 | -1.06 | Apigenin 5-O-glucoside |  | 477.1039 | 477.1034 | 4.85 | NEG | 5455.23752 | 4613.239589 | 4413.360848 | 0.000729847 | 0.000628167 | 0.000579215 | 0.000645743 | ZFPMFULXUJZHFG-QNDFHXLGSA-N | C1(O)=CC2OC(C3C=CC(O)=CC=3)=CC(=O)C=2C(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=C1 |  |  | LMPK12110339 |  | 14730806 |  | 芹菜素-5-O-葡萄糖苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DA0115 | HPLC≥98% | level2 |
| compound00501 | 4.65\_535.1428m/z | M+H | C25H26O13 | 44.2 | 0 | -3.47 | Apigenin-6-C-beta-D-xylopyranosyl-8-C-alpha-L-arabinopyranoside |  | 535.1446 | 535.1428 | 4.65 | POS | 5216.186545 | 4988.822047 | 5147.550027 | 0.000697865 | 0.000679309 | 0.000675571 | 0.000684248 | LDVNKZYMYPZDAI-LUCKJMCUSA-N | O=c1cc(-c2ccc(O)cc2)oc2c([C@H]3OC[C@H](O)[C@H](O)[C@H]3O)c(O)c([C@@H]3OC[C@@H](O)[C@H](O)[C@H]3O)c(O)c12 |  |  |  |  |  | 85700-46-5 | 6-甲氧基-2-[2-(3’-甲氧基苯) 乙基]色原酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DQ0456-0005 | HPLC≥98% | level2 |
| compound00502 | 4.26\_623.1619m/z | M+FA-H | C27H30O14 | 58.8 | 92.3 | 0.18 | Apigenin-8-C-glucoside-2'-rhamnoside | 312.0639, 383.0772, 413.0876, 623.1617 | 623.1618 | 623.1619 | 4.26 | NEG | 645754.7149 | 641886.6098 | 641003.4463 | 0.086394401 | 0.08740328 | 0.084126085 | 0.085974589 | LYGPBZVKGHHTIE-NQQFNCMQSA-N | C[C@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]2c2c(O)cc(O)c3c(=O)cc(-c4ccc(O)cc4)oc23)[C@@H](O)[C@@H](O)[C@@H]1O |  |  |  |  | 53486256 | 64820-99-1 |  |  |  |  |  |  |  | level2 |
| compound00503 | 8.74\_332.1618n | M+NH4, M+Na, M+H, M+H-H2O | C19H24O5 | 47.3 | 5.52 | -1.81 | Arnicolide D | 307.13, 315.159, 333.1691, 349.1983 | 333.1697 | 333.169 | 8.74 | POS | 296143.2063 | 297893.1353 | 299127.9409 | 0.039620485 | 0.040562985 | 0.039257921 | 0.039813797 | NZESEVTYUVXOTC-APDQSUQKSA-N | O=C(OC1C2C(OC(=O)C2C)CC(C)C3C=CC(=O)C13C)C(=C)C |  |  |  |  |  |  | 山金车内酯 D | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | HY-N6843 | HPLC≥98% | level2 |
| compound00504 | 7.91\_321.1095m/z | M+K | C15H22O5 | 55.5 | 0 | -1.18 | artemisinin g |  | 321.1099 | 321.1095 | 7.91 | POS | 18365.9476 | 18247.15829 | 19055.04265 | 0.002457148 | 0.002484647 | 0.002500807 | 0.002480867 | GUSFNHMDMCPUPO-DYLBMRNYSA-N | C[C@@H]1CC[C@H]2[C@H](C(=O)O[C@@H]([C@@]23[C@H]1CCO3)OC(=O)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00505 | 0.87\_218.1136m/z | M+H | C8H15N3O4 | 40.1 | 0 | 0.34 | Alanyglutamine |  | 218.1135 | 218.1136 | 0.87 | POS | 5083.842032 | 4197.345826 | 5352.348218 | 0.000680158 | 0.000571537 | 0.000702449 | 0.000651381 | HJCMDXDYPOUFDY-WHFBIAKZSA-N | C[C@H](N)C(=O)N[C@@H](CCC(N)=O)C(O)=O | HMDB0028685 | 85601 |  |  | 123935 | 39537-23-0 | L-丙氨酸-L-谷氨酰胺 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-W014102 | HPLC≥98% | level2 |
| compound00506 | 4.88\_317.1028m/z | M-H | C17H18O6 | 46.6 | 0 | -0.67 | Agarotetrol |  | 317.1031 | 317.1028 | 4.88 | NEG | 9121.273846 | 9601.676098 | 10138.38706 | 0.001220319 | 0.001307424 | 0.001330574 | 0.001286106 | CWMIROLCTHMEEO-JJXSEGSLSA-N | O=c1cc(CCc2ccccc2)oc2c1[C@H](O)[C@@H](O)[C@@H](O)[C@@H]2O |  |  |  |  |  | 69809-22-9 | 沉香四醇 | 其他 |  | Others |  | HY-N1468 | HPLC≥98% | level2 |
| compound00507 | 4.22\_319.0823m/z | M+FA-H | C15H14O5 | 41.5 | 6.05 | -0.2 | Afzelechin | 241.0506, 242.0571, 245.0814, 256.0735, 257.0815, 271.0972, 275.0923, 318.1497, 319.0446, 319.0830 | 319.0823 | 319.0823 | 4.22 | NEG | 11239.16861 | 11367.13894 | 11714.49285 | 0.001503669 | 0.00154782 | 0.001537425 | 0.001529638 | RSYUFYQTACJFML-DZGCQCFKSA-N | C1(O)C=C2O[C@]([H])(C3C=CC(O)=CC=3)[C@@]([H])(O)CC2=C(O)C=1 |  | 47251 | LMPK12020035 | C09320 | 442154 |  | 阿夫儿茶精 | 酚类 | 多酚类 | Phenols | Polyphenols | B30001-5mg | HPLC≥98% | level2 |
| compound00508 | 6.71\_295.0610m/z | M-H2O-H | C17H14O6 | 56.5 | 66.9 | -0.71 | Aflatoxin B2 alpha | 251.1064, 254.9843, 280.0377, 295.0609 | 295.0612 | 295.061 | 6.71 | NEG | 15602.01147 | 15251.71079 | 16064.23161 | 0.002087366 | 0.002076768 | 0.00210829 | 0.002090808 | WWSYXEZEXMQWHT-UHFFFAOYSA-N | COC1=CC2=C(C3CCOC3O2)C2=C1C1=C(C(=O)CC1)C(=O)O2 | HMDB0035208 |  |  | C16753 | 23648 | 7220-81-7 |  |  |  |  |  |  |  | level2 |
| compound00509 | 7.04\_267.0650m/z | M+H-H2O | C16H12O5 | 51.7 | 0 | -0.67 | 7,4'-Dihydroxy-8-methoxyisoflavone |  | 267.0652 | 267.065 | 7.04 | POS | 13275.7619 | 13449.73031 | 12339.2235 | 0.001776141 | 0.001831399 | 0.001619415 | 0.001742318 | UBLJWIMJOYYSCU-UHFFFAOYSA-N | COC1=C(C=CC2=C1OC=C(C2=O)C3=CC=C(C=C3)O)O |  | 972960 |  |  | 71428798 |  |  |  |  |  |  |  |  | level2 |
| compound00510 | 5.71\_291.1202m/z | M+Na | C14H20O5 | 53.6 | 0 | -0.53 | 7,8-dihydroxy-isobutyryl-thymol |  | 291.1203 | 291.1202 | 5.71 | POS | 3562.364026 | 4209.828627 | 4596.089029 | 0.000476602 | 0.000573236 | 0.000603196 | 0.000551012 | OHCHAAIKJDAFAY-UHFFFAOYSA-N | CC(C)C(=O)OCC(C)(C1=C(C=C(C=C1)CO)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00511 | 10.11\_328.1902m/z | M+NH4 | C20H22O3 | 50.1 | 0 | -1.65 | 7-(4-Hydroxy-3-methoxyphenyl)-1-phenylhept-4-en-3-one |  | 328.1907 | 328.1902 | 10.11 | POS | 3706.116579 | 3781.349948 | 4179.235419 | 0.000495835 | 0.000514892 | 0.000548488 | 0.000519738 | NOHMOWQGVDSLNY-UHFFFAOYSA-N | COC1=C(C=CC(=C1)CCC=CC(=O)CCC2=CC=CC=C2)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00512 | 5.77\_207.0653m/z | M+H | C11H10O4 | 54.4 | 41 | 0.47 | 7-Methoxy-4-methyl-coumarin-8-ol | 207.065 | 207.0652 | 207.0653 | 5.77 | POS | 34947.87719 | 35296.49545 | 33906.00815 | 0.004675616 | 0.004806191 | 0.004449866 | 0.004643891 | HHSJFOILNWMNFO-UHFFFAOYSA-N | O=C1C=C(C)C2=CC=C(OC)C(O)=C2O1 |  |  |  |  |  | 22084-94-2 | 4-甲基瑞香素7-甲基醚 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N10015 | HPLC≥98% | level2 |
| compound00513 | 8.45\_311.2227m/z | M-H2O-H | C18H34O5 | 59.2 | 40.4 | -0.36 | 8,11,12-trihydroxyoctadec-9-enoic acid | 174.9551, 223.1122, 267.1024, 293.2124, 311.0926, 311.2225 | 311.2228 | 311.2227 | 8.45 | NEG | 91869.01715 | 92323.45704 | 95131.40629 | 0.012290996 | 0.012571337 | 0.012485163 | 0.012449166 | YFCZLXRIKFCQFU-UHFFFAOYSA-N | CCCCCCC(C(C=CC(CCCCCCC(=O)O)O)O)O |  |  |  |  | 5321949 |  |  |  |  |  |  |  |  | level2 |
| compound00514 | 4.69\_383.1321m/z | M+Na | C16H24O9 | 44.2 | 0 | 2.27 | 8-epideoxyloganic acid |  | 383.1312 | 383.1321 | 4.69 | POS | 9979.939763 | 9561.260352 | 10562.0311 | 0.001335199 | 0.001301921 | 0.001386174 | 0.001341098 | DSXFHNSGLYXPNG-SPLNBZCLSA-N | C[C@@H]1CC[C@@H]2C(C(=O)O)=CO[C@@H](O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)C21 |  |  |  |  |  | 88668-99-9 | 8-表-脱氧马钱酸 | 萜类 | 单萜类 | Terpenes | Monoterpenes | B31123-5mg | HPLC≥98% | level2 |
| compound00515 | 5.98\_755.1580m/z | M+Na | C37H32O16 | 40.7 | 0 | -0.39 | 9'''-MethyllithosperMateB |  | 755.1583 | 755.158 | 5.98 | POS | 16431.81029 | 15814.29753 | 16333.50335 | 0.002198383 | 0.002153373 | 0.002143629 | 0.002165129 | HBYGJMZNCIGGFN-CNJKJOQLSA-N | COC(=O)[C@@H](Cc1ccc(O)c(O)c1)OC(=O)/C=C/c1ccc(O)c2c1[C@@H](C(=O)O[C@H](Cc1ccc(O)c(O)c1)C(=O)O)[C@H](c1ccc(O)c(O)c1)O2 |  |  |  |  |  | 1167424-31-8 | 9'''-丹酚酸B单甲酯 | 酚类 | 多酚类 | Phenols | Polyphenols | DD0017 | HPLC≥98% | level2 |
| compound00516 | 7.86\_327.2176m/z | M-H | C18H32O5 | 53 | 47.4 | -0.27 | 9,10,11-trihydroxyoctadeca-12,15-dienoic acid | 155.1064, 171.1017, 185.118, 197.1175, 201.112, 209.118, 309.206, 327.1237, 327.2174 | 327.2177 | 327.2176 | 7.86 | NEG | 504000.2827 | 511635.3628 | 507955.9801 | 0.067429322 | 0.069667459 | 0.066664771 | 0.067920517 | KFINXCASWPGHEW-UHFFFAOYSA-N | CCC=CCC=CC(C(C(CCCCCCCC(=O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00517 | 6.45\_247.0973m/z | M-H | C14H16O4 | 51.7 | 47.8 | -1.03 | 6beta-hydroxyfraxinellone | 147.0447, 147.0805, 176.9973, 178.9565, 178.9918, 203.1071, 206.9871, 226.9933, 247.0013, 247.0972 | 247.0976 | 247.0973 | 6.45 | NEG | 7297.667934 | 7107.308715 | 7119.062323 | 0.000976342 | 0.000967775 | 0.000934315 | 0.000959477 | ZCEUBPHEBYXFLM-VHRBIJSZSA-N | CC1=C2C(=O)O[C@H]([C@@]2(CC[C@@H]1O)C)C3=COC=C3 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00518 | 8.98\_345.1706m/z | M-H | C20H26O5 | 54.2 | 2.86 | -0.47 | [(3aR,4S,6E,9S,10Z,11aR)-9-hydroxy-6,10-dimethyl-3-methylene-2-oxo-3a,4,5,8,9,11a-hexahydrocyclodeca[b]furan-4-yl] (E)-2-methylbut-2-enoate | 330.1466, 345.0001, 345.1711 | 345.1707 | 345.1706 | 8.98 | NEG | 170300.899 | 177075.7169 | 176656.7684 | 0.022784261 | 0.024111733 | 0.023184653 | 0.023360216 | QFINJHBXXJQKPB-PJCXTRSKSA-N | C/C=C(\C)/C(=O)O[C@H]1C/C(=C/C[C@@H](/C(=C\[C@@H]2[C@@H]1C(=C)C(=O)O2)/C)O)/C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00519 | 0.78\_209.0295m/z | M-H | C6H10O8 | 54.4 | 80.5 | -3.85 | a hexaric acid | 71.0128, 85.0285, 87.0077, 89.0234, 111.0076, 129.0184, 133.0134, 159.0291, 191.0192, 209.0315 | 209.0303 | 209.0295 | 0.78 | NEG | 59148.53917 | 57484.63469 | 57530.65209 | 0.00791338 | 0.007827466 | 0.007550394 | 0.007763747 | DSLZVSRJTYRBFB-UHFFFAOYSA-N | C(C(C(C(=O)O)O)O)(C(C(=O)O)O)O | HMDB0029881 | 3343 |  | C00818 | 607 | 87-73-0 |  |  |  |  |  |  |  | level2 |
| compound00520 | 5.56\_493.2286m/z | M+FA-H | C21H36O10 | 40.7 | 0 | -1.07 | A-D-Glucopyranoside |  | 493.2291 | 493.2286 | 5.56 | NEG | 13707.58733 | 12843.85761 | 14941.36697 | 0.001833914 | 0.0017489 | 0.001960923 | 0.001847912 | RVQFSOHDFFWTLD-ZZUMIZGVSA-N | CC1(C)[C@H]2CC[C@]1(C)[C@H](O[C@@H]1OC(CO[C@@H]3OC[C@](O)(CO)[C@H]3O)[C@@H](O)[C@H](O)[C@H]1O)C2 |  |  |  |  |  | 88700-35-0 | 龙脑7-O-[β-D-呋喃芹菜糖基-(1→6)]-β-D-吡喃葡萄糖苷 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | DL0126 | HPLC≥98% | level2 |
| compound00521 | 3.91\_219.1131m/z | M+H | C12H14N2O2 | 41.1 | 0 | 1.31 | Abrine |  | 219.1128 | 219.1131 | 3.91 | POS | 2620.858514 | 2338.835805 | 2685.576738 | 0.00035064 | 0.00031847 | 0.000352458 | 0.000340523 | CZCIKBSVHDNIDH-NSHDSACASA-N | CNC(CC1=CNC2=CC=CC=C21)C(=O)O |  | 44665 |  | C02983 | 160511 | 526-31-8 | 相思子碱 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino Acids | HY-N1436 | HPLC≥98% | level2 |
| compound00522 | 1.35\_297.1191m/z | M+FA-H | C10H20O7 | 54.1 | 69.1 | 0.08 | Acetoin glucoside | 135.0438, 159.0287, 161.0438, 208.0709, 210.1248, 213.0017, 251.1131, 252.1454, 297.0605, 297.1184 | 297.1191 | 297.1191 | 1.35 | NEG | 225505.5834 | 223655.5364 | 228159.3744 | 0.03017 | 0.030454331 | 0.029943919 | 0.030189417 | ZLXYJEYKAQYNPV-UHFFFAOYSA-N | CC(O)C(C)OC1OC(CO)C(O)C(O)C1O | HMDB0040822 | 95284 |  |  | 78171387 | 146763-54-4 |  |  |  |  |  |  |  | level2 |
| compound00523 | 5.20\_179.0701m/z | M+H-H2O | C10H12O4 | 43 | 0 | -0.94 | Acetosyringone |  | 179.0703 | 179.0701 | 5.2 | POS | 2916.133148 | 3095.128731 | 2926.866624 | 0.000390144 | 0.000421452 | 0.000384126 | 0.000398574 | OJOBTAOGJIWAGB-UHFFFAOYSA-N | CC(=O)C1=CC(=C(C(=C1)OC)O)OC |  | 43832 |  | C10664 | 17198 | 2478-38-8 | 乙酰丁香酮 | 其他 |  | Others |  | HY-W009884 | HPLC≥98% | level2 |
| compound00524 | 7.67\_347.1863m/z | M-H | C20H28O5 | 53.9 | 60 | -0.4 | adenostemmoic acid b | 317.1761, 347.1473, 347.1857 | 347.1864 | 347.1863 | 7.67 | NEG | 184457.4061 | 193072.999 | 190463.587 | 0.024678236 | 0.026290022 | 0.024996677 | 0.025321645 | UVEPVLCUQGRNSH-UHFFFAOYSA-N | CC1(CCCC2(C1CCC34C2(C(CC(C3)C(=C)C4=O)O)O)C)C(=O)O |  |  |  |  | 21672519 |  |  |  |  |  |  |  |  | level2 |
| compound00525 | 6.17\_347.1863m/z | M-H2O-H | C20H30O6 | 59.2 | 86.6 | -0.26 | Adenostemmoic acid D | 255.1387, 303.1962, 347.1485, 347.1873 | 347.1864 | 347.1863 | 6.17 | NEG | 55461.9764 | 56442.91716 | 57409.19534 | 0.007420161 | 0.007685619 | 0.007534454 | 0.007546745 | QDNKMJSMTIFSMN-UHFFFAOYSA-N | CC12CCCC(C1CCC34C2C(CC(C3)C(C4=O)(CO)O)O)(C)C(=O)O |  |  |  |  | 23260141 |  |  |  |  |  |  |  |  | level2 |
| compound00526 | 7.56\_329.1394m/z | M-H2O-H | C19H24O6 | 57.6 | 73.7 | -0.03 | 9-Hydroxyglabratolide | 139.1119, 171.1018, 211.1333, 229.1442, 241.1598, 255.1392, 285.1493, 299.1274, 329.1418 | 329.1394 | 329.1394 | 7.56 | NEG | 547087.5333 | 547525.049 | 534408.5156 | 0.07319389 | 0.074554422 | 0.070136435 | 0.072628249 | YAVQKFOMLWQFEM-JWCOLNTHSA-N | C/C/1=C\C2C(C(C(/C(=C\CC1)/C=O)O)OC(=O)C(C)C)C(=C)C(=O)O2 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00527 | 8.56\_272.0915m/z | M+NH4 | C15H10O4 | 43.8 | 0 | -1.04 | 4',5-Dihydroxyflavone |  | 272.0918 | 272.0915 | 8.56 | POS | 7463.184347 | 7880.968624 | 7464.871687 | 0.000998486 | 0.001073122 | 0.000979699 | 0.001017102 | OKRNDQLCMXUCGG-UHFFFAOYSA-N | C1=CC(=C2C(=C1)OC(=CC2=O)C3=CC=C(C=C3)O)O |  | 359320 |  |  | 165521 |  | 5,4 '-二羟基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N1881 | HPLC≥98% | level2 |
| compound00528 | 8.57\_313.1069m/z | M+H | C18H16O5 | 43.5 | 0 | -0.38 | 4',5,7-Trimethoxyflavone |  | 313.1071 | 313.1069 | 8.57 | POS | 3039.893419 | 3288.024755 | 2705.914103 | 0.000406702 | 0.000447718 | 0.000355128 | 0.000403183 | ZXJJBDHPUHUUHD-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC(OC)=CC=3)=CC(=O)C=2C(OC)=C1 | HMDB0030842 | 43862 | LMPK12111071 |  | 79730 | 5631-70-9 | 4',5,7-三甲氧基黄酮 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N6818 | HPLC≥98% | level2 |
| compound00529 | 8.90\_311.1273m/z | M+H | C19H18O4 | 62.3 | 95.4 | -1.45 | 3α-hydroxytanshinone iia | 265.1203, 267.1374, 275.1061, 283.1311, 293.1143, 311.1251 | 311.1278 | 311.1273 | 8.9 | POS | 2441818.034 | 2438059.405 | 2398863.164 | 0.32668659 | 0.331981359 | 0.314829769 | 0.32449924 | PTDUBPDLRWKSBQ-UHFFFAOYSA-N | CC1=COC2=C1C(=O)C(=O)C3=C2C=CC4=C3CCC(C4(C)C)O |  |  |  |  | 14610644 |  |  |  |  |  |  |  |  | level2 |
| compound00530 | 4.51\_371.0984m/z | M+FA-H | C15H18O8 | 53.1 | 53.8 | 0.02 | (z)-8-β-d-glucopyranosyloxycinnamicacid | 113.0237, 121.0285, 249.0612, 371.0974 | 371.0984 | 371.0984 | 4.51 | NEG | 119452.4523 | 118640.2382 | 117796.4014 | 0.015981336 | 0.016154794 | 0.015459745 | 0.015865292 | IFJZNZBKGRGNSP-UHFFFAOYSA-N | C1=CC=C(C=C1)C=C(C(=O)O)OC2C(C(C(C(O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00531 | 6.00\_301.2019m/z | M+FA-H | C15H28O3 | 56.2 | 3.1 | -0.46 | 1 beta,4 beta,7 alpha-trihydroxyeudcsmane | 143.0711, 183.1018, 197.0026, 300.9968, 301.109, 301.1447, 301.2033 | 301.2021 | 301.2019 | 6 | NEG | 11505.62652 | 11831.05763 | 12029.02767 | 0.001539318 | 0.001610991 | 0.001578704 | 0.001576338 | HZQODNRPUJAVLV-QRTUWBSPSA-N | CC(C)[C@@]1(CC[C@]2([C@@H](CC[C@]([C@H]2C1)(C)O)O)C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00532 | 1.16\_989.3193m/z | M-H | C36H62O31 | 40.5 | 0 | -0.9 | 1,1,1,1-Kestohexaose |  | 989.3202 | 989.3193 | 1.16 | NEG | 18944.20261 | 20129.05129 | 18133.44257 | 0.002534512 | 0.002740897 | 0.002379855 | 0.002551755 | BWRYDXSZCCQXIF-TWMOFSFSSA-N | OC[C@H]1O[C@H](O[C@]2(CO[C@]3(CO[C@]4(CO[C@]5(CO[C@]6(CO)O[C@H](CO)[C@@H](O)[C@@H]6O)O[C@H](CO)[C@@H](O)[C@@H]5O)O[C@H](CO)[C@@H](O)[C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)O[C@H](CO)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O |  |  |  |  |  | 62512-19-0 | 去甲槟榔次碱 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N6838 | HPLC≥98% | level2 |
| compound00533 | 9.90\_263.1651m/z | M+FA-H | C15H22O | 54.9 | 0 | -0.93 | 1,1,7,7a-tetramethyl-1a,2,4,6,7,7b-hexahydrocyclopropa[a]naphthalen-5-one | 242.9847, 262.9888, 263.1648 | 263.1653 | 263.1651 | 9.9 | NEG | 21638.87645 | 23407.88424 | 23432.04607 | 0.002895028 | 0.003187363 | 0.003075251 | 0.003052547 | NYVDTZCCCWPPPG-UHFFFAOYSA-N | CC1CC(=O)CC2=CCC3C(C12C)C3(C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00534 | 8.74\_350.1728n | M-H2O-H, M-H | C19H26O6 | 51 | 0 | -0.3 | 1,6-O,O-diacetylbritannilactone | 257.1555, 269.1549, 283.17, 287.1651, 301.1807, 330.2364, 331.1526 | 331.1551 | 331.155 | 8.74 | NEG | 289452.6057 | 292149.8577 | 298576.5721 | 0.038725361 | 0.039780945 | 0.039185559 | 0.039230622 | MVCCWTMPDBIKCJ-IMKJFWDFSA-N | CC1=C([C@@H]([C@H]2[C@@H](C1)OC(=O)C2=C)OC(=O)C)[C@@H](C)CCCOC(=O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00535 | 4.28\_435.0931m/z | M-H | C20H20O11 | 51 | 0.866 | -0.48 | 1-(2'-γ-pyranone)-6-caffeoyl-α-d-pyranoglucose | 151.0392, 167.0341, 175.0393, 179.0342, 193.0500, 195.0293, 197.0450, 373.0924, 417.0820, 435.0927 | 435.0933 | 435.0931 | 4.28 | NEG | 86579.30377 | 86734.54522 | 86888.67509 | 0.011583295 | 0.011810316 | 0.011403377 | 0.011598996 | CLFSHBHNICRSDA-UHFFFAOYSA-N | C1=CC(=C(C=C1C=CC(=O)OCC2C(C(C(C(O2)OC3=COC=CC3=O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00536 | 9.36\_281.1179m/z | M-H | C18H18O3 | 55.7 | 69 | -1.41 | 1-(3,7-dihydroxy-2,8-dimethyl-9,10-dihydrophenanthren-4-yl)ethanone | 281.1181 | 281.1183 | 281.1179 | 9.36 | NEG | 45686.54139 | 41168.31028 | 40571.02978 | 0.006112323 | 0.005605734 | 0.005324592 | 0.005680883 | KDADJLHRXRSXQU-UHFFFAOYSA-N | CC1=CC2=C(C3=C(CC2)C(=C(C=C3)O)C)C(=C1O)C(=O)C |  |  |  |  |  | 77305-81-8 |  |  |  |  |  |  |  | level2 |
| compound00537 | 3.07\_353.0842m/z | M+Na | C14H18O9 | 51.7 | 52.3 | -0.2 | 1-(3-o-β-d-glucopyranosyl-4,5-dihydroxy-phenyl)-ethanone | 130.0497, 225.0359, 353.0842 | 353.0843 | 353.0842 | 3.07 | POS | 61694.15356 | 62240.15874 | 68641.73874 | 0.008253954 | 0.008475008 | 0.009008627 | 0.008579196 | QLFNMRWROGMDLF-UHFFFAOYSA-N | CC(=O)C1=CC(=C(C(=C1)OC2C(C(C(C(O2)CO)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00538 | 1.09\_245.0768m/z | M+H | C9H12N2O6 | 51.9 | 0 | -0.06 | 1-[(2R,3S,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione | 70.0656, 86.0968, 113.0347, 116.0707, 130.0498, 133.0607 | 245.0768 | 245.0768 | 1.09 | POS | 58807.74231 | 59030.93372 | 60488.65365 | 0.007867786 | 0.00803802 | 0.007938606 | 0.007948137 | DRTQHJPVMGBUCF-VXUIKNBNSA-N | C1=CN(C(=O)NC1=O)[C@H]2[C@H]([C@@H]([C@@H](O2)CO)O)O |  |  |  |  |  | 3083-77-0 |  |  |  |  |  |  |  | level2 |
| compound00539 | 4.30\_176.0707m/z | M+H-H2O | C10H11NO3 | 57.9 | 0 | 0.55 | 1-[2-(furan-2-yl)-2-oxoethyl]pyrrolidin-2-one |  | 176.0706 | 176.0707 | 4.3 | POS | 5842.716513 | 5739.30661 | 5485.920365 | 0.000781687 | 0.0007815 | 0.000719979 | 0.000761055 | UICNWMCGFJXCHN-UHFFFAOYSA-N | C1CC(=O)N(C1)CC(=O)C2=CC=CO2 |  |  |  |  | 62018463 |  |  |  |  |  |  |  |  | level2 |
| compound00540 | 1.27\_289.0676m/z | M+FA-H | C9H12N2O6 | 40.4 | 0 | -0.48 | 1-beta-D-Arabinofuranosyluracil |  | 289.0678 | 289.0676 | 1.27 | NEG | 6287.458723 | 5546.472629 | 6938.767639 | 0.000841188 | 0.000755242 | 0.000910652 | 0.000835694 | DRTQHJPVMGBUCF-CCXZUQQUSA-N | C1=CN(C(=O)NC1=O)C2C(C(C(O2)CO)O)O |  |  |  | C16745 | 18323 |  | 阿糖尿苷 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N6652 | HPLC≥98% | level2 |
| compound00541 | 4.78\_267.0872m/z | M-H | C13H16O6 | 59.7 | 91.1 | -0.8 | 1-feruloyl-sn-glycerol | 134.0362, 149.06, 175.0393, 193.05, 252.0636, 267.0874 | 267.0874 | 267.0872 | 4.78 | NEG | 27194.85786 | 26292.96947 | 26325.71599 | 0.003638353 | 0.003580215 | 0.00345502 | 0.003557862 | QXRAHTFDPBQKIM-GFAPAMAISA-N | COC1=C(C=CC(=C1)/C=C/C(=O)OC[C@H](CO)O)O |  |  |  |  |  | 120601-65-2 |  |  |  |  |  |  |  | level2 |
| compound00542 | 9.50\_343.1186m/z | M-H | C19H20O6 | 57.7 | 0 | -0.21 | 1-methyl-acetylshikonin |  | 343.1187 | 343.1186 | 9.5 | NEG | 5388.774302 | 4382.215975 | 4332.672853 | 0.000720955 | 0.00059671 | 0.000568625 | 0.000628763 | SCIUCADXFKAPEB-UHFFFAOYSA-N | CC(=CCC(C1=CC(=C2C(=O)C=CC(=O)C2=C1OC)O)OC(=O)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00543 | 4.46\_219.1131m/z | M+H | C12H14N2O2 | 54.2 | 0 | 1.5 | 1-Methyl-L-tryptophan |  | 219.1128 | 219.1131 | 4.46 | POS | 2501.678316 | 2281.359692 | 1880.756567 | 0.000334695 | 0.000310644 | 0.000246833 | 0.000297391 | ZADWXFSZEAPBJS-JTQLQIEISA-N | CN1C=C(C2=CC=CC=C21)CC(C(=O)O)N |  | 44695 |  |  | 676159 | 21339-55-9 | 1-甲基- L -色氨酸 | 氨基酸及多肽类 | 氨基酸类 | Amino Acids, Peptides and derivatives | Amino acids | B21359-20mg | HPLC≥98% | level2 |
| compound00544 | 4.66\_237.0765m/z | M-H | C12H14O5 | 60.2 | 90.9 | -1.5 | 1-O-(4-Hydroxycinnamoyl)-L-glycerol | 119.0491, 145.0285, 163.0391, 237.0763 | 237.0768 | 237.0765 | 4.66 | NEG | 45375.27097 | 46416.02676 | 44593.27602 | 0.006070679 | 0.006320295 | 0.005852477 | 0.00608115 | YUQSZTOOHLGKGG-GQOHGMTASA-N | C1=CC(=CC=C1/C=C/C(=O)OC[C@H](CO)O)O |  |  |  |  |  | 106055-11-2 |  |  |  |  |  |  |  | level2 |
| compound00545 | 4.29\_253.0715m/z | M-H | C12H14O6 | 58.3 | 81.6 | -1.01 | 1-o-caffeoylglycerol | 135.0441, 161.0235, 179.0343, 253.0715 | 253.0718 | 253.0715 | 4.29 | NEG | 20109.08634 | 20829.32768 | 20066.61818 | 0.00269036 | 0.002836251 | 0.002633568 | 0.00272006 | NOHROAYVCRHDHO-DUXPYHPUSA-N | C1=CC(=C(C=C1/C=C/C(=O)OCC(CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00546 | 3.70\_313.0914m/z | M+H-H2O | C14H18O9 | 53.4 | 0 | -1.19 | 1-O-vanilloyl-β-D-glucoside |  | 313.0918 | 313.0914 | 3.7 | POS | 2710.009233 | 3880.604965 | 3138.69723 | 0.000362567 | 0.000528407 | 0.000411927 | 0.0004343 | YROOZUQRTLHXIO-UHFFFAOYSA-N | O=C(OC1OC(CO)C(O)C(O)C1O)C2=CC=C(O)C(OC)=C2 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00547 | 3.89\_361.1503m/z | M-H | C16H26O9 | 51.2 | 54.5 | -0.19 | 1-o-β-d-glucopyranosylamplexin | 73.0284, 89.0233, 101.0236, 113.0232, 161.0446, 197.0446, 293.1543, 317.1604, 361.1030, 361.1497 | 361.1504 | 361.1503 | 3.89 | NEG | 10098.98966 | 10253.88098 | 10456.93689 | 0.001351126 | 0.001396232 | 0.001372381 | 0.001373247 | ISPPLOMGZOFTJR-UHFFFAOYSA-N | C=CC(COC1C(C(C(C(O1)CO)O)O)O)C2CCOC(=O)C2CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00548 | 4.19\_325.1396m/z | M+H | C15H20N2O6 | 55.4 | 64.3 | 0.52 | 1-ribityl-2,3-diketo-1,2,3,4-tetrahydro-6,7-dimethyl-quinoxaline | 81.0340, 116.0706, 175.0865, 191.0813, 211.1057, 307.1282, 324.1888, 325.1235, 325.1320, 325.1412 | 325.1394 | 325.1396 | 4.19 | POS | 20690.87874 | 20278.18528 | 19505.50389 | 0.002768197 | 0.002761204 | 0.002559926 | 0.002696442 | SLOQSNHEHSCLGS-UHFFFAOYSA-N | O=C1NC=2C=C(C(=CC2N(C1=O)CC(O)C(O)C(O)CO)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00549 | 10.26\_297.1857m/z | M-H2O-H | C20H28O3 | 50.9 | 0 | -0.88 | 10,18-Epoxyros-15-ene-7,18-dione | 282.1622, 297.1514, 297.1856 | 297.186 | 297.1857 | 10.26 | NEG | 30222.28096 | 31900.93391 | 34589.62029 | 0.004043386 | 0.00434383 | 0.004539585 | 0.004308934 | HWECMADGHQKSLK-UHFFFAOYSA-N | CC1(CCC2(C(C1)C(=O)CC3C24CCCC3(C(=O)O4)C)C)C=C |  |  |  |  | 90473942 | 508-71-4 |  |  |  |  |  |  |  | level2 |
| compound00550 | 7.97\_251.0922m/z | M+FA-H | C12H14O3 | 54.8 | 67.7 | -1.55 | (z)-6,7-epoxy-6,7-dihydroligustilide | 182.9866, 207.1019, 210.9803, 210.9982, 223.0963, 230.9849, 231.0060, 250.1441, 250.9907, 251.0941 | 251.0926 | 251.0922 | 7.97 | NEG | 9519.776333 | 10001.85898 | 9544.465857 | 0.001273634 | 0.001361915 | 0.001252628 | 0.001296059 | ZCTBULGQERTBEG-UHFFFAOYSA-N | CCCC=C1C2=C(C3C(O3)CC2)C(=O)O1 |  |  |  |  | 5317139 |  |  |  |  |  |  |  |  | level2 |
| compound00551 | 5.65\_295.0606m/z | M-H2O-H | C17H14O6 | 57.4 | 46.2 | -1.94 | (Z)-3-[2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3,4-dihydroxy-phenyl]acrylic acid | 109.0284, 185.0237, 186.0306, 295.0607 | 295.0612 | 295.0606 | 5.65 | NEG | 72271.50272 | 71143.61593 | 70507.12783 | 0.009669079 | 0.009687358 | 0.009253443 | 0.009536626 | PULWRMOKQNWQBD-UJURIKRHSA-N | C1=CC(=C(C=C1/C=C/C2=C(C=CC(=C2O)O)/C=C\C(=O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00552 | 4.00\_395.1708m/z | 2M-H | C10H14O4 | 54.6 | 0 | -0.85 | (S)-Guaiphenesin |  | 395.1711 | 395.1708 | 4 | NEG | 20846.00673 | 20684.79391 | 21114.32506 | 0.002788951 | 0.00281657 | 0.00277107 | 0.002792197 | HSRJKNPTNIJEKV-QMMMGPOBSA-N | COC1=CC=CC=C1OC[C@H](CO)O |  |  |  |  |  | 93-14-1 |  |  |  |  |  |  |  | level2 |
| compound00553 | 6.37\_359.1499m/z | 2M-H | C10H12O3 | 56.8 | 0 | -0.29 | (S)-2-Phenyl-3-hydroxypropanoic acid methyl ester |  | 359.15 | 359.1499 | 6.37 | NEG | 10503.40417 | 10741.85299 | 11016.30453 | 0.001405232 | 0.001462678 | 0.001445793 | 0.001437901 | OLEWRQVKIUHEJP-SECBINFHSA-N | COC(=O)[C@H](CO)C1=CC=CC=C1 |  |  |  |  |  | 3967-53-1 |  |  |  |  |  |  |  | level2 |
| compound00554 | 6.31\_397.1258m/z | M+Na | C20H22O7 | 40.5 | 0 | 0.04 | (+)-Nortrachelogenin |  | 397.1258 | 397.1258 | 6.31 | POS | 6146.300649 | 5892.905804 | 6970.347365 | 0.000822303 | 0.000802415 | 0.000914797 | 0.000846505 | ZITBJWXLODLDRH-JLTOFOAXSA-N | COc1cc(C[C@@H]2COC(=O)[C@@]2(O)Cc2ccc(O)c(OC)c2)ccc1O |  |  |  |  |  | 61521-74-2 | 荛花酚 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | B32845-5mg | HPLC≥97% | level2 |
| compound00555 | 10.65\_295.2276m/z | M-H | C18H32O3 | 59.6 | 79.8 | -1.05 | (+/-)9-HODE | 171.1019, 277.2167, 295.2275 | 295.2279 | 295.2276 | 10.65 | NEG | 100188.8837 | 105782.9998 | 97625.11267 | 0.013404097 | 0.014404072 | 0.012812441 | 0.013540203 | NPDSHTNEKLQQIJ-UHFFFAOYSA-N | C(CCCCCCCC(O)C=CC=CCCCCC)(=O)O |  |  | LMFA02000318 |  | 1927 |  |  |  |  |  |  |  |  | level2 |
| compound00556 | 4.70\_517.0984m/z | M+FA-H | C23H20O11 | 48.2 | 0 | -0.78 | (-)-EGCG-3''-O-ME |  | 517.0988 | 517.0984 | 4.7 | NEG | 24977.24401 | 27202.1527 | 26958.43795 | 0.003341662 | 0.003704015 | 0.003538059 | 0.003527912 | WVRDOLPMKOCJRJ-DENIHFKCSA-N | C1(O)C=C2O[C@H](C3C=C(O)C(O)=C(O)C=3)[C@H](OC(C3C=C(OC)C(O)=C(O)C=3)=O)CC2=C(O)C=1 | HMDB0038363 | 47337 | LMPK12020121 |  | 9804842 | 83104-87-4 | 表没食子儿茶素 3-O-(3-O-甲基)没食子酸酯 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | DJ0050-0005 | HPLC≥98% | level2 |
| compound00557 | 4.58\_583.2032m/z | M+FA-H | C26H34O12 | 51.1 | 0 | -0.06 | (-)-olivil 4'-o-beta-d-glucopyranoside |  | 583.2032 | 583.2032 | 4.58 | NEG | 9569.400727 | 5631.911647 | 9102.41425 | 0.001280273 | 0.000766876 | 0.001194612 | 0.001080587 | OXHVZEZYYQQCRJ-CTQTXEDXSA-N | COC1=C(C=CC(=C1)C[C@]2(CO[C@@H]([C@H]2CO)C3=CC(=C(C=C3)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)OC)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00558 | 5.55\_413.1571m/z | M+K | C18H30O8 | 53 | 0 | -0.42 | (1r,2r)-p-menth-4(5)-ene-1,2-diol1-o-β-d-(6-o-acetyl)glucopyranoside |  | 413.1572 | 413.1571 | 5.55 | POS | 7381.36982 | 6594.812795 | 8022.622728 | 0.000987541 | 0.000897991 | 0.001052899 | 0.000979477 | JGXUYPSOOTZEGY-UHFFFAOYSA-N | CC(C)C1=CCC(C(C1)O)(C)OC2C(C(C(C(O2)COC(=O)C)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00559 | 5.20\_357.0614m/z | M-H | C18H14O8 | 59.8 | 22.2 | -0.59 | (1S,2R)-1-(3,4-dihydroxyphenyl)-6,7-dihydroxy-1,2-dihydronaphthalene-2,3-dicarboxylic acid | 207.0293, 207.9767, 221.0450, 269.0817, 269.1187, 313.0718, 313.1091, 321.0406, 356.2559, 357.0612 | 357.0616 | 357.0614 | 5.2 | NEG | 22083.13023 | 20329.8657 | 20072.53255 | 0.002954464 | 0.002768241 | 0.002634344 | 0.002785683 | WJMFXQBNYLYADA-HOTGVXAUSA-N | C1=CC(=C(C=C1[C@@H]2[C@H](C(=CC3=CC(=C(C=C23)O)O)C(=O)O)C(=O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00560 | 3.97\_239.0556m/z | M+FA-H | C10H10O4 | 53.2 | 65.9 | -2.6 | (1S,2S)-1,2-Di(2-furyl)-1,2-ethanediol | 135.0441, 179.0342, 197.0448 | 239.0562 | 239.0556 | 3.97 | NEG | 10532.31406 | 11348.55332 | 11172.18924 | 0.0014091 | 0.00154529 | 0.001466252 | 0.001473547 | PAGAJWBCCKFHIT-NXEZZACHSA-N | C1=COC(=C1)[C@H]([C@@H](C2=CC=CO2)O)O |  |  |  |  |  | 98-00-0 |  |  |  |  |  |  |  | level2 |
| compound00561 | 5.10\_377.1815m/z | M+FA-H | C16H28O7 | 55.7 | 73.5 | -0.72 | (1S,2S,4R)-1,8-Epoxy-p-menthan-2-ol glucoside | 71.0128, 101.0234, 135.044, 161.0447, 164.0706, 331.1761, 376.2238, 377.0082, 377.1782 | 377.1817 | 377.1815 | 5.1 | NEG | 60620.63802 | 57720.45399 | 61133.63996 | 0.00811033 | 0.007859577 | 0.008023255 | 0.00799772 | NWZYTZHMCGWGOF-UHFFFAOYSA-N | CC1(C)OC2(C)CCC1CC2OC1OC(CO)C(O)C(O)C1O | HMDB0033110 | 89001 |  |  | 73815050 | 155836-26-3 |  |  |  |  |  |  |  | level2 |
| compound00562 | 4.87\_455.2252m/z | M+Na | C21H36O9 | 50.7 | 0 | 0.03 | (1s,4s,5s,7r,10r)-10,11,14-trihydroxyguai-3-one 11-o-β-d-glucopyranoside |  | 455.2252 | 455.2252 | 4.87 | POS | 46530.24838 | 49642.18406 | 46293.14446 | 0.006225201 | 0.006759589 | 0.00607557 | 0.006353453 | KWDNQVRRYNIDTM-UHFFFAOYSA-N | CC1C2CC(CCC(C2CC1=O)(CO)O)C(C)(C)OC3C(C(C(C(O3)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00563 | 5.43\_491.2136m/z | M+FA-H | C21H34O10 | 53.4 | 50.7 | 0.55 | (1s,5r,7r,10r)-secoatractylolactone11-o-β-d-glucopyranoside | 179.0334, 197.0448, 207.9690, 267.0638, 293.0454, 295.0600, 311.0558, 313.1652, 445.2083, 491.0993 | 491.2134 | 491.2136 | 5.43 | NEG | 10409.7644 | 9109.023138 | 7609.146396 | 0.001392704 | 0.001240341 | 0.000998634 | 0.00121056 | HIJTUHQXWSDVSN-UHFFFAOYSA-N | CC(=O)C1CC(CCC2(C1CC(=O)O2)CO)C(C)(C)OC3C(C(C(C(O3)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00564 | 4.06\_385.1135m/z | M-H2O-H | C17H24O11 | 43.1 | 0 | -1.27 | 10-Hydroxymajoroside |  | 385.114 | 385.1135 | 4.06 | NEG | 31740.04846 | 31663.19552 | 29245.3207 | 0.004246446 | 0.004311458 | 0.003838192 | 0.004132032 | IWDXNCIWSRAIAR-OCGKWZSUSA-N | COC(=O)C1=CO[C@H](C2=C([C@H](C[C@H]12)O)CO)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O |  |  |  |  |  | 259753-12-3 | 10-羟基大车前草苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | Y54765-5mg | HPLC≥98% | level2 |
| compound00565 | 6.99\_261.1130m/z | M-H | C15H18O4 | 58.8 | 54.2 | -0.91 | (1α,2β,5α,8α10α)-1,10-epoxy-2-hydroxy-3,7(11)-guaiadien-12,8-olide | 154.9919, 161.0604, 161.0964, 217.1227, 220.9835, 240.988, 260.9966, 261.1128 | 261.1132 | 261.113 | 6.99 | NEG | 12764.90163 | 12175.32849 | 12423.35004 | 0.001707794 | 0.001657869 | 0.001630456 | 0.001665373 | QKIQAUSGMKJYFS-UHFFFAOYSA-N | CC1=CC(C23C1CC4=C(C(=O)OC4CC2(O3)C)C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00566 | 4.64\_189.0762m/z | M-H | C8H14O5 | 56.1 | 77.7 | -3.65 | (2R)-2-butoxybutanedioic acid | 99.0804, 127.0755, 129.0547, 145.0656, 145.0859, 171.0652, 188.9973, 189.076 | 189.0768 | 189.0762 | 4.64 | NEG | 9719.126169 | 10124.80697 | 9508.989667 | 0.001300305 | 0.001378657 | 0.001247972 | 0.001308978 | UDLOAJGWSDUKME-ZCFIWIBFSA-N | CCCCO[C@H](CC(=O)O)C(=O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00567 | 5.12\_433.1135m/z | M-H | C21H22O10 | 60.3 | 80 | -1.1 | (2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]chroman-4-one | 61.9873, 151.0029, 271.0613, 433.1138 | 433.114 | 433.1135 | 5.12 | NEG | 32119.57084 | 34099.21631 | 33589.17296 | 0.004297222 | 0.004643162 | 0.004408285 | 0.004449556 | VPQWOQSQAVBHEV-PFGOOLOPSA-N | C1[C@@H](OC2=C(C(=CC(=C2C1=O)O)O)[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)C4=CC=C(C=C4)O |  |  |  |  |  | 278614-44-1 |  |  |  |  |  |  |  | level2 |
| compound00568 | 6.13\_269.0456m/z | M-H2O-H | C15H12O6 | 52.8 | 0 | 0.27 | (2r,3r)-2',3,5,7-tetrahydroxyflavanone |  | 269.0456 | 269.0456 | 6.13 | NEG | 4170.769543 | 4258.633704 | 4032.798199 | 0.000558 | 0.000579882 | 0.000529269 | 0.000555717 | BJNCWLSOQIVKIX-UHFFFAOYSA-N | C1=CC=C(C(=C1)C2C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00569 | 1.03\_274.0920m/z | M+Na | C10H13N5O3 | 56.9 | 88.1 | 3.93 | (2R,3R,4S)-2-(6-aminopurin-9-yl)-4-(hydroxymethyl)oxolan-3-ol | 154.0497, 164.0704, 192.0653, 226.0708, 238.0708, 256.0812, 256.1249, 273.1194, 274.0923, 274.1018 | 274.091 | 274.092 | 1.03 | POS | 2965911.479 | 2889511.031 | 2724242.306 | 0.396804141 | 0.393453825 | 0.357532931 | 0.382596966 | KQLDDLUWUFBQHP-WVBSTYLSSA-N | C1[C@@H]([C@H]([C@@H](O1)N2C=NC3=C(N=CN=C32)N)O)CO |  |  |  |  |  | 73-03-0 |  |  |  |  |  |  |  | level2 |
| compound00570 | 4.20\_349.1867m/z | M-H | C16H30O8 | 51 | 0 | -0.21 | (3s,6r)-6,7-dihydroxy-6,7-dihydrolinalool-3-o-β-d-glucopyranoside |  | 349.1868 | 349.1867 | 4.2 | NEG | 16665.02058 | 17616.28427 | 17246.22816 | 0.002229584 | 0.002398743 | 0.002263416 | 0.002297248 | BWEHDKNACKAKFC-UHFFFAOYSA-N | CC(C)(C(CCC(C)(C=C)OC1C(C(C(C(O1)CO)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00571 | 11.36\_317.2119m/z | M-H | C20H30O3 | 53.1 | 34.8 | -1.11 | (3Z)-3-[2-[(1R,2S,4aS,8aS)-5,5,8a-trimethylspiro[decalin-2,2'-oxirane]-1-yl]ethylidene]tetrahydrofuran-2-one | 112.9845, 180.9721, 317.2119 | 317.2122 | 317.2119 | 11.36 | NEG | 30442.13283 | 30881.86448 | 33466.45947 | 0.0040728 | 0.004205067 | 0.00439218 | 0.004223349 | MBPTXJNHCBXMBP-IGOJNLFMSA-N | C[C@]12CCCC([C@@H]1CC[C@]3([C@@H]2C/C=C\4/CCOC4=O)CO3)(C)C |  |  |  |  |  | 482-38-2 |  |  |  |  |  |  |  | level2 |
| compound00572 | 7.36\_337.1045m/z | M+Na | C18H18O5 | 50.3 | 0 | -0.54 | (6aS,11aS)-6a-ethoxymedicarpin |  | 337.1047 | 337.1045 | 7.36 | POS | 14002.62049 | 15216.25108 | 16092.93874 | 0.001873386 | 0.00207194 | 0.002112057 | 0.002019128 | XLMJRHLKCZWROJ-ZWKOTPCHSA-N | CCO[C@@]12COC3=C([C@@H]1OC4=C2C=CC(=C4)OC)C=CC(=C3)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00573 | 4.59\_439.1821m/z | M+FA-H | C17H30O10 | 57.1 | 81.5 | -0.12 | (e)-2-hexenyl-α-l-arabinopyranosyl-(1→2)-β-d-glucopyranoside | 59.0128, 71.0127, 89.0234, 101.0234, 149.0447, 371.0979, 393.1763, 439.1819 | 439.1821 | 439.1821 | 4.59 | NEG | 84946.44675 | 84016.74245 | 82581.74046 | 0.011364837 | 0.011440243 | 0.01083813 | 0.011214403 | MOOXSHZEQJWTJN-UHFFFAOYSA-N | CCCC=CCOC1C(C(C(CO1)O)O)OC2C(C(C(C(O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00574 | 1.14\_188.0919m/z | M+NH4 | C8H10O4 | 58.9 | 94.2 | 0.7 | (R)-3,4-dihydroxyphenylethyleneglycol | 125.0597, 134.0599, 135.0439, 142.0498, 142.0861, 152.0705, 153.0544, 170.0810, 171.0649, 188.0915 | 188.0917 | 188.0919 | 1.14 | POS | 42129.17601 | 42406.45678 | 40533.50891 | 0.005636389 | 0.005774327 | 0.005319668 | 0.005576795 | MTVWFVDWRVYDOR-QMMMGPOBSA-N | C1=CC(=C(C=C1[C@H](CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00575 | 5.25\_701.1498m/z | M-H2O-H | C36H32O16 | 63.3 | 47.2 | -1.99 | (2R)-2-[3-[(2S,3S)-3-[(1S)-1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]carbonyl-2-(3,4-dihydroxyphenyl)-7-hydroxy-2,3-dihydro-1-benzofuran-4-yl]propanoyloxy]-3-(3,4-dihydroxyphenyl)propanoic acid | 295.0592, 297.0766, 321.0404, 339.0493, 341.0659, 359.0769, 503.0985, 519.0925, 701.1522, 701.1697 | 701.1512 | 701.1498 | 5.25 | NEG | 285143.8597 | 278684.4966 | 286593.2602 | 0.038148901 | 0.037947417 | 0.037612854 | 0.037903058 | JUFYZLWTPPZFMH-JTOFGFGCSA-N | C1=CC(=C(C=C1C[C@H](C(=O)O)OC(=O)CCC2=C3[C@@H]([C@H](OC3=C(C=C2)O)C4=CC(=C(C=C4)O)O)C(=O)O[C@@H](CC5=CC(=C(C=C5)O)O)C(=O)O)O)O |  |  |  |  |  | 122021-74-3 |  |  |  |  |  |  |  | level2 |
| compound00576 | 9.95\_357.2051m/z | M+Na | C20H30O4 | 51.6 | 0 | 4.49 | 10β-hydroxyfuranoeremophilan-6β-yl-2'ξ-methylbutanoate | 199.0751, 229.122, 241.1218, 255.1378, 297.1843, 357.1078, 357.2029 | 357.2035 | 357.2051 | 9.95 | POS | 37548.68647 | 37512.18105 | 38314.33506 | 0.005023573 | 0.005107892 | 0.005028421 | 0.005053296 | ZGSGPGJJWNVAIA-UHFFFAOYSA-N | CCC(C)C(=O)OC1C2=C(CC3(C1(C(CCC3)C)C)O)OC=C2C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00577 | 7.51\_303.1954m/z | M+H | C19H26O3 | 48.8 | 13.8 | -0.37 | 11-Beta-hydroxyandrostenedione | 303.1561, 303.1945 | 303.1955 | 303.1954 | 7.51 | POS | 15151.62173 | 16054.34242 | 15515.16922 | 0.002027109 | 0.002186059 | 0.00203623 | 0.002083133 | WSCUHXPGYUMQEX-KCZNZURUSA-N | [C@]12([H])[C@@H](O)C[C@]3(C)C(CC[C@@]3([H])[C@]1([H])CCC1=CC(CC[C@]21C)=O)=O | HMDB0006773 |  | LMST02020066 | C05284 | 94141 | 382-44-5 | 4-雄烯-11β-醇-3,17-二酮 | 甾体类 | 其他甾体类 | Steroids | Other steroids | HY-114464 | HPLC≥98% | level2 |
| compound00578 | 8.13\_331.1913m/z | M-H | C20H28O4 | 57 | 0 | -0.56 | 14-Deoxy-11,12-didehydroandrographolide |  | 331.1915 | 331.1913 | 8.13 | NEG | 7748.097547 | 6935.470063 | 7639.286763 | 0.001036605 | 0.000944377 | 0.001002589 | 0.000994524 | XMJAJFVLHDIEHF-AATRIKPKSA-N | C=C1CCC2C(C)(CO)C(O)CCC2(C)C1/C=C/C1=CCOC1=O |  |  |  |  |  | 42895-58-9 | 14-去氧-11;12-二去氢穿心莲内酯 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N1490 | HPLC≥98% | level2 |
| compound00579 | 5.76\_269.0455m/z | M-H2O-H | C15H12O6 | 56.5 | 0 | -0.08 | 3,4,5,2',4'-Pentahydroxychalcone |  | 269.0455 | 269.0455 | 5.76 | NEG | 3905.594755 | 4065.804768 | 4108.54923 | 0.000522523 | 0.000553625 | 0.000539211 | 0.000538453 | NLAXFZHJXUCLDR-UHFFFAOYSA-N | C1=CC(=C(C=C1O)O)C(=O)C=CC2=CC(=C(C(=C2)O)O)O |  |  |  |  | 2763155 |  |  |  |  |  |  |  |  | level2 |
| compound00580 | 6.09\_221.0809m/z | M+H-H2O | C12H14O5 | 40.7 | 0 | 0.37 | 3,4,5-Trimethoxycinnamic acid |  | 221.0808 | 221.0809 | 6.09 | POS | 2278.422713 | 2415.268557 | 2395.581273 | 0.000304826 | 0.000328878 | 0.000314399 | 0.000316034 | YTFVRYKNXDADBI-SNAWJCMRSA-N | COC1=CC(\C=C\C(O)=O)=CC(OC)=C1OC | HMDB0002511 | 6705 |  |  | 735755 | 90-50-6 | 3,4,5-三甲氧基肉桂酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-W012123 | HPLC≥98% | level2 |
| compound00581 | 5.95\_221.0814m/z | M-H2O-H | C12H16O5 | 42.6 | 0 | -2.17 | 3,4,5-Trimethoxyhydrocinnamic acid |  | 221.0819 | 221.0814 | 5.95 | NEG | 2509.213143 | 2459.621081 | 2541.457946 | 0.000335703 | 0.000334917 | 0.000333544 | 0.000334722 | ZCYXGVJUZBKJAI-UHFFFAOYSA-N | COC1=CC(CCC(O)=O)=CC(OC)=C1OC | HMDB0030254 | 86836 |  |  | 64860 | 25173-72-2 | 3-(3,4,5-三甲氧基苯基)丙酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-W022390 | HPLC≥98% | level2 |
| compound00582 | 3.53\_195.0293m/z | M-H | C9H8O5 | 52.9 | 59.2 | -2.95 | 3,4,6-trihydroxycinnamic acid | 66.034, 123.0441, 128.0344, 130.9916, 151.0391, 165.0186, 195.0296 | 195.0299 | 195.0293 | 3.53 | NEG | 4604.948699 | 5534.785851 | 5118.613701 | 0.000616088 | 0.000753651 | 0.000671773 | 0.000680504 | GUOJZFSYQUIYCN-UHFFFAOYSA-N | C1=C(C(=CC(=C1O)O)O)C=CC(=O)O |  |  |  |  | 25244000 |  |  |  |  |  |  |  |  | level2 |
| compound00583 | 1.76\_347.0982m/z | M+FA-H | C13H18O8 | 52 | 60.8 | -0.67 | 3,4-Dihydroxybenzyl alcohol-4-glucoside | 139.0389, 142.9949, 161.0441, 211.0211, 279.1099, 300.9911, 301.0925, 346.1587, 346.1654, 347.0906 | 347.0984 | 347.0982 | 1.76 | NEG | 52231.76946 | 50496.07361 | 51391.70105 | 0.006987998 | 0.00687586 | 0.00674471 | 0.006869523 | AWHHJEGHYHOVRN-UHFFFAOYSA-N | C1=CC(=C(C=C1CO)O)OC2C(C(C(C(O2)CO)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00584 | 5.78\_191.0704m/z | M+H-H2O | C11H12O4 | 41.8 | 0 | 0.55 | 3,4-Dimethoxycinnamic acid |  | 191.0703 | 191.0704 | 5.78 | POS | 2143.092119 | 2041.231723 | 1910.06264 | 0.000286721 | 0.000277947 | 0.000250679 | 0.000271782 | HJBWJAPEBGSQPR-GQCTYLIASA-N | COC1=C(OC)C=C(\C=C\C(O)=O)C=C1 | HMDB0034315 | 43817 |  |  | 717531 | 14737-89-4 | 3,4-二甲氧基肉桂酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1778 | HPLC≥98% | level2 |
| compound00585 | 4.33\_197.0810m/z | M+H-H2O | C10H14O5 | 42.2 | 0 | 0.97 | 3,4-O-Isopropylidene-shikimic acid |  | 197.0809 | 197.081 | 4.33 | POS | 7338.90262 | 7638.128523 | 7255.460867 | 0.000981859 | 0.001040055 | 0.000952216 | 0.000991377 | PILATNHSTHZMCA-UHFFFAOYSA-N | CC1(C)OC2C=C(C(=O)O)CC(O)C2O1 |  |  |  |  |  | 183075-03-8 | 3,4-O-异亚丙基莽草酸 | 羧酸及衍生物 |  | Carboxylic acid and derivatives |  | HY-N1782 | HPLC≥98% | level2 |
| compound00586 | 3.75\_359.0773m/z | 2M-H | C9H8O4 | 50.8 | 0 | 0.04 | 3,7-dihydroxy-2,3-dihydrochromen-4-one |  | 359.0772 | 359.0773 | 3.75 | NEG | 14155.36259 | 14546.74291 | 13400.35174 | 0.001893821 | 0.001980775 | 0.001758679 | 0.001877758 | GLPDBGACWOZVNL-UHFFFAOYSA-N | C1C(C(=O)C2=C(O1)C=C(C=C2)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00587 | 7.75\_269.1170m/z | M+H | C17H16O3 | 59.7 | 86.5 | -0.65 | 3,7-dihydroxy-2,8-dimethyl-9,10-dihydrophenanthrene-4-carbaldehyde | 195.1171, 213.0542, 223.1117, 233.0967, 251.1062, 251.1997, 269.0801, 269.1167 | 269.1172 | 269.117 | 7.75 | POS | 73980.14989 | 75575.19555 | 75155.2476 | 0.009897676 | 0.010290789 | 0.009863468 | 0.010017311 | RDCKNSFRNNWMTK-UHFFFAOYSA-N | CC1=CC2=C(C3=C(CC2)C(=C(C=C3)O)C)C(=C1O)C=O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00588 | 4.47\_611.1970m/z | M+H | C28H34O15 | 52 | 52.5 | -0.03 | 3',5-dihydroxy-4'-methoxyflavone 7-o-α- rhamnosesyl(1.6)-β-d-glucoside | 177.0544, 195.0286, 263.0543, 303.0857, 345.0960, 369.0954, 413.1233, 449.1432, 592.3787, 610.3895 | 611.197 | 611.197 | 4.47 | POS | 46553.19956 | 49285.98319 | 48499.0683 | 0.006228272 | 0.006711087 | 0.006365078 | 0.006434812 | QUQPHWDTPGMPEX-IHAPIEOYSA-N | C[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=CC(=C4C(=O)C[C@H](OC4=C3)C5=CC(=C(C=C5)OC)O)O)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00589 | 4.98\_221.0447m/z | M-H | C11H10O5 | 60.9 | 89.7 | -3.87 | 3-(4-acetyloxy-3-hydroxyphenyl)prop-2-enoic acid | 162.0313, 177.055, 206.0212, 221.045 | 221.0455 | 221.0447 | 4.98 | NEG | 9778.687431 | 10403.49621 | 10644.64525 | 0.001308274 | 0.001416605 | 0.001397016 | 0.001373965 | QNXWCFJSFNQQDN-UHFFFAOYSA-N | CC(=O)OC1=C(C=C(C=C1)C=CC(=O)O)O |  |  |  |  | 14818630 |  |  |  |  |  |  |  |  | level2 |
| compound00590 | 7.55\_331.1914m/z | M-H | C20H28O4 | 59 | 79.6 | -0.36 | 3-dehydrodeoxyandrographolide | 261.0895, 287.0687, 287.1652, 287.2017, 305.0794, 330.1416, 330.2364, 331.0588, 331.1544, 331.1924 | 331.1915 | 331.1914 | 7.55 | NEG | 129755.0649 | 129436.6247 | 129005.4651 | 0.017359705 | 0.017624897 | 0.016930837 | 0.017305146 | ROPZFDGMJDAXOR-UHFFFAOYSA-N | CC12CCC(=O)C(C1CCC(=C)C2CCC3=CCOC3=O)(C)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00591 | 1.50\_426.1271m/z | M+FA-H | C14H23NO11 | 56.6 | 0 | 4.63 | 3-deoxy-D-ribHexNAc(b1-4)b-GlcA |  | 426.1251 | 426.1271 | 1.5 | NEG | 7671.268893 | 7778.92884 | 7161.826302 | 0.001026326 | 0.001059227 | 0.000939927 | 0.001008493 | WCDDVEOXEIYWFB-VXORFPGASA-N | CC(=O)N[C@@H]1C[C@@H]([C@H](O[C@H]1O[C@H]2[C@@H]([C@H]([C@@H](O[C@@H]2C(=O)O)O)O)O)CO)O |  |  |  |  |  | 9004-61-9 |  |  |  |  |  |  |  | level2 |
| compound00592 | 4.51\_367.1034m/z | M-H | C17H20O9 | 48.4 | 34 | -0.2 | 3-Feruloylquinic acid | 173.0096, 173.0447, 175.0392, 191.0190, 191.0553, 193.0500, 323.0776, 366.1161, 366.1877, 367.1064 | 367.1035 | 367.1034 | 4.51 | NEG | 25253.67669 | 26204.01426 | 24637.03674 | 0.003378646 | 0.003568102 | 0.003233395 | 0.003393381 | RAGZUCNPTLULOL-UHFFFAOYSA-N | O=C(OC1CC(O)(C(=O)O)CC(O)C1O)C=CC2=CC=C(O)C(OC)=C2 |  |  |  |  |  |  | 3-O-阿魏酰奎宁酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N6599 | HPLC≥98% | level2 |
| compound00593 | 10.84\_485.3269m/z | M-H | C30H46O5 | 50.8 | 18.8 | -0.66 | 3-Hydroxy-12-oleanene-23,28-dioic acid | 485.3217 | 485.3272 | 485.3269 | 10.84 | NEG | 75584.6661 | 68064.90915 | 73427.29294 | 0.010112341 | 0.009268142 | 0.009636689 | 0.009672391 | PAIBKVQNJKUVCE-HCXGXNEWSA-N | C[C@]12CC[C@H]([C@@]([C@@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)C)(C)C(=O)O)O |  |  |  |  |  | 91652-87-8 |  |  |  |  |  |  |  | level2 |
| compound00594 | 1.03\_110.0604m/z | M+H | C6H7NO | 43.4 | 18.9 | 3.52 | 3-Hydroxy-2-methylpyridine | 67.0548, 81.034, 82.0656, 83.0495, 89.5071, 98.5123, 109.0762, 109.1015, 110.0602 | 110.06 | 110.0604 | 1.03 | POS | 147879.7683 | 150668.5859 | 157837.2416 | 0.019784577 | 0.020515973 | 0.020714755 | 0.020338435 | AQSRRZGQRFFFGS-UHFFFAOYSA-N | CC1=C(C=CC=N1)O |  | 103463 |  |  | 70719 | 1121-25-1 | 3-羟基-2-甲基吡啶 | 生物碱 |  | Alkaloids |  | HY-W002339 | HPLC≥98% | level2 |
| compound00595 | 9.43\_287.1276m/z | M+H-H2O | C17H20O5 | 51 | 0 | -0.76 | 3-methoxy-4-acetoxycinnamyl angelate |  | 287.1278 | 287.1276 | 9.43 | POS | 4153.06322 | 3834.450083 | 4068.284592 | 0.000555631 | 0.000522123 | 0.000533927 | 0.000537227 | GZZZGYBTVVSDGQ-UHFFFAOYSA-N | CC=C(C)C(=O)OCC=CC1=CC(=C(C=C1)OC(=O)C)OC |  |  |  |  | 5319394 |  |  |  |  |  |  |  |  | level2 |
| compound00596 | 5.87\_241.1078m/z | M-H | C12H18O5 | 58.8 | 76.7 | -1.47 | 3-n-butyl-3-hydroxy-4,5,6,7-tetrahydro-6,7-dihydroxy phthalide | 173.1176, 197.1176, 220.9834, 241.1078 | 241.1081 | 241.1078 | 5.87 | NEG | 23072.35554 | 21693.1269 | 22910.1159 | 0.00308681 | 0.002953871 | 0.003006752 | 0.003015811 | ZZFPYEQIYOWDGH-UHFFFAOYSA-N | CCCCC1(C2=C(C(C(CC2)O)O)C(=O)O1)O |  |  |  |  | 5315568 |  |  |  |  |  |  |  |  | level2 |
| compound00597 | 3.88\_165.0185m/z | M-H2O-H | C8H8O5 | 44.3 | 0 | -4.49 | 3-O-Methylgallic acid |  | 165.0192 | 165.0185 | 3.88 | NEG | 4831.615786 | 5137.280434 | 5042.489429 | 0.000646413 | 0.000699524 | 0.000661783 | 0.00066924 | KWCCUYSXAYTNKA-UHFFFAOYSA-N | COC1=CC(=CC(=C1O)O)C(=O)O |  |  |  | C05616 | 19829 |  | 3-O-甲基没食子酸 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N2009 | HPLC≥98% | level2 |
| compound00598 | 7.78\_212.1412n | M+H-H2O, M+H | C12H20O3 | 61.5 | 39.6 | 0.02 | 3-oxo-2-pentylcyclopentaneacetic acid | 149.1325, 154.9670, 159.1171, 163.0388, 177.0544, 177.1264, 177.1636, 195.0847, 195.1142, 195.1376 | 195.138 | 195.138 | 7.78 | POS | 22975.99531 | 21856.05202 | 23004.68263 | 0.003073918 | 0.002976056 | 0.003019163 | 0.003023046 | PQEYTAGBXNEUQL-UHFFFAOYSA-N | CCCCCC1C(CC(O)=O)CCC1=O | HMDB0033601 | 44409 |  |  | 107126 | 98674-52-3 | 二氢茉莉酸 | 其他 |  | Others |  | Y35128-1g | HPLC≥98% | level2 |
| compound00599 | 0.74\_138.0549m/z | M+H | C7H7NO2 | 44.5 | 23.3 | -0.24 | 3-Pyridineacetic acid | 68.9976, 111.0078, 138.0548 | 138.055 | 138.0549 | 0.74 | POS | 252606.8173 | 262014.9358 | 266370.3143 | 0.033795827 | 0.035677586 | 0.03495877 | 0.034810728 | WGNUNYPERJMVRM-UHFFFAOYSA-N | OC(=O)CC1=CN=CC=C1 | HMDB0001538 | 6308 |  |  | 108 | 501-81-5 | 3-吡啶乙酸 | 羧酸及衍生物 |  | Carboxylic acid and derivatives |  | HY-W015806 | HPLC≥98% | level2 |
| compound00600 | 5.43\_269.0814m/z | M-H2O-H | C16H16O5 | 56.1 | 79 | -1.71 | 3-(4-hydroxybenzyl)-3,4,7-chromantriol | 109.0284, 147.0442, 159.0442, 254.0582, 269.0461, 269.0815 | 269.0819 | 269.0814 | 5.43 | NEG | 73970.0193 | 69221.1883 | 73636.64111 | 0.00989632 | 0.009425588 | 0.009664164 | 0.009662024 | IYAYKNOVHBOSPH-UHFFFAOYSA-N | C1C(C(C2=C(O1)C=C(C=C2)O)O)(CC3=CC=C(C=C3)O)O |  |  |  |  | 13846660 |  |  |  |  |  |  |  |  | level2 |
| compound00601 | 9.97\_411.1046m/z | M+Na | C20H20O8 | 49.6 | 0 | -1.22 | Artemitin |  | 411.1051 | 411.1046 | 9.97 | POS | 17803.12581 | 18014.03668 | 19427.43992 | 0.002381849 | 0.002452903 | 0.002549681 | 0.002461478 | RIGYMJVFEJNCKD-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=C(OC)C(OC)=CC=3)=C(OC)C(=O)C=2C(O)=C1OC | HMDB0030095 | 51429 | LMPK12113017 |  | 5320351 | 479-90-3 | 艾黄素 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N3017 | HPLC≥98% | level2 |
| compound00602 | 8.38\_296.1047n | M+Na, M+K, M+H, M+H-H2O | C18H16O4 | 57.1 | 0 | -0.67 | 3''-methoxyasparenydiol | 319.0936 | 319.0941 | 319.0939 | 8.38 | POS | 676293.3782 | 677468.0527 | 672786.492 | 0.090480115 | 0.092248271 | 0.088297332 | 0.090341906 | CFTKDOICDIITEC-DUXPYHPUSA-N | COC1=C(C=CC(=C1)C#C/C=C/COC2=CC=C(C=C2)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00603 | 9.53\_315.1966m/z | M-H | C20H28O3 | 57.7 | 0 | -0.03 | 15-Hydroxydehydroabietic acid |  | 315.1966 | 315.1966 | 9.53 | NEG | 4369.168094 | 3650.797771 | 4231.923431 | 0.000584543 | 0.000497115 | 0.000555403 | 0.000545687 | ILQLITDRYFHAGM-NSISKUIASA-N | CC12CCCC(C1CCC3=C2C=CC(=C3)C(C)(C)O)(C)C(=O)O |  | 985438 |  |  | 14487943 |  | 15-羟基去氢松香酸 | 萜类 | 二萜类 | Terpenes | Diterpenes | DQ0045 | HPLC≥98% | level2 |
| compound00604 | 4.31\_231.1129m/z | M+H | C13H14N2O2 | 51 | 48.2 | 0.38 | 1beta-Methyl-1,2,3,4-tetrahydro-beta-carboline-3beta-carboxylic acid | 130.0651, 144.0807, 146.06, 158.0963, 168.0806, 188.0704, 214.0861, 231.0638, 231.1128 | 231.1128 | 231.1129 | 4.31 | POS | 30516.59963 | 29234.87 | 29751.80744 | 0.004082763 | 0.003980802 | 0.003904664 | 0.00398941 | ZUPHXNBLQCSEIA-RDDDGLTNSA-N | C[C@@H]1C2=C(C[C@@H](N1)C(=O)O)C3=CC=CC=C3N2 |  |  |  |  |  | 40678-46-4 |  |  |  |  |  |  |  | level2 |
| compound00605 | 6.91\_314.0791n | M-H, M+FA-H | C17H14O6 | 68.7 | 78.3 | 0.16 | 2',7-Dihydroxy-4',5'-dimethoxyisoflavone | 151.0387, 161.0236, 313.0724 | 313.0718 | 313.0718 | 6.91 | NEG | 479842.472 | 470497.7538 | 494789.9751 | 0.06419729 | 0.064065906 | 0.064936848 | 0.064400015 | UYOJEKMKWXYOEQ-UHFFFAOYSA-N | COC1=CC(O)=C(C=C1OC)C1=COC2=C(C=CC(O)=C2)C1=O | HMDB0041644 | 96007 |  |  | 5316763 |  |  |  |  |  |  |  |  | level2 |
| compound00606 | 4.19\_217.0975m/z | M+H | C12H12N2O2 | 63.3 | 94.2 | 1.47 | 2,3,4,9-Tetrahydro-1H-beta-carboline-3-carboxylic acid | 144.0806, 217.0967 | 217.0972 | 217.0975 | 4.19 | POS | 258499.713 | 260068.0084 | 256560.8026 | 0.034584227 | 0.03541248 | 0.033671357 | 0.034556022 | FSNCEEGOMTYXKY-UHFFFAOYSA-N | OC(=O)C1CC2=C(CN1)NC1=CC=CC=C21 | HMDB0035665 | 90929 |  |  | 98285 | 42438-90-4 |  |  |  |  |  |  |  | level2 |
| compound00607 | 5.01\_448.1363n | M+H-H2O, M+H | C22H24O10 | 61.7 | 87.2 | -1.46 | 2,3,5,4'-tetrahydroxystilbene-2-o-(6''-o-acetyl)-beta-d-glucopyranoside | 245.0441, 263.0546, 281.0651, 315.0856, 327.0856, 369.0963, 395.1118, 413.1223, 430.3316, 431.1327 | 449.1442 | 449.1436 | 5.01 | POS | 3185111.275 | 3078825.869 | 3239621.219 | 0.426130501 | 0.419232113 | 0.425171897 | 0.423511503 | NDTPPCMMWLHFIY-UHFFFAOYSA-N | CC(=O)OCC1C(C(C(C(O1)OC2=C(C=C(C=C2C=CC3=CC=C(C=C3)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00608 | 7.63\_359.1500m/z | M+FA-H | C19H22O4 | 67.5 | 50.2 | -0.17 | 2,3-Didehydro-gibberellin A9 | 161.0235, 197.0442, 254.9862, 274.9925, 315.1232, 315.1604, 358.9958, 359.1509 | 359.15 | 359.15 | 7.63 | NEG | 29593.48238 | 30486.55919 | 29141.32819 | 0.003959261 | 0.00415124 | 0.003824544 | 0.003978348 | NJHXRWOUQCGQAV-YGNOGLJPSA-N |  |  |  | LMPR0104170023 | C11866 | 443459 |  |  |  |  |  |  |  |  | level2 |
| compound00609 | 8.52\_325.1079m/z | M-H2O-H | C19H20O6 | 54.9 | 0 | -0.72 | 2,5,7-Trihydroxy-6,8-dimethyl-3-(4'-methoxybenzyl)chroman-4-one | 264.9900, 281.0814, 281.1177, 283.0608, 304.9799, 304.9863, 307.1914, 324.9908, 325.0697, 325.1078 | 325.1081 | 325.1079 | 8.52 | NEG | 25885.94075 | 27740.04563 | 26577.45496 | 0.003463235 | 0.003777257 | 0.003488058 | 0.003576184 | PLNGZQZXHIURST-UHFFFAOYSA-N | CC1=C(C(=C2C(=C1O)C(=O)C(C(O2)O)CC3=CC=C(C=C3)OC)C)O |  |  |  |  | 5322061 |  |  |  |  |  |  |  |  | level2 |
| compound00610 | 4.86\_275.0559m/z | 2M-H | C7H6O3 | 42.2 | 0 | -0.89 | 2,5-Dihydroxybenzaldehyde |  | 275.0561 | 275.0559 | 4.86 | NEG | 6799.896029 | 7306.852465 | 8815.213094 | 0.000909746 | 0.000994947 | 0.001156919 | 0.001020537 | CLFRCXCBWIQVRN-UHFFFAOYSA-N | OC1=CC(C=O)=C(O)C=C1 | HMDB0004062 | 44699 |  | C05585 | 70949 | 1194-98-5 | 2,5-二羟基苯甲醛 | 其他 |  | Others |  | HY-N1673 | HPLC≥98% | level2 |
| compound00611 | 7.55\_300.0875m/z | M+FA-H | C15H13NO3 | 55.6 | 0 | -1.14 | 2,6-dimethoxy-9H-carbazole-3-carbaldehyde |  | 300.0878 | 300.0875 | 7.55 | NEG | 5221.2419 | 5360.42947 | 5014.532796 | 0.000698541 | 0.000729909 | 0.000658113 | 0.000695521 | WCKFRKXQABCDRE-UHFFFAOYSA-N | COC1=CC2=C(C=C1)NC3=C2C=C(C(=C3)OC)C=O |  |  |  |  | 182690 |  |  |  |  |  |  |  |  | level2 |
| compound00612 | 9.10\_283.1324m/z | M+H | C18H18O3 | 52.6 | 0 | -1.65 | 3''-methoxynyasol |  | 283.1329 | 283.1324 | 9.1 | POS | 5209.157584 | 5324.540911 | 4784.709081 | 0.000696924 | 0.000725023 | 0.000627951 | 0.000683299 | APVUNYPUJLEPIY-UHFFFAOYSA-N | COC1=C(C=CC(=C1)C(C=C)C=CC2=CC=C(C=C2)O)O |  | 973350 |  |  | 71429202 |  |  |  |  |  |  |  |  | level2 |
| compound00613 | 5.12\_163.0393m/z | M-H2O-H | C9H10O4 | 49.2 | 0 | -4.23 | 2,6-Dimethoxybenzoic acid |  | 163.04 | 163.0393 | 5.12 | NEG | 1886.438854 | 1484.184409 | 1632.816896 | 0.000252383 | 0.000202096 | 0.000214293 | 0.000222924 | MBIZFBDREVRUHY-UHFFFAOYSA-N | COC1=CC=CC(OC)=C1C(O)=O | HMDB0029273 | 86145 |  |  | 15109 | 1466-76-8 | 2,6-二甲氧基苯甲酸 | 羧酸及衍生物 |  | Carboxylic acid and derivatives |  | HY-76504 | HPLC≥98% | level2 |
| compound00614 | 7.13\_212.1405n | M+H-H2O, M+H | C12H20O3 | 53.1 | 61.1 | -3.72 | 2-(3-hydroxy-2-pent-2-enylcyclopentyl)acetic acid | 151.1115, 154.9669, 159.1166, 163.0388, 177.0544, 177.1272, 177.1635, 195.0832, 195.1137, 195.1375 | 213.1485 | 213.1477 | 7.13 | POS | 168936.737 | 168218.6782 | 160978.786 | 0.022601752 | 0.022905703 | 0.021127055 | 0.022211504 | LYSGIJUGUGJIPS-UHFFFAOYSA-N | CCC=CCC1C(CCC1O)CC(=O)O |  |  |  |  | 11171865 |  |  |  |  |  |  |  |  | level2 |
| compound00615 | 9.47\_239.1285m/z | M+FA-H | C12H18O2 | 57.8 | 76.9 | -2.08 | 2-[(1R)-4-methyl-1-cyclohex-3-enyl]prop-2-enyl acetate | 101.0599, 102.9557, 154.0628, 195.1383, 218.9879, 238.9913, 239.0696, 239.1261 | 239.129 | 239.1285 | 9.47 | NEG | 19144.76358 | 17436.31034 | 17280.52196 | 0.002561345 | 0.002374237 | 0.002267917 | 0.002401166 | BCTDJPZNMXPMIA-LBPRGKRZSA-N | CC1=CC[C@@H](CC1)C(=C)COC(=O)C |  |  |  |  |  | 15111-97-4 |  |  |  |  |  |  |  | level2 |
| compound00616 | 4.44\_195.0293m/z | M+FA-H | C8H6O3 | 41.3 | 1.86 | -3.96 | 2-Carboxybenzaldehyde | 130.9915, 136.0155, 151.0391, 180.0056, 195.0292 | 195.0301 | 195.0293 | 4.44 | NEG | 12366.60332 | 12811.97622 | 12766.80851 | 0.001654506 | 0.001744559 | 0.001675532 | 0.001691532 | DYNFCHNNOHNJFG-UHFFFAOYSA-N | C1=CC=C(C(=C1)C=O)C(=O)O |  | 65893 |  | C03057 | 8406 | 119-67-5 | 2-羧基苯甲醛 | 其他 |  | Others |  | HY-Y1771 | HPLC≥98% | level2 |
| compound00617 | 4.67\_241.0973m/z | M+H | C14H12N2O2 | 57.9 | 0 | 0.64 | 2-Ethyl-2-vinylcyclobutanone |  | 241.0972 | 241.0973 | 4.67 | POS | 2126.068525 | 2029.469828 | 1938.190399 | 0.000284443 | 0.000276345 | 0.000254371 | 0.00027172 | CNUHEVWYPKFJHH-UHFFFAOYSA-N | C1=CC=C2C(=C1)C3=C(N2)C(=NC=C3)CCC(=O)O |  |  |  |  | 5375436 |  |  |  |  |  |  |  |  | level2 |
| compound00618 | 5.00\_261.1339m/z | M-H | C12H22O6 | 57.8 | 88.7 | -1.91 | 2-hex-2-enoxy-6-(hydroxymethyl)oxane-3,4,5-triol | 125.0962, 187.097, 261.1342 | 261.1344 | 261.1339 | 5 | NEG | 21065.34579 | 18323.84556 | 19700.61086 | 0.002818296 | 0.002495089 | 0.002585533 | 0.002632973 | GZDNGWOBFHUEOM-UHFFFAOYSA-N | CCCC=CCOC1C(C(C(C(O1)CO)O)O)O |  |  |  |  | 6450053 |  |  |  |  |  |  |  |  | level2 |
| compound00619 | 6.37\_447.1084m/z | M-H2O-H | C25H22O9 | 67.6 | 94.4 | -0.36 | 2-Hydroxy-2,2-diphenylaceticacid | 109.0285, 173.0235, 185.0236, 267.066, 277.0508, 293.0817, 295.0609, 337.0716, 403.1186, 447.1085 | 447.1085 | 447.1084 | 6.37 | NEG | 83355.08366 | 84191.9672 | 84163.97114 | 0.011151932 | 0.011464103 | 0.011045784 | 0.011220606 | CRPGUMMYQABYES-UHFFFAOYSA-N | COC1=C(O)C=CC(=C1)C1OC2=C(OC1CO)C=C(C=C2)C1CC(=O)C2=C(O1)C=C(O)C=C2O | HMDB0033325 |  |  | C08600 | 4481258 | 70815-32-6 |  |  |  |  |  |  |  | level2 |
| compound00620 | 5.96\_349.1656m/z | M-H | C19H26O6 | 41.7 | 0 | -0.24 | 2-Propenoic acid, 2-methyl-2,3,3a,4,5,8,9,10,11,11a-decahydro-6,10-bis (hydroxymethyl)-3-methylene-2-oxocyc lodeca[b]furan-4-yl ester |  | 349.1657 | 349.1656 | 5.96 | NEG | 7174.354243 | 7579.891885 | 7882.343916 | 0.000959844 | 0.001032125 | 0.001034489 | 0.001008819 | PIRNIYXVCYUDEY-RZGVYQARSA-N | CC(=C)C(=O)O[C@@H]1C/C(=C\CC[C@H](C[C@@H]2[C@@H]1C(=C)C(=O)O2)CO)/CO |  |  |  |  |  | 1380680-89-6 | 香叶草基阿魏酸酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | DP0084-0005 | HPLC≥98% | level2 |
| compound00621 | 8.77\_295.0971m/z | M-H2O-H | C18H18O5 | 41.4 | 0 | -1.45 | 2E)-1-(4-hydroxyphenyl)-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one |  | 295.0976 | 295.0971 | 8.77 | NEG | 4754.95973 | 5793.028591 | 5461.75947 | 0.000636158 | 0.000788815 | 0.000716808 | 0.000713927 | UJQJEKOZLIGAHH-CMDGGOBGSA-N | COc1cc(OC)c(/C=C/C(=O)c2ccc(O)cc2)c(OC)c1 |  |  |  |  |  | 1389310-69-3 |  | 其他 |  | Others |  | DH0344 | HPLC≥98% | level2 |
| compound00622 | 6.56\_313.0718m/z | M-H | C17H14O6 | 60.9 | 41.8 | 0.19 | 2-(3,4-dihydroxyphenyl)ethenyl 3-(3,4-dihydroxyphenyl)prop-2-enoate | 151.0392, 161.0235, 269.0821, 283.0974, 312.0936, 313.0709 | 313.0718 | 313.0718 | 6.56 | NEG | 52714.78961 | 53836.6302 | 55717.62632 | 0.00705262 | 0.007330731 | 0.00731245 | 0.007231934 | GFZFUVWXGQWUGX-UHFFFAOYSA-N | C1=CC(=C(C=C1C=CC(=O)OC=CC2=CC(=C(C=C2)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00623 | 7.07\_303.1238m/z | M-H | C17H20O5 | 55.7 | 0 | 0.12 | Artilesin A |  | 303.1238 | 303.1238 | 7.07 | NEG | 3133.245198 | 3066.127073 | 3217.203582 | 0.000419191 | 0.000417503 | 0.00042223 | 0.000419641 | QONYNSMAVSRIRD-UHFFFAOYSA-N | CC1C2C(OC1=O)C1C(C)=CC(=O)C1=C(C)CC2OC(C)=O | HMDB0035790 |  |  |  | 627631 | 5989-43-5 |  |  |  |  |  |  |  | level2 |
| compound00624 | 0.96\_337.0775m/z | M-H | C12H18O11 | 40.5 | 0 | -0.54 | Ascorbyl glucoside |  | 337.0776 | 337.0775 | 0.96 | NEG | 17873.42117 | 17513.3967 | 17335.84472 | 0.002391254 | 0.002384733 | 0.002275178 | 0.002350388 | MLSJBGYKDYSOAE-DCWMUDTNSA-N | C(C1C(C(C(C(O1)OC2=C(C(OC2=O)C(CO)O)O)O)O)O)O |  | 72159 |  | C18339 | 54693473 | 129499-78-1 | 2-O-α-D-葡萄糖基-L-抗坏血 酸 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | B65164-100mg | HPLC≥98% | level2 |
| compound00625 | 0.79\_133.0608m/z | M+H | C4H8N2O3 | 51.8 | 54.7 | 0.08 | asparagin | 88.0761, 112.0218, 113.0298, 116.0343, 116.0708, 123.0792, 132.0771, 132.0910, 132.1021, 133.0613 | 133.0608 | 133.0608 | 0.79 | POS | 38098.19138 | 40618.04147 | 41917.05925 | 0.005097091 | 0.005530806 | 0.005501247 | 0.005376381 | DCXYFEDJOCDNAF-UHFFFAOYSA-N | NC(CC(O)=N)C(O)=O | HMDB0251512 |  |  | C16438 |  |  |  |  |  |  |  |  |  | level2 |
| compound00626 | 4.95\_791.1454m/z | M+FA-H | C37H30O17 | 52.2 | 0 | -1.46 | epigallocatechin-(4bata-8)-epicatechin-3-o-gallate ester |  | 791.1466 | 791.1454 | 4.95 | NEG | 54149.16412 | 66832.65751 | 65083.01139 | 0.007244523 | 0.009100351 | 0.008541575 | 0.008295483 | LQQNPVZIFKLQPE-UHFFFAOYSA-N | C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)O)C6=CC(=C(C=C6)O)O)OC(=O)C7=CC(=C(C(=C7)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00627 | 4.09\_595.1665m/z | M-H2O-H | C27H34O16 | 55 | 69.9 | -0.54 | epigeoside | 313.0727, 355.0822, 385.0927, 475.1238, 595.1669 | 595.1668 | 595.1665 | 4.09 | NEG | 46761.90966 | 48451.15105 | 45092.05102 | 0.006256195 | 0.006597411 | 0.005917937 | 0.006257181 | WQZUHCMKCSWRNS-UHFFFAOYSA-N | C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)OC4C(C(C(C(O4)COC5C(C(C(C(O5)CO)O)O)O)O)O)O |  |  |  |  | 131795 |  |  |  |  |  |  |  |  | level2 |
| compound00628 | 7.12\_437.1207m/z | M+Na | C22H22O8 | 44.5 | 0 | 0.07 | Epipodophyllotoxin |  | 437.1207 | 437.1207 | 7.12 | POS | 16397.16004 | 16703.86278 | 16106.67499 | 0.002193748 | 0.002274502 | 0.00211386 | 0.002194037 | YJGVMLPVUAXIQN-LGWHJFRWSA-N | COc1cc([C@@H]2c3cc4c(cc3[C@@H](O)[C@H]3COC(=O)[C@H]23)OCO4)cc(OC)c1OC |  |  |  |  |  | 4375-07-9 | 表鬼臼毒素 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | B25498-10mg | HPLC≥98% | level2 |
| compound00629 | 5.45\_535.0871m/z | M+H-H2O | C27H20O13 | 47.6 | 0 | -0.05 | Epitheaflagallin 3-O-gallate |  | 535.0871 | 535.0871 | 5.45 | POS | 8540.012419 | 8191.768431 | 9158.130173 | 0.001142553 | 0.001115442 | 0.001201924 | 0.001153307 | CMGRMMSVGCHWOK-UHFFFAOYSA-N | OC1=CC(O)=C2CC(OC(=O)C3=CC(O)=C(O)C(O)=C3)C(OC2=C1)C1=CC(=O)C(O)=C2C(O)=C(O)C(O)=CC2=C1 | HMDB0033288 | 89146 |  |  | 14520971 | 102067-92-5 | 表茶黄棓灵 3-O-没食子酸酯 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | DE0145 | HPLC≥98% | level2 |
| compound00630 | 4.62\_596.1747n | M+H-H2O, M+Na | C27H32O15 | 41 | 0 | 1.01 | Eriocitrin |  | 619.1633 | 619.1639 | 4.62 | POS | 49895.92699 | 46075.00099 | 44406.03927 | 0.006675489 | 0.006273859 | 0.005827904 | 0.006259084 | OMQADRGFMLGFJF-XMOPVOFBSA-N | CC1O[C@@H](OCC2O[C@@H](Oc3cc(O)c4c(c3)OC(c3ccc(O)c(O)c3)CC4=O)C(O)C(O)[C@@H]2O)C(O)C(O)[C@H]1O |  |  |  |  |  | 13463-28-0 | 圣草次甙 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0636 | HPLC≥98% | level2 |
| compound00631 | 3.84\_339.0721m/z | M-H | C15H16O9 | 40.3 | 0 | -0.15 | Esculin |  | 339.0722 | 339.0721 | 3.84 | NEG | 3355.451903 | 3654.631648 | 3403.490523 | 0.00044892 | 0.000497637 | 0.000446678 | 0.000464412 | XHCADAYNFIFUHF-TVKJYDDYSA-N | OC[C@H]1O[C@@H](OC2=C(O)C=C3OC(=O)C=CC3=C2)[C@H](O)[C@@H](O)[C@@H]1O | HMDB0030820 | 43929 |  | C09264 | 5281417 | 531-75-9 | 秦皮甲素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0188 | HPLC≥98% | level2 |
| compound00632 | 6.45\_209.0811m/z | M+H | C11H12O4 | 44.7 | 0 | 1.26 | Ethyl Caffeic acid |  | 209.0808 | 209.0811 | 6.45 | POS | 2241.617892 | 2290.607468 | 1919.725006 | 0.000299902 | 0.000311903 | 0.000251947 | 0.000287918 | WDKYDMULARNCIS-GQCTYLIASA-N | CCOC(=O)\C=C\C1=CC(O)=C(O)C=C1 | HMDB0301712 |  |  |  |  | 102-37-4 | 咖啡酸乙酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N6966 | HPLC≥98% | level2 |
| compound00633 | 4.96\_199.0599m/z | M+H | C9H10O5 | 43.1 | 0 | -0.85 | Ethyl gallate |  | 199.0601 | 199.0599 | 4.96 | POS | 7584.488407 | 7611.778583 | 8561.605112 | 0.001014716 | 0.001036467 | 0.001123636 | 0.001058273 | VFPFQHQNJCMNBZ-UHFFFAOYSA-N | CCOC(=O)C1=CC(O)=C(O)C(O)=C1 | HMDB0033836 | 89560 |  |  | 13250 | 831-61-8 | 没食子酸乙酯 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0525 | HPLC≥98% | level2 |
| compound00634 | 7.88\_173.1172m/z | M+H | C9H16O3 | 44.7 | 0 | 0.06 | Ethyl pivaloylacetate |  | 173.1172 | 173.1172 | 7.88 | POS | 2829.717622 | 2544.260223 | 2745.718654 | 0.000378583 | 0.000346442 | 0.000360352 | 0.000361792 | VUYNTIDSHCJIKF-UHFFFAOYSA-N | CCOC(=O)CC(=O)C(C)(C)C |  | 359560 |  |  | 86950 |  | 特戊酰基乙酸乙酯 | 其他 |  | Others |  | HY-W076971 | HPLC≥98% | level2 |
| compound00635 | 5.72\_149.0597m/z | M+H-H2O | C9H10O3 | 43.8 | 0 | 0.16 | Ethyl vanillin |  | 149.0597 | 149.0597 | 5.72 | POS | 2825.407821 | 2596.440359 | 3107.177782 | 0.000378006 | 0.000353547 | 0.00040779 | 0.000379781 | CBOQJANXLMLOSS-UHFFFAOYSA-N | CCOC1=C(O)C=CC(C=O)=C1 | HMDB0029665 | 86409 |  |  | 8467 | 121-32-4 | 乙基香兰素 | 其他 |  | Others |  | B27123-100mg | HPLC≥98% | level2 |
| compound00636 | 7.64\_337.1044m/z | M+Na | C18H18O5 | 52.1 | 0 | -0.93 | ETHYL-PHOSPHINICACID |  | 337.1047 | 337.1044 | 7.64 | POS | 20147.61701 | 21626.44113 | 23432.58751 | 0.002695515 | 0.002944791 | 0.003075322 | 0.002905209 | TYFJTEPDESMEHE-UHFFFAOYSA-N | COC1=CC=C(C=C1)CCC2CC3=C(C(=CC(=C3)O)O)C(=O)O2 |  |  |  |  | 15558543 |  |  |  |  |  |  |  |  | level2 |
| compound00637 | 9.36\_326.1153n | M-H, M+FA-H, 2M-H | C19H18O5 | 55.2 | 0 | -0.32 | Eucalyptin | 281.1181, 325.1078 | 325.1081 | 325.108 | 9.36 | NEG | 821299.6455 | 743335.5193 | 746522.3933 | 0.109880252 | 0.101217196 | 0.097974522 | 0.10302399 | NHMMAMIRMITGRD-UHFFFAOYSA-N | C1(OC)=C(C)C2OC(C3C=CC(OC)=CC=3)=CC(=O)C=2C(O)=C1C |  | 49455 | LMPK12111028 |  | 76573 |  |  |  |  |  |  |  |  | level2 |
| compound00638 | 7.81\_287.1288m/z | M-H2O-H | C17H22O5 | 51 | 0 | -0.41 | eupaformonin |  | 287.1289 | 287.1288 | 7.81 | NEG | 8341.735995 | 9260.5753 | 8651.106019 | 0.001116026 | 0.001260978 | 0.001135382 | 0.001170795 | UYVDDCCDZKMLBM-IGERJXIRSA-N | CC1=CCC(C(=CC2C(C(C1)O)C(=C)C(=O)O2)C)OC(=O)C |  | 67690 |  | C09431 | 11953933 | 55520-20-2 |  |  |  |  |  |  |  | level2 |
| compound00639 | 8.63\_325.0714m/z | M-H2O-H | C18H16O7 | 41.1 | 0 | -0.98 | Eupatilin |  | 325.0717 | 325.0714 | 8.63 | NEG | 5446.74302 | 5044.418776 | 5729.174917 | 0.00072871 | 0.000686879 | 0.000751904 | 0.000722498 | DRRWBCNQOKKKOL-UHFFFAOYSA-N | C1(O)=CC2OC(C3C=C(OC)C(OC)=CC=3)=CC(=O)C=2C(O)=C1OC | HMDB0029469 | 49653 | LMPK12111228 | C10040 | 5273755 | 22368-21-4 | 异泽兰黄素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0783 | HPLC≥98% | level2 |
| compound00640 | 6.11\_331.1540m/z | M+H-H2O | C19H24O6 | 51.2 | 0 | 0.03 | Eurycomalactone |  | 331.154 | 331.154 | 6.11 | POS | 5933.712166 | 5670.208153 | 5683.228811 | 0.000793861 | 0.000772091 | 0.000745874 | 0.000770609 | OGHYZHNTIINXEO-UHFFFAOYSA-N | CC1=CC(=O)C(O)C2(C)C1CC(=O)C1(C)C3C(=O)OC(C3C)C(O)C12 |  |  |  |  |  | 23062-24-0 | 东革内酯 | 萜类 | 三萜类 | Terpenes | Triterpenes | DD0109 | HPLC≥98% | level2 |
| compound00641 | 3.99\_487.1437m/z | M+H | C21H26O13 | 40.5 | 0 | -1.97 | Fabiatrin |  | 487.1446 | 487.1437 | 3.99 | POS | 15862.09179 | 16010.01222 | 16810.23809 | 0.002122162 | 0.002180023 | 0.002206196 | 0.00216946 | AHBJPGDMGKOLJC-OJHUANBKSA-N | COc1cc2ccc(=O)oc2cc1O[C@@H]1O[C@H](CO[C@@H]2OC[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 18309-73-4 | 法筚枝苷 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DF0020 | HPLC≥98% | level2 |
| compound00642 | 0.83\_130.0862m/z | M+H-H2O | C6H13NO3 | 59.7 | 14.7 | -0.6 | Fagomine | 70.0657, 84.0448, 84.0812, 112.0871, 130.0501, 130.0863 | 130.0862 | 130.0862 | 0.83 | POS | 1061457.374 | 1035769.459 | 1035413.267 | 0.142010537 | 0.141036823 | 0.135888918 | 0.139645426 | YZNNBIPIQWYLDM-HSUXUTPPSA-N | OC[C@H]1NCC[C@@H](O)[C@@H]1O | HMDB0033453 | 68150 |  | C10144 | 72259 | 53185-12-9 | (2R,3R,4R)-2-羟甲基哌啶-3,4-二醇 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-13005 | HPLC≥98% | level2 |
| compound00643 | 11.89\_280.2631m/z | M+NH4 | C18H30O | 59.9 | 80.2 | -1.64 | Farnesylacetone | 161.1324, 163.1479, 165.1635, 175.1481, 179.1798, 245.2263, 263.2366, 279.2312, 280.1020, 280.2634 | 280.2635 | 280.2631 | 11.89 | POS | 42650.91155 | 42530.79574 | 42603.25041 | 0.005706191 | 0.005791258 | 0.005591303 | 0.005696251 | LTUMRKDLVGQMJU-UHFFFAOYSA-N | CC(=CCCC(=CCCC(=CCCC(=O)C)C)C)C |  | 341180 |  |  | 61206 |  |  |  |  |  |  |  |  | level2 |
| compound00644 | 5.81\_372.1207n | M-H2O-H, M-H | C20H20O7 | 57.9 | 73.9 | -0.65 | fibraurin | 235.9262, 267.0643, 279.0670, 323.0572, 327.1254, 338.0787, 341.1028, 353.1024, 371.0142, 371.1139 | 371.1136 | 371.1134 | 5.81 | NEG | 25324.23641 | 25121.96902 | 24378.34847 | 0.003388086 | 0.003420764 | 0.003199445 | 0.003336098 | XUFRUKAPNGPYSR-TZGNGTQESA-N | C[C@@]12CC=C3C(=O)O[C@H](C[C@]3([C@@H]1[C@H]4[C@H]5[C@@H]([C@@]2(C(=O)O4)O)O5)C)C6=COC=C6 |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00645 | 9.98\_303.1965m/z | M-H | C19H28O3 | 57.1 | 74.4 | -0.26 | ent-15,16-epoxy-3-oxa-kauran-2-one | 259.2065, 282.9789, 302.9838, 303.1965 | 303.1966 | 303.1965 | 9.98 | NEG | 12482.6127 | 13193.61926 | 14449.61191 | 0.001670027 | 0.001796525 | 0.001896385 | 0.001787646 | LLKRJRVDKASBCG-UHFFFAOYSA-N | CC1(C2CCC34CC(CCC3C2(CC(=O)O1)C)C5(C4O5)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00646 | 5.23\_731.1606m/z | M+FA-H | C36H30O14 | 54.6 | 47.7 | -1.63 | elgnica | 321.0404, 335.0564, 339.0509, 353.0674, 489.0827, 493.1150, 519.0925, 533.1102, 537.1025, 731.1609 | 731.1618 | 731.1606 | 5.23 | NEG | 278717.8115 | 275396.8212 | 276394.5593 | 0.037289172 | 0.037499747 | 0.036274364 | 0.037021094 | KDDWZKWJBCZABZ-RGJYXDCBSA-N | C1=CC2=C(C(=C1)O)C(=O)C3=C([C@]2([C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)C5=C(C6=C(C=C5)C(=O)C7=C(C6=O)C(=CC(=C7)CO)O)O)C=C(C=C3O)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00647 | 4.83\_636.3751m/z | M+FA-H | C33H53NO8 | 40.3 | 0.00265 | -0.44 | Edpetiline | 315.0147, 330.038, 493.0985, 535.1089, 575.1408, 636.3752 | 636.3753 | 636.3751 | 4.83 | NEG | 126000.6071 | 126359.7877 | 118299.1832 | 0.016857402 | 0.017205936 | 0.015525731 | 0.01652969 | DHQFYEJMFMYGCV-RRIRULBESA-N | C[C@H]1CC[C@@H]2N(C1)C[C@@H]1[C@H](CC[C@H]3[C@@H]4CC(=O)[C@H]5C[C@@H](O[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6O)CC[C@]5(C)[C@H]4C[C@H]31)[C@]2(C)O |  |  |  |  |  | 32685-93-1 | 西贝母碱苷 | 生物碱 |  | Alkaloids |  | HY-N1921 | HPLC≥98% | level2 |
| compound00648 | 6.91\_271.0963m/z | M+H | C16H14O4 | 42.6 | 0 | -0.65 | Echinatin |  | 271.0965 | 271.0963 | 6.91 | POS | 1176.901276 | 1234.656413 | 1290.506164 | 0.000157456 | 0.000168119 | 0.000169368 | 0.000164981 | QJKMIJNRNRLQSS-WEVVVXLNSA-N | C1(O)=CC=C(C(=O)/C=C/C2C=CC(O)=CC=2OC)C=C1 |  | 52234 | LMPK12120431 |  | 6442675 |  | 刺甘草查尔酮 | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | HY-N0269 | HPLC≥98% | level2 |
| compound00649 | 10.25\_315.1601m/z | M+FA-H | C18H22O2 | 53.6 | 0 | -0.26 | deoxodehydrocyclopiloselloidone | 112.9845, 180.9723, 248.9599, 271.1701, 272.1733, 315.155 | 315.1602 | 315.1601 | 10.25 | NEG | 141372.5962 | 146648.1592 | 149444.4618 | 0.018913994 | 0.019968527 | 0.019613276 | 0.019498599 | WFXJDXJXOHZQRD-UHFFFAOYSA-N | CC(=CCC1=C2C(=CC(=C1)C(=O)C)C=CC(O2)(C)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00650 | 8.44\_315.1966m/z | M-H2O-H | C20H30O4 | 44 | 0 | -0.03 | Deoxyandrographolide |  | 315.1966 | 315.1966 | 8.44 | NEG | 18457.34042 | 18401.75752 | 20026.99128 | 0.002469375 | 0.002505698 | 0.002628367 | 0.00253448 | DAXSYTVXDSOSIE-HNJRGHQBSA-N | CC1=C(CCC2=CCOC2=O)[C@]2(C)CC[C@@H](O)[C@@](C)(CO)[C@H]2CC1 |  |  |  |  |  | 79233-15-1 | 去氧穿心莲内酯 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N0857 | HPLC≥98% | level2 |
| compound00651 | 10.22\_303.1951m/z | M+H | C19H26O3 | 54.2 | 0 | -1.24 | deoxycapillartemisin |  | 303.1955 | 303.1951 | 10.22 | POS | 20536.38704 | 34190.85698 | 46984.7729 | 0.002747528 | 0.00465564 | 0.00616634 | 0.004523169 | KRXZPYDOSGHFEM-UHFFFAOYSA-N | CC(=CCC1=CC(=CC(=C1O)CC=C(C)C)CCC(=O)O)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00652 | 4.92\_149.0597m/z | M+H-H2O | C9H10O3 | 41.7 | 0 | 0.05 | Desaminotyrosine |  | 149.0597 | 149.0597 | 4.92 | POS | 5939.401636 | 6654.852449 | 6868.84481 | 0.000794622 | 0.000906166 | 0.000901476 | 0.000867421 | NMHMNPHRMNGLLB-UHFFFAOYSA-N | OC(=O)CCC1=CC=C(O)C=C1 | HMDB0002199 | 4148 |  | C01744 | 10394 | 501-97-3 | 对羟基苯丙酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-W015346 | HPLC≥98% | level2 |
| compound00653 | 6.23\_387.1437m/z | M+H-H2O | C21H24O8 | 41.7 | 0 | -0.38 | Desoxyrhaponticin |  | 387.1438 | 387.1437 | 6.23 | POS | 5360.76816 | 5205.957295 | 5185.121429 | 0.000717208 | 0.000708876 | 0.000680502 | 0.000702195 | MFMQRDLLSRLUJY-UHFFFAOYSA-N | COc1ccc(C=Cc2cc(O)cc(OC3OC(CO)C(O)C(O)C3O)c2)cc1 |  |  |  |  |  | 30197-14-9 | 脱氧土大黄苷 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N2486 | HPLC≥98% | level2 |
| compound00654 | 5.63\_278.1152n | M+Na, M+K, M+H-H2O | C15H18O5 | 65 | 69.7 | -0.93 | dictamdiol B | 301.1052 | 301.1047 | 301.1044 | 5.63 | POS | 120243.3376 | 121591.0691 | 119987.8104 | 0.016087147 | 0.016556598 | 0.015747349 | 0.016130364 | XWGNIHFUPLLNBR-GVUJHPQVSA-N | CC1=C2[C@@H](C(=O)O[C@H]([C@@]2(CC[C@H]1O)C)C3=COC=C3)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00655 | 7.84\_181.1222m/z | M+H | C11H16O2 | 50.5 | 47.3 | -0.33 | Dihydroactinidiolide | 107.0858, 111.9685, 121.101, 135.1166, 139.9631, 163.1113, 181.0645, 181.0989, 181.122 | 181.1223 | 181.1222 | 7.84 | POS | 14018.4133 | 13522.0441 | 13714.43622 | 0.001875499 | 0.001841246 | 0.0017999 | 0.001838881 | IMKHDCBNRDRUEB-UHFFFAOYSA-N | CC12CCCC(C)(C)C1=CC(=O)O2 | HMDB0035240 | 90552 |  |  | 27209 | 15356-74-8 | 二氢猕猴桃内酯 | 萜类 | 胡萝卜素 | Terpenes | Carotenoids | HY-W041301 | HPLC≥98% | level2 |
| compound00656 | 4.29\_181.0500m/z | M-H | C9H10O4 | 51.2 | 0 | -3.39 | Dihydrocaffeic acid |  | 181.0506 | 181.05 | 4.29 | NEG | 1519.22605 | 1462.1518 | 1140.006949 | 0.000203255 | 0.000199096 | 0.000149616 | 0.000183989 | DZAUWHJDUNRCTF-UHFFFAOYSA-N | OC(=O)CCC1=CC(O)=C(O)C=C1 | HMDB0000423 | 5412 |  | C10447 | 348154 | 1078-61-1 | 二氢咖啡酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N2406 | HPLC≥98% | level2 |
| compound00657 | 4.96\_155.0702m/z | M+H | C8H10O3 | 54.9 | 0 | -0.78 | Filicinsaure |  | 155.0703 | 155.0702 | 4.96 | POS | 10074.26825 | 10295.47454 | 11057.7142 | 0.001347819 | 0.001401896 | 0.001451228 | 0.001400314 | ZAQQZMZXYOTJAB-UHFFFAOYSA-N | CC1(C(=CC(=CC1=O)O)O)C |  |  |  |  | 550690 | 2065-00-1 |  |  |  |  |  |  |  | level2 |
| compound00658 | 5.69\_257.0806m/z | M+H | C15H12O4 | 40.4 | 0 | -0.98 | Dihydrodaidzein |  | 257.0808 | 257.0806 | 5.69 | POS | 2653.220627 | 3366.307711 | 3486.52455 | 0.00035497 | 0.000458377 | 0.000457576 | 0.000423641 | JHYXBPPMXZIHKG-CYBMUJFWSA-N | O=C1c2ccc(O)cc2OC[C@@H]1c1ccc(O)cc1 |  |  |  |  |  | 17238-05-0 | 二氢大豆苷元 | 黄酮类 | 二氢异黄酮类 | Flavonoids | isoflavanones | HY-N1461 | HPLC≥98% | level2 |
| compound00659 | 4.73\_433.1134m/z | M+H-H2O | C21H22O11 | 55.2 | 0 | 1.01 | Dihydrokaempferol-3-glucoside |  | 433.1129 | 433.1134 | 4.73 | POS | 28207.55098 | 28643.74911 | 26846.78137 | 0.003773839 | 0.003900311 | 0.003523405 | 0.003732518 | VWBWQPAZMNABMR-UHFFFAOYSA-N | C1=CC(=CC=C1C2C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00660 | 8.39\_215.1066m/z | M+H-H2O | C14H16O3 | 41.2 | 0 | -0.08 | Dihydrokavain |  | 215.1067 | 215.1066 | 8.39 | POS | 2480.644125 | 2658.31266 | 2567.870665 | 0.000331881 | 0.000361972 | 0.000337011 | 0.000343621 | VOOYTQRREPYRIW-UHFFFAOYSA-N | COC1=CC(=O)OC(CCC2=CC=CC=C2)C1 | HMDB0029504 |  |  |  | 98356 | 587-63-3 | 二氢醉椒素 | 其他 |  | Others |  | HY-N0920 | HPLC≥98% | level2 |
| compound00661 | 8.17\_315.0625m/z | M+K | C15H16O5 | 44.1 | 1.31 | -1.62 | Dihydromethysticin | 213.091, 214.094, 252.1455, 255.1738, 269.1521, 296.2289, 314.144, 315.0613 | 315.063 | 315.0625 | 8.17 | POS | 87416.98823 | 91237.6914 | 98356.66583 | 0.011695367 | 0.012423493 | 0.012908451 | 0.012342437 | RSIWXFIBHXYNFM-NSHDSACASA-N | COC1=CC(=O)OC(C1)CCC2=CC3=C(C=C2)OCO3 |  | 68016 |  | C09926 | 88308 | 19902-91-1 | 二氢麻醉椒素 | 其他 |  | Others |  | HY-N0921 | HPLC≥98% | level2 |
| compound00662 | 10.05\_278.0940n | M+Na, M+K, M+H, M+H-H2O | C18H14O3 | 48.5 | 29.7 | -1.15 | Dihydrotanshinone I | 301.0829 | 301.0835 | 301.0832 | 10.05 | POS | 6643100.194 | 6807683.087 | 6805580.155 | 0.888768827 | 0.926976544 | 0.893172759 | 0.90297271 | HARGZZNYNSYSGJ-JTQLQIEISA-N | Cc1cccc2c3c(ccc12)C1=C(C(=O)C3=O)[C@@H](C)CO1 |  |  |  |  |  | 87205-99-0 | 二氢丹参酮 I | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-N0360 | HPLC≥98% | level2 |
| compound00663 | 6.36\_237.0757m/z | M+H | C12H12O5 | 41.5 | 0 | -0.22 | Dimethylfraxetin |  | 237.0758 | 237.0757 | 6.36 | POS | 1951.94251 | 1639.405983 | 1780.003195 | 0.000261147 | 0.000223232 | 0.00023361 | 0.00023933 | RAYQKHLZHPFYEJ-UHFFFAOYSA-N | COC1=C(C(=C2C(=C1)C=CC(=O)O2)OC)OC |  | 43772 |  |  | 3083928 |  | 二甲基白蜡树亭 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0085 | HPLC≥98% | level2 |
| compound00664 | 10.56\_455.3515m/z | M+H-H2O | C30H48O4 | 51.5 | 0 | -0.97 | disacoside B qt |  | 455.352 | 455.3515 | 10.56 | POS | 4331.088003 | 3360.783325 | 3197.969762 | 0.000579449 | 0.000457625 | 0.000419706 | 0.000485593 | PGOYMURMZNDHNS-GBTZXOCISA-N | C[C@]12CC[C@@H]([C@@]([C@@H]1CC[C@@]3([C@H]2CC=C4[C@]3(CC[C@@]5([C@@H]4CC(CC5)(C)C)C(=O)O)C)C)(C)CO)O |  |  |  |  |  | 140360-29-8 |  |  |  |  |  |  |  | level2 |
| compound00665 | 7.36\_333.1695m/z | M+H | C19H24O5 | 56.6 | 74.3 | -0.6 | diversoside qt | 267.1372, 269.1531, 297.1483, 314.1452, 315.1581, 332.1512, 332.1936, 333.0724, 333.1099, 333.1658 | 333.1697 | 333.1695 | 7.36 | POS | 82297.69588 | 81661.69308 | 82264.94947 | 0.011010466 | 0.011119565 | 0.010796554 | 0.010975528 | QYYKWTUUCOTGNS-RTGRKSDTSA-N | C/C(=C\COC1=CC2=C(C=C1)C=CC(=O)O2)/CC[C@@H](C(C)(C)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00666 | 4.55\_279.0872m/z | M-H2O-H | C14H18O7 | 52.3 | 0 | -0.64 | dofuranuronic acid |  | 279.0874 | 279.0872 | 4.55 | NEG | 1103.947505 | 1247.706295 | 1154.355689 | 0.000147695 | 0.000169895 | 0.000151499 | 0.000156363 | RAAPRDZMRIATKY-UHFFFAOYSA-N | COC(=O)C(C1C(C(C(O1)O)O)OCC2=CC=CC=C2)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00667 | 6.88\_267.1015m/z | M+H | C17H14O3 | 52 | 0 | -0.15 | Dracorhodin perchloric acid |  | 267.1016 | 267.1015 | 6.88 | POS | 2308.417129 | 2593.950252 | 2276.429844 | 0.000308839 | 0.000353208 | 0.000298761 | 0.00032027 | UCZJPQIEFFTIEV-UHFFFAOYSA-N | COC1=C(C)C(=O)C=C2OC(=CC=C12)C1=CC=CC=C1 | HMDB0251617 | 348602 |  |  | 69509 |  | 血竭素髙氯酸盐 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-N0726 | HPLC≥98% | level2 |
| compound00668 | 9.29\_299.1274m/z | M+H-H2O | C18H20O5 | 58.4 | 40.3 | -1.27 | Dihydroechinofuran | 197.0596, 217.0859, 239.1065, 253.1584, 255.1739, 257.1169, 299.127 | 299.1278 | 299.1274 | 9.29 | POS | 31944.71268 | 31264.81855 | 31545.14168 | 0.004273828 | 0.004257212 | 0.004140023 | 0.004223688 | IMZVJDUASUPZQK-UHFFFAOYSA-N | CC(=O)OC(CC=C(C)C)c1coc(-c2cc(O)ccc2O)c1 |  |  |  |  |  | 85022-66-8 | 紫草呋喃A | 醌类 | 苯醌类 | Quinones | Benzoquinones | JOT-10519 | HPLC≥98% | level2 |
| compound00669 | 4.25\_387.1297m/z | M-H | C17H24O10 | 53.2 | 26.4 | 0.06 | fissistigmoside | 161.0447, 179.0554, 191.0190, 207.1015, 209.0298, 319.0814, 341.1086, 357.2142, 386.0785, 387.0826 | 387.1297 | 387.1297 | 4.25 | NEG | 27493.22689 | 26632.34808 | 27194.32838 | 0.003678271 | 0.003626426 | 0.003569017 | 0.003624572 | UYXZFQQYRZUIEJ-UHFFFAOYSA-N | COC1=CC(=CC(=C1O)OC)C2C(OC3C(C(C(OC3O2)CO)O)O)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00670 | 4.36\_449.1086m/z | M-H | C21H22O11 | 42.5 | 0 | -0.63 | Flavanomarein |  | 449.1089 | 449.1086 | 4.36 | NEG | 11667.02008 | 12264.50142 | 11100.53242 | 0.00156091 | 0.001670011 | 0.001456848 | 0.00156259 | DGGOLFCPSUVVHX-RTHJTPBESA-N | O=C1C2=CC=C(OC3OC(CO)C(O)C(O)C3O)C(O)=C2OC(C4=CC=C(O)C(O)=C4)C1 |  |  |  |  |  | 577-38-8 | 黄诺马苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N7675 | HPLC≥98% | level2 |
| compound00671 | 11.11\_313.1079m/z | M-H | C18H18O5 | 45.5 | 0 | -0.85 | Flavokawain A |  | 313.1081 | 313.1079 | 11.11 | NEG | 2688.541079 | 2750.570828 | 2061.319426 | 0.000359695 | 0.000374535 | 0.00027053 | 0.00033492 | CGIBCVBDFUTMPT-RMKNXTFCSA-N | COC1=CC=C(\C=C\C(=O)C2=C(O)C=C(OC)C=C2OC)C=C1 | HMDB0033586 | 52124 |  |  | 5355469 | 3420-72-2 | 2'-羟基-4,4',6'-甲氧基查尔酮 | 黄酮类 | 查尔酮类 | Flavonoids | Chalcones | 0 | HPLC≥98% | level2 |
| compound00672 | 1.45\_212.0560m/z | M+FA-H | C8H9NO3 | 55.9 | 81.3 | -2.57 | griffonin qt | 128.0343, 138.0549, 143.0252, 144.0656, 145.0495, 150.0549, 164.0344, 168.0656, 182.0452, 212.0555 | 212.0566 | 212.056 | 1.45 | NEG | 15247.24268 | 15200.97899 | 15322.76011 | 0.002039902 | 0.00206986 | 0.002010978 | 0.002040247 | SIKDHUUZRZDYPO-ZXHNMSBYSA-N | C1=C/C(=C\C#N)/[C@@H]([C@@H]([C@@H]1O)O)O |  |  |  |  |  | 63492-69-3 |  |  |  |  |  |  |  | level2 |
| compound00673 | 10.20\_329.1741m/z | M+H | C20H24O4 | 42 | 0 | -2.09 | Guaiacin |  | 329.1747 | 329.1741 | 10.2 | POS | 4929.297716 | 4955.181738 | 5229.236536 | 0.000659482 | 0.000674728 | 0.000686291 | 0.000673501 | TZAAYUCUPIYQBR-JGRMJRGVSA-N | CC1CC2=CC(=C(C=C2C(C1C)C3=CC(=C(C=C3)O)OC)O)OC | HMDB0034178 | 89757 |  |  | 11724027 | 36531-08-5 | 愈创木素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DY0171-0005 | HPLC≥98% | level2 |
| compound00674 | 5.04\_107.0493m/z | M+H-H2O | C7H8O2 | 46.6 | 0 | 1.22 | Guaiacol |  | 107.0492 | 107.0493 | 5.04 | POS | 1359.51904 | 1242.49916 | 1407.633128 | 0.000181888 | 0.000169186 | 0.00018474 | 0.000178605 | LHGVFZTZFXWLCP-UHFFFAOYSA-N | COC1=C(O)C=CC=C1 | HMDB0001398 | 6217 |  | C15572 | 460 | 90-05-1 | 愈创木酚 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1380 | HPLC≥98% | level2 |
| compound00675 | 4.99\_221.0792m/z | M+Na | C10H14O4 | 48.7 | 0 | 3.65 | Guaifenesin |  | 221.0783 | 221.0792 | 4.99 | POS | 1549.09591 | 1623.888191 | 1530.910013 | 0.000207251 | 0.000221119 | 0.000200919 | 0.000209763 | HSRJKNPTNIJEKV-UHFFFAOYSA-N | COC1=CC=CC=C1OCC(O)CO | HMDB0004998 | 4057 |  |  | 3516 | 93-14-1 | 愈创甘油醚 | 其他 |  | Others |  | HY-B0264 | HPLC≥98% | level2 |
| compound00676 | 0.84\_127.0635n | M+H-H2O, M+H | C6H9NO2 | 40.9 | 4.1 | 1.09 | Guvacine | 67.0548, 82.0656, 110.0602 | 128.0706 | 128.0707 | 0.84 | POS | 61193.1243 | 63857.51175 | 64691.48666 | 0.008186922 | 0.008695237 | 0.008490191 | 0.00845745 | QTDZOWFRBNTPQR-UHFFFAOYSA-N | C1CNCC(=C1)C(=O)O |  | 44304 |  | C10149 | 3532 |  | 去甲槟榔次碱 | 生物碱 |  | Alkaloids |  | HY-100809 | HPLC≥98% | level2 |
| compound00677 | 6.77\_345.1343m/z | M-H | C19H22O6 | 57.1 | 0.544 | -0.28 | hallactone a | 227.1073, 227.1437, 257.1587, 283.1339, 301.1442, 345.1336 | 345.1344 | 345.1343 | 6.77 | NEG | 41145.15192 | 40436.13634 | 41998.22926 | 0.005504738 | 0.005506036 | 0.0055119 | 0.005507558 | WXJASYTWXBVSQZ-UOMNFSLCSA-N | CC(C)C1=C2CC3C4C(C(C5C(C4(C2=CC(=O)O1)C)O5)O)(C(=O)O3)C |  | 67430 |  | C09104 | 442035 | 41787-72-8 |  |  |  |  |  |  |  | level2 |
| compound00678 | 4.70\_213.1025m/z | M+H | C13H12N2O | 40.1 | 0 | 1.28 | Harmine |  | 213.1022 | 213.1025 | 4.7 | POS | 4863.434862 | 5098.043419 | 4962.229199 | 0.00065067 | 0.000694181 | 0.000651249 | 0.000665367 | BXNJHAXVSOCGBA-UHFFFAOYSA-N | COC1=CC=C2C(NC3=C2C=CN=C3C)=C1 | HMDB0030311 | 43924 |  | C06538 | 5280953 | 442-51-3 | 肉叶云香碱 | 生物碱 |  | Alkaloids |  | HY-N0737A | HPLC≥98% | level2 |
| compound00679 | 3.03\_345.1190m/z | M-H2O-H | C15H24O10 | 40.9 | 0 | -0.25 | Harpagide |  | 345.1191 | 345.119 | 3.03 | NEG | 6433.507382 | 6328.951797 | 6140.878754 | 0.000860728 | 0.00086179 | 0.000805937 | 0.000842818 | XUWSHXDEJOOIND-PDTKEKFYSA-N | C[C@@]1(O)C[C@H](O)[C@@]2(O)C=CO[C@H](O[C@H]3O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]3O)C12 |  |  |  |  |  | 6926-08-5 | 哈巴苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N0397 | HPLC≥98% | level2 |
| compound00680 | 3.84\_413.1421m/z | M+Na | C17H26O10 | 63.6 | 91 | 0.69 | harpagide acetate | 136.0616, 162.0409, 281.0989, 413.1402 | 413.1418 | 413.1421 | 3.84 | POS | 22632.98848 | 23266.60052 | 23217.80358 | 0.003028028 | 0.003168125 | 0.003047133 | 0.003081096 | WULASHYSJRHJKR-UHFFFAOYSA-N | CC(=O)OCC1CC(C2C1C(OC=C2)OC3C(C(C(C(O3)CO)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00681 | 4.45\_579.1356m/z | M-H | C26H28O15 | 43.6 | 15.1 | 0.18 | Graveobioside A | 191.0187, 197.0444, 309.04, 327.0508, 357.0616, 429.0817, 459.0904, 579.134 | 579.1355 | 579.1356 | 4.45 | NEG | 151482.3542 | 153811.9155 | 147787.205 | 0.020266561 | 0.020943989 | 0.019395776 | 0.020202108 | YSXNEFJASLJGTK-YRCFQSNFSA-N | C1(O[C@H]2[C@H](O[C@H]3[C@H](O)[C@](CO3)(CO)O)[C@@H](O)[C@H](O)[C@@H](CO)O2)=CC2OC(C3C=C(O)C(O)=CC=3)=CC(=O)C=2C(O)=C1 | HMDB0301864 | 93155 | LMPK12110657 |  | 101248035 | 63808-23-1 | 药芹二糖苷A | 黄酮类 | 黄酮 | Flavonoids | Flavones | DM0081-0020 | HPLC≥98% | level2 |
| compound00682 | 10.91\_455.3515m/z | M+H-H2O | C30H48O4 | 54.5 | 0 | -1.02 | Hederagenin |  | 455.352 | 455.3515 | 10.91 | POS | 5769.486505 | 6569.031754 | 4262.627487 | 0.00077189 | 0.00089448 | 0.000559433 | 0.000741934 | PGOYMURMZNDHNS-MYPRUECHSA-N | CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)CO)O)C)C)C2C1)C)C(=O)O)C |  | 44384 |  |  | 73299 | 465-99-6 | 常春藤皂苷元 | 萜类 | 三萜类 | Terpenes | Triterpenes | HY-N0256 | HPLC≥98% | level2 |
| compound00683 | 10.19\_337.1770m/z | M+Na | C20H26O3 | 54.9 | 0 | -1.44 | helioscopinolide e |  | 337.1774 | 337.177 | 10.19 | POS | 7856.344835 | 7748.61182 | 9110.520165 | 0.001051087 | 0.001055099 | 0.001195676 | 0.001100621 | JFINBCWMRIJTDN-NLDJYOPPSA-N | CC1=C2C=C3CC[C@H]4[C@]([C@@H]3C[C@H]2OC1=O)(CCC(=O)C4(C)C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00684 | 3.76\_347.0773m/z | M+FA-H | C16H14O6 | 40.9 | 0 | 0.15 | Hematoxylin |  | 347.0772 | 347.0773 | 3.76 | NEG | 6426.648194 | 5894.458971 | 6064.145229 | 0.00085981 | 0.000802626 | 0.000795866 | 0.000819434 | WZUVPPKBWHMQCE-CJNGLKHVSA-N | Oc1cc2c(cc1O)[C@H]1c3ccc(O)c(O)c3OC[C@@]1(O)C2 |  |  |  |  |  | 517-28-2 | 苏木精 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0116 | HPLC≥98% | level2 |
| compound00685 | 4.62\_435.1291m/z | M+H | C21H22O10 | 43.8 | 0 | 1.12 | Hemiphloin |  | 435.1286 | 435.1291 | 4.62 | POS | 15361.15781 | 13947.83959 | 13967.96988 | 0.002055143 | 0.001899225 | 0.001833174 | 0.00192918 | QKPKGDDHOGIEOO-JVVVWQBKSA-N | C1(O)=CC2O[C@H](C3C=CC(O)=CC=3)CC(=O)C=2C(O)=C1[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1 |  | 52711 | LMPK12140223 |  | 160711 |  | 半皮桉苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | DB0342 | HPLC≥95% | level2 |
| compound00686 | 4.87\_434.1212n | M+H-H2O, M+H | C21H22O10 | 57 | 78.3 | -0.21 | hemipholin | 147.0439, 153.0181, 273.0753 | 435.1286 | 435.1285 | 4.87 | POS | 142842.9267 | 141460.2408 | 137136.7611 | 0.019110707 | 0.019262108 | 0.017997998 | 0.018790271 | QKPKGDDHOGIEOO-UHFFFAOYSA-N | C1C(OC2=CC(=C(C(=C2C1=O)O)C3C(C(C(C(O3)CO)O)O)O)O)C4=CC=C(C=C4)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00687 | 4.65\_465.1032m/z | M+H | C21H20O12 | 57.4 | 0 | 0.96 | Herbacetrin |  | 465.1028 | 465.1032 | 4.65 | POS | 9564.062699 | 8516.863136 | 9446.447299 | 0.001279559 | 0.001159709 | 0.001239763 | 0.001226344 | RSPZVQZNRINVPE-UHFFFAOYSA-N | C1=CC(=CC=C1C2=C(C(=O)C3=C(O2)C(=C(C=C3O)OC4C(C(C(C(O4)CO)O)O)O)O)O)O |  |  |  |  | 5318021 | 35815-07-7 |  |  |  |  |  |  |  | level2 |
| compound00688 | 5.30\_503.0967m/z | M+K | C22H24O11 | 57 | 0 | 3.69 | Hesperetin 5-glucoside |  | 503.0949 | 503.0967 | 5.3 | POS | 103392.8552 | 103827.1517 | 101479.3613 | 0.01383275 | 0.014137752 | 0.013318277 | 0.013762926 | QSLBWGKNSBMTJL-UHFFFAOYSA-N | C1(O)=CC2OC(C3C=C(O)C(OC)=CC=3)CC(=O)C=2C(OC2OC(CO)C(O)C(O)C2O)=C1 | HMDB0037535 | 52861 | LMPK12140377 |  | 18625123 | 69651-80-5 |  |  |  |  |  |  |  | level2 |
| compound00689 | 5.24\_463.1242m/z | M-H | C22H24O11 | 40.6 | 0 | -0.81 | Hesperetin 7-O-glucoside |  | 463.1246 | 463.1242 | 5.24 | NEG | 27706.61945 | 26435.02672 | 29430.29834 | 0.00370682 | 0.003599558 | 0.003862469 | 0.003722949 | ADSYMQORONDIDD-ZJHVPRRPSA-N | COC1=C(C=C(C=C1)C2CC(=O)C3=C(C=C(C=C3O2)OC4C(C(C(C(O4)CO)O)O)O)O)O |  | 64212 |  | C16422 | 147394 | 31712-49-9 | 橙皮素-7-O-葡萄糖苷 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-125130 | HPLC≥98% | level2 |
| compound00690 | 1.37\_161.0447m/z | M-H2O-H | C6H12O6 | 56.9 | 88.3 | -4.52 | hexulose | 73.0285, 83.0128, 85.0285, 87.0077, 89.0233, 99.0441, 101.0233, 131.0340, 143.0341, 161.0447 | 161.0455 | 161.0447 | 1.37 | NEG | 163530.625 | 168593.3683 | 180272.8383 | 0.021878478 | 0.022956723 | 0.02365923 | 0.022831477 | BJHIKXHVCXFQLS-UHFFFAOYSA-N | OCC(O)C(O)C(O)C(=O)CO | HMDB0246950 |  |  | C01452 | 1101 |  |  |  |  |  |  |  |  | level2 |
| compound00691 | 9.24\_331.1914m/z | M-H | C20H28O4 | 68.7 | 58.8 | -0.37 | hedychilactone c | 257.154, 269.1544, 287.1644, 330.9938, 331.152, 331.1912 | 331.1915 | 331.1914 | 9.24 | NEG | 29036.88939 | 28408.9866 | 29043.20944 | 0.003884795 | 0.003868345 | 0.003811667 | 0.003854935 | LAIHLMZBILKPIA-UGXIPXOPSA-N | C[C@@]12CCCC([C@@H]1C(=O)[C@@H](C(=C)C2C/C=C/3\CCOC3=O)O)(C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00692 | 8.99\_253.0832m/z | M+Na | C14H14O3 | 41.1 | 0 | -1.55 | Demethylsuberosin |  | 253.0836 | 253.0832 | 8.99 | POS | 4893.283547 | 5096.185261 | 5135.038273 | 0.000654664 | 0.000693928 | 0.000673929 | 0.000674174 | FIDUIAPDSKSUGO-UHFFFAOYSA-N | CC(C)=CCC1=CC2=C(OC(=O)C=C2)C=C1O | HMDB0304330 | 72018 |  | C18083 | 5316525 | 21422-04-8 | 7-去甲基软木花椒素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N2488 | HPLC≥98% | level2 |
| compound00693 | 5.93\_263.1287m/z | M-H | C15H20O4 | 55.5 | 50.6 | -0.54 | granilin | 219.1008, 219.1382, 222.9811, 235.0759, 242.9868, 262.9891, 263.0676, 263.0902, 263.1163, 263.1281 | 263.1289 | 263.1287 | 5.93 | NEG | 72333.35527 | 72262.2369 | 71979.35263 | 0.009677354 | 0.009839676 | 0.009446659 | 0.009654563 | ZEIYNPAINVEWGP-NQHOMTGGSA-N | CC12CC3C(CC1C(=C)C(CC2O)O)C(=C)C(=O)O3 |  | 67727 |  | C09470 | 442254 | 40737-97-1 |  |  |  |  |  |  |  | level2 |
| compound00694 | 10.76\_299.2014m/z | M-H2O-H | C20H30O3 | 50.2 | 0 | -0.81 | Gradifloric acid | 299.2012 | 299.2016 | 299.2014 | 10.76 | NEG | 96470.74918 | 94185.48457 | 91413.31278 | 0.012906654 | 0.012824882 | 0.011997196 | 0.012576244 | GVGJRXSJJHLPGZ-UHFFFAOYSA-N | CC12CCCC(C)(C1CCC13CC(CCC21)C(=C)C3O)C(O)=O | HMDB0036930 | 71957 |  | C17956 | 131752096 | 22338-69-8 |  |  |  |  |  |  |  | level2 |
| compound00695 | 4.39\_617.1486m/z | M+Na | C27H30O15 | 53 | 0 | 1.58 | Flavonoid LP |  | 617.1477 | 617.1486 | 4.39 | POS | 13379.56514 | 14010.33444 | 14209.74429 | 0.001790029 | 0.001907734 | 0.001864904 | 0.001854223 | SFNFQCXADNWOCI-UHFFFAOYSA-N | C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C=C(C(=C3O)C4C(C(C(C(O4)CO)O)O)O)O)OC5C(C(C(C(O5)CO)O)O)O |  |  |  |  | 73981632 | 19416-87-6 |  |  |  |  |  |  |  | level2 |
| compound00696 | 4.13\_393.0795m/z | M+Na | C16H18O10 | 40.2 | 0 | 0.86 | Fraxin |  | 393.0792 | 393.0795 | 4.13 | POS | 22174.54034 | 20418.14376 | 20901.45871 | 0.002966693 | 0.002780262 | 0.002743133 | 0.002830029 | CRSFLLTWRCYNNX-YJADWKFMSA-N | COc1cc2ccc(=O)oc2c(O[C@@H]2OC(CO)[C@@H](O)[C@@H](O)C2O)c1O |  |  |  |  |  | 524-30-1 | 秦皮甙 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0579 | HPLC≥98% | level2 |
| compound00697 | 0.70\_543.1318m/z | M+K | C18H32O16 | 57.4 | 89.9 | -0.8 | Fructomaltose | 381.0785, 543.1316 | 543.1322 | 543.1318 | 0.7 | POS | 6536423.804 | 6323693.965 | 6371242.822 | 0.874496779 | 0.86107357 | 0.83616979 | 0.857246713 | FVVCFHXLWDDRHG-UHFFFAOYSA-N | OCC1OC(CO)(OC2OC(CO)C(OC3OC(CO)C(O)C(O)C3O)C(O)C2O)C(O)C1O | HMDB0029930 | 86595 |  |  | 21932711 |  |  |  |  |  |  |  |  | level2 |
| compound00698 | 3.98\_111.0445m/z | M+H-H2O | C6H8O3 | 40.8 | 2.56 | 3.75 | Furaneol | 88.0046, 89.5071, 93.0338, 93.0702, 94.0654, 98.5123, 99.5124, 110.0602, 111.0205, 111.0442 | 111.0441 | 111.0445 | 3.98 | POS | 6818.416482 | 6616.658131 | 8541.531356 | 0.000912224 | 0.000900965 | 0.001121001 | 0.000978064 | INAXVXBDKKUCGI-UHFFFAOYSA-N | CC1OC(C)=C(O)C1=O | HMDB0040594 | 95077 |  |  | 19309 |  | 呋喃酮 | 其他 |  | Others |  | HY-N7093 | HPLC≥98% | level2 |
| compound00699 | 5.68\_123.0442m/z | M+H-H2O | C7H8O3 | 55.4 | 0 | 0.92 | Furfurylacetate |  | 123.0441 | 123.0442 | 5.68 | POS | 4028.315528 | 4459.051888 | 4444.862371 | 0.000538941 | 0.000607172 | 0.000583349 | 0.000576488 | CKOYRRWBOKMNRG-UHFFFAOYSA-N | CC(=O)OCC1=CC=CO1 | HMDB0034246 | 89800 |  |  | 12170 | 623-17-6 |  |  |  |  |  |  |  | level2 |
| compound00700 | 4.93\_179.0945n | M+H-H2O, M+H | C10H13NO2 | 47 | 16.7 | -0.67 | Fusaric acid | 103.0544, 120.0808, 131.049, 133.0283, 134.0962, 135.0439, 162.091 | 180.1019 | 180.1018 | 4.93 | POS | 120754.4757 | 124195.7384 | 123928.6632 | 0.016155531 | 0.016911266 | 0.016264551 | 0.016443783 | DGMPVYSXXIOGJY-UHFFFAOYSA-N | CCCCC1=CN=C(C=C1)C(O)=O | HMDB0252556 | 68152 |  | C10146 | 3442 | 536-69-6 | 萎蔫酸 | 生物碱 |  | Alkaloids |  | HY-128483 | HPLC≥98% | level2 |
| compound00701 | 10.51\_497.3271m/z | M-H2O-H | C31H48O6 | 51.8 | 0 | -0.19 | Fusidine |  | 497.3272 | 497.3271 | 10.51 | NEG | 23851.65369 | 24073.16962 | 20825.5721 | 0.003191071 | 0.003277953 | 0.002733174 | 0.003067399 | IECPWNUMDGFDKC-MZJAQBGESA-N | C1C[C@]2(C)[C@]3([H])[C@H](O)C[C@@]4([H])/C(=C(\CC/C=C(\C)/C)/C(=O)O)/[C@@H](OC(C)=O)C[C@]4(C)[C@@]3(C)CC[C@@]2([H])[C@H](C)[C@@H]1O | HMDB0015570 | 2984 | LMPR0106040001 | C06694 | 3000226 | 6990-06-3 |  |  |  |  |  |  |  | level2 |
| compound00702 | 5.71\_371.1469m/z | M+Na | C19H24O6 | 51.7 | 0 | 0.98 | GA16 |  | 371.1465 | 371.1469 | 5.71 | POS | 10574.97101 | 11034.98031 | 10782.69968 | 0.001414807 | 0.001502592 | 0.001415135 | 0.001444178 | ZGHAVKULRAPSKM-NRESNZGCSA-N | C[C@@]12[C@H](C[C@@H]([C@@]3([C@@H]1[C@@H]([C@]45[C@H]3CC[C@H](C4)C(=C)C5)C(=O)O)OC2=O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00703 | 9.38\_317.1391m/z | M-H | C18H22O5 | 44.1 | 0 | -1.02 | Zearalenone |  | 317.1394 | 317.1391 | 9.38 | NEG | 4137.65549 | 4069.243568 | 3219.844792 | 0.00055357 | 0.000554094 | 0.000422576 | 0.00051008 | MBMQEIFVQACCCH-QBODLPLBSA-N | C12C=CCCCC(CCC[C@H](C)OC(=O)C1=C(O)C=C(O)C=2)=O |  | 40980 | LMPK04000016 | C09981 | 5281576 |  | 玉米烯酮 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-103447 | HPLC≥98% | level2 |
| compound00704 | 4.77\_457.0777m/z | M-H | C22H18O11 | 40.4 | 0 | 0.11 | Gallocatechin gallate |  | 457.0776 | 457.0777 | 4.77 | NEG | 12225.49404 | 13439.95623 | 12786.87393 | 0.001635628 | 0.001830068 | 0.001678165 | 0.00171462 | WMBWREPUVVBILR-NQIIRXRSSA-N | OC1=CC(O)=C2C[C@@H](OC(=O)C3=CC(O)=C(O)C(O)=C3)[C@@H](OC2=C1)C1=CC(O)=C(O)C(O)=C1 | HMDB0301673 |  |  |  | 199472 | 68-22-4 | 没食子儿茶素没食子酸酯 | 黄酮类 | 黄烷醇类 | Flavonoids | Flavanols | HY-N0522 | HPLC≥98% | level2 |
| compound00705 | 1.03\_256.0934m/z | M-H2O-H | C10H17N3O6 | 56.6 | 86.9 | -1.86 | gamma-Glu-ala-gly | 128.0343, 194.093, 238.083, 256.0944 | 256.0939 | 256.0934 | 1.03 | NEG | 14059.17249 | 10991.31683 | 13127.60873 | 0.001880952 | 0.001496646 | 0.001722884 | 0.001700161 | RPVCUZZJCXVVDW-WDSKDSINSA-N | C[C@H](NC(=O)CC[C@H](N)C(O)=O)C(=O)NCC(O)=O | HMDB0005766 | 58301 |  |  | 5489007 | 1116-21-8 |  |  |  |  |  |  |  | level2 |
| compound00706 | 0.78\_275.1129n | M+H-H2O, M+H | C10H17N3O6 | 48.1 | 51.1 | 4.23 | gamma-l-glutamyl-glutamine | 104.1072, 124.9998, 144.1017, 184.0732, 211.0712, 240.1217, 258.1081 | 258.1085 | 258.1096 | 0.78 | POS | 365307.7859 | 361944.9299 | 368383.2571 | 0.048873894 | 0.049284677 | 0.048347074 | 0.048835215 | JBFYFLXEJFQWMU-UHFFFAOYSA-N | C(CC(=O)NC(CCC(=O)N)C(=O)O)C(C(=O)O)N |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00707 | 4.53\_485.1078m/z | M+K | C19H26O12 | 57.3 | 0 | 4.98 | Gaultherin |  | 485.1054 | 485.1078 | 4.53 | POS | 24611.52477 | 25196.24239 | 24973.09089 | 0.003292733 | 0.003430877 | 0.003277499 | 0.003333703 | VHUNCYDAXJGCLO-UHFFFAOYSA-N | COC(=O)c1ccccc1OC1OC(COC2OCC(O)C(O)C2O)C(O)C(O)C1O |  |  |  |  |  | 490-67-5 | 冬绿苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N1965 | HPLC≥98% | level2 |
| compound00708 | 4.13\_411.1265m/z | M+Na | C17H24O10 | 40.2 | 0 | 0.92 | Geniposide |  | 411.1261 | 411.1265 | 4.13 | POS | 12462.86975 | 11440.3957 | 11182.20483 | 0.001667386 | 0.001557796 | 0.001467566 | 0.001564249 | IBFYXTRXDNAPMM-ZYTZASFUSA-N | COC(=O)C1=CO[C@@H](OC2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H]2C(CO)=CC[C@H]12 |  |  |  |  |  | 24512-63-8 | 栀子苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N0009 | HPLC≥98% | level2 |
| compound00709 | 4.39\_337.0931m/z | M-H2O-H | C16H20O9 | 45.5 | 0 | 0.6 | Gentiopicroside |  | 337.0929 | 337.0931 | 4.39 | NEG | 6279.458671 | 6564.716362 | 6188.974359 | 0.000840118 | 0.000893893 | 0.000812249 | 0.000848753 | DUAGQYUORDTXOR-GPQRQXLASA-N | O([C@@H]1OC=C2C(=O)OCC=C2[C@H]1C=C)[C@H]1[C@H](O)[C@H]([C@H](O)[C@@H](CO)O1)O |  | 41154 | LMPR0102070009 | C09782 | 88708 |  | 龙胆苦苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N0494 | HPLC≥98% | level2 |
| compound00710 | 6.29\_375.1450m/z | M+FA-H | C19H22O5 | 53.8 | 0 | 0.15 | gibberellin 7 |  | 375.1449 | 375.145 | 6.29 | NEG | 6314.862884 | 6173.493214 | 5615.494769 | 0.000844855 | 0.000840621 | 0.000736984 | 0.000807487 | SEEGHKWOBVVBTQ-NFMPGMCNSA-N | CC12C(C=CC3(C1C(C45C3CCC(C4)C(=C)C5)C(=O)O)OC2=O)O |  | 41236 | LMPR0104170024 | C11867 | 443460 |  |  |  |  |  |  |  |  | level2 |
| compound00711 | 3.98\_341.0876m/z | M-H2O-H | C15H20O10 | 58.5 | 83.2 | -0.63 | Glucosyringicacid | 135.0441, 179.0343, 341.086 | 341.0878 | 341.0876 | 3.98 | NEG | 50610.77516 | 51776.26323 | 50519.27246 | 0.006771128 | 0.007050179 | 0.006630212 | 0.006817173 | BLKMDORKRDACEI-OVKLUEDNSA-N | COC1=CC(=CC(=C1O[C@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CO)O)O)O)OC)C(=O)O |  |  |  |  |  | 33228-65-8 |  |  |  |  |  |  |  | level2 |
| compound00712 | 3.92\_359.0982m/z | M+FA-H | C14H18O8 | 43 | 0.129 | -0.62 | Glucovanillin | 211.0608, 224.0319, 239.0559, 269.0665, 271.0981, 291.1452, 299.0769, 315.0852, 359.0880, 359.0932 | 359.0984 | 359.0982 | 3.92 | NEG | 10287.84666 | 10676.17262 | 10798.39046 | 0.001376393 | 0.001453734 | 0.001417194 | 0.001415774 | LPRNQMUKVDHCFX-RKQHYHRCSA-N | COC1=C(C=CC(=C1)C=O)OC2C(C(C(C(O2)CO)O)O)O |  | 73372 |  | C19808 | 6452133 | 494-08-6 | 4-(β-D-葡萄糖基)-3-甲氧基苯甲醛 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N6667 | HPLC≥98% | level2 |
| compound00713 | 5.70\_347.1498m/z | M-H | C19H24O6 | 56.4 | 0 | -0.55 | GA54 | 229.1597, 255.1387, 303.159, 303.1964, 346.231, 347.1502 | 347.15 | 347.1498 | 5.7 | NEG | 61849.82164 | 64608.72056 | 63168.89214 | 0.00827478 | 0.008797526 | 0.008290364 | 0.008454223 | ZGHAVKULRAPSKM-LYQBYBLHSA-N | [H][C@@]12CC[C@@H]3C[C@]1(CC3=C)[C@@H](C(O)=O)[C@]1([H])[C@@]3(C)[C@@H](O)C[C@@H](O)[C@@]21OC3=O | HMDB0035048 |  |  |  | 101603122 | 72533-75-6 |  |  |  |  |  |  |  | level2 |
| compound00714 | 5.03\_491.0982m/z | 2M-H | C13H10O5 | 57.3 | 3.07 | -0.32 | Hispidin | 135.0441, 267.0663, 293.0456, 311.0562, 447.1091, 491.0979 | 491.0984 | 491.0982 | 5.03 | NEG | 70057.01769 | 71288.39557 | 74382.25255 | 0.009372807 | 0.009707072 | 0.009762019 | 0.009613966 | SGJNQVTUYXCBKH-UHFFFAOYSA-N | OC1=CC(=O)OC(C=CC2=CC=C(O)C(O)=C2)=C1 | HMDB0253181 |  |  |  | 54722180 |  | 牛奶树碱 | 生物碱 |  | Alkaloids |  | HY-100618 | HPLC≥98% | level2 |
| compound00715 | 9.80\_327.1236m/z | M-H | C19H20O5 | 57.3 | 75.7 | -0.61 | Deltoin | 146.9371, 190.9275, 242.9855, 255.1385, 283.1339, 306.9832, 309.206, 326.984, 327.1231 | 327.1238 | 327.1236 | 9.8 | NEG | 20280.79603 | 21046.47686 | 21224.42454 | 0.002713332 | 0.002865819 | 0.00278552 | 0.002788224 | HHNCJFKRMZDTHW-WQRDJFRPSA-N | CC=C(C)C(=O)OC(C)(C)C1CC2=C(O1)C=C3C(=C2)C=CC(=O)O3 |  | 71725 |  | C17482 | 906525 | 19662-71-6 |  |  |  |  |  |  |  | level2 |
| compound00716 | 0.95\_160.1332m/z | M+H | C8H17NO2 | 42.3 | 0 | -0.18 | delta-Valerobetaine |  | 160.1332 | 160.1332 | 0.95 | POS | 10414.3857 | 11081.13427 | 10370.34302 | 0.001393323 | 0.001508876 | 0.001361017 | 0.001421072 | CDLVFVFTRQPQFU-UHFFFAOYSA-N | C[N+](C)(C)CCCCC([O-])=O | HMDB0240732 |  |  |  | 14274897 |  |  | 其他 |  | Others |  | HY-114202 | HPLC≥98% | level2 |
| compound00717 | 9.69\_414.2036n | M+H, M+NH4, M+K | C24H30O6 | 50.8 | 42.7 | -1.54 | caesaldekarin e | 119.0856, 415.2104 | 415.2115 | 415.2109 | 9.69 | POS | 442987.9861 | 454301.4409 | 461002.2043 | 0.059266593 | 0.061860515 | 0.0605025 | 0.060543202 | VVJWDPJDEOTQOZ-AWAHEQQVSA-N | CC1=C2CC[C@@]3([C@@](C2=CC4=C1C=CO4)([C@H](C[C@H](C3(C)C)OC(=O)C)OC(=O)C)C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00718 | 9.84\_315.1964m/z | M-H | C20H28O3 | 45.9 | 0 | -0.43 | Cafestol |  | 315.1966 | 315.1964 | 9.84 | NEG | 15114.98172 | 16542.48408 | 14699.78305 | 0.002022207 | 0.002252528 | 0.001929218 | 0.002067984 | DNJVYWXIDISQRD-HWUKTEKMSA-N | CC12CCC3=C(C1CCC45C2CCC(C4)C(C5)(CO)O)C=CO3 |  | 67399 |  | C09066 | 108052 | 469-83-0 | 咖啡油醇 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N6257 | HPLC≥98% | level2 |
| compound00719 | 9.18\_285.1117m/z | M+H | C17H16O4 | 51.1 | 0 | -1.43 | Caffeic acid phenethyl ester |  | 285.1121 | 285.1117 | 9.18 | POS | 17598.15452 | 17936.72564 | 17104.27944 | 0.002354427 | 0.002442376 | 0.002244787 | 0.002347197 | SWUARLUWKZWEBQ-VQHVLOKHSA-N | [H]\C(=C(\[H])C1=CC(O)=C(O)C=C1)C(=O)OCCC1=CC=CC=C1 | HMDB0302344 |  |  | C10484 | 5281787 |  | 咖啡酸苯乙酯 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N0274 | HPLC≥98% | level2 |
| compound00720 | 4.80\_491.1178m/z | M+FA-H | C22H22O10 | 44.4 | 0 | -3.78 | Calycosin-7-O-beta-D-glucoside |  | 491.1197 | 491.1178 | 4.8 | NEG | 5070.928433 | 3148.401686 | 5718.200964 | 0.000678431 | 0.000428706 | 0.000750464 | 0.0006192 | WACBUPFEGWUGPB-UHFFFAOYSA-N | COC1=CC=C(C=C1O)C1=COC2=CC(OC3OC(CO)C(O)C(O)C3O)=CC=C2C1=O | HMDB0038821 | 93458 |  |  | 91973796 | 114272-30-9 | 毛蕊异黄酮苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | HY-N0520 | HPLC≥98% | level2 |
| compound00721 | 4.56\_726.2007n | M+H, M+Na | C32H38O19 | 44.7 | 0 | -0.08 | Camelliaside B |  | 727.208 | 727.2079 | 4.56 | POS | 91811.81106 | 86747.26923 | 91534.52716 | 0.012283343 | 0.011812049 | 0.012013105 | 0.012036165 | LLPRITPJQPQXIR-BVDHFOMSSA-N | CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC=C(C=C5)O)OC6C(C(C(CO6)O)O)O)O)O)O)O)O |  | 50166 |  |  | 25115190 |  | 山茶甙 B | 黄酮类 | 黄酮 | Flavonoids | Flavones | B21117-10mg | HPLC≥98% | level2 |
| compound00722 | 5.16\_223.0937m/z | M+Na | C10H16O4 | 57.1 | 0 | -1.71 | Camphoric acid |  | 223.0941 | 223.0937 | 5.16 | POS | 6531.902555 | 6215.504976 | 6305.286672 | 0.000873892 | 0.000846342 | 0.000827514 | 0.000849249 | LSPHULWDVZXLIL-QUBYGPBYSA-N | CC1(C)[C@H](C(=O)O)CC[C@]1(C)C(=O)O |  |  |  |  |  | 560-09-8 | L-樟脑酸 | 羧酸及衍生物 |  | Carboxylic acid and derivatives |  | HY-122808 | HPLC≥98% | level2 |
| compound00723 | 5.34\_329.1376m/z | M+H-H2O | C19H22O6 | 52 | 0 | -2.19 | canavalia gibberellin ii |  | 329.1383 | 329.1376 | 5.34 | POS | 5008.056558 | 5417.254602 | 5069.42769 | 0.000670019 | 0.000737647 | 0.000665318 | 0.000690995 | UPCTWJNMQCQZPT-AODVQFRNSA-N | [H][C@@]12CC[C@]3(O)C[C@]1(CC3=C)[C@@H](C(O)=O)[C@]1([H])[C@@]3(CO)C=CC[C@@]21OC3=O | HMDB0036891 | 91889 |  |  | 101603107 | 18450-94-7 |  |  |  |  |  |  |  | level2 |
| compound00724 | 8.07\_231.1378m/z | M+H-H2O | C15H20O3 | 53.3 | 0 | -0.54 | Carabrone |  | 231.1379 | 231.1378 | 8.07 | POS | 9393.303944 | 9554.889682 | 9392.831765 | 0.001256714 | 0.001301053 | 0.001232727 | 0.001263498 | AGIQIKMGJVLKMA-NLRWUALESA-N | C=C1C(=O)O[C@@H]2C[C@]3(C)[C@@H](CCC(C)=O)[C@@H]3C[C@H]12 |  |  |  |  |  | 1748-81-8 | 天名精内酯酮 | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | HY-N5020 | HPLC≥98% | level2 |
| compound00725 | 10.66\_331.1913m/z | M-H | C20H28O4 | 58.3 | 72.2 | -0.46 | Carnosicacid | 163.0749, 244.1473, 287.2015, 331.1913 | 331.1915 | 331.1913 | 10.66 | NEG | 50153.57891 | 50867.1155 | 48608.69457 | 0.00670996 | 0.006926383 | 0.006379465 | 0.006671936 | QRYRORQUOLYVBU-UHFFFAOYSA-N | CC(C)C1=C(C(=C2C(=C1)CCC3C2(CCCC3(C)C)C(=O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00726 | 5.14\_621.1463m/z | M+FA-H | C27H28O14 | 55.1 | 0 | 0.37 | cassiaoccidentalin b | 291.0637, 299.0197, 314.0434, 315.0507, 335.0539, 477.1030, 515.0951, 519.1144, 559.0775, 621.1404 | 621.1461 | 621.1463 | 5.14 | NEG | 82952.85348 | 80952.641 | 86820.30052 | 0.011098118 | 0.011023016 | 0.011394404 | 0.011171846 | WGIMZJFXUGTVFX-RUYCBFJTSA-N | C1(C2C=CC(O)=C(O)C=2)=CC(=O)C2C(O)=C([C@]3([H])[C@@H](O[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)C(=O)[C@@H](O)[C@H](C)O3)C(O)=CC=2O1 |  | 48953 | LMPK12110522 |  | 70698280 |  |  |  |  |  |  |  |  | level2 |
| compound00727 | 5.75\_566.1637n | M+H, M+Na | C26H30O14 | 42.2 | 0 | 0.29 | Cassiaside B |  | 567.1708 | 567.171 | 5.75 | POS | 72438.28773 | 67203.86988 | 66149.48981 | 0.009691393 | 0.009150898 | 0.008681541 | 0.00917461 | NIVCJAYDAMQSJO-UHFFFAOYSA-N | COc1cc(OC2OC(COC3OCC(O)(CO)C3O)C(O)C(O)C2O)c2c(O)c3c(=O)cc(C)oc3cc2c1 |  |  |  |  |  | 119170-51-3 | 决明子苷 B | 醌类 | 萘醌类 | Quinones | Naphthoquinones | B52097-5mg | HPLC≥98% | level2 |
| compound00728 | 7.47\_341.1361m/z | M+Na | C18H22O5 | 53.4 | 0 | 0.5 | celaphanol b | 323.0888, 323.1271, 340.1224, 341.1364 | 341.1359 | 341.1361 | 7.47 | POS | 21701.85644 | 23625.01872 | 24439.45381 | 0.002903454 | 0.00321693 | 0.003207464 | 0.003109283 | KJOVGUXTTUZJSJ-QZTJIDSGSA-N | C[C@@]1(CCC[C@]2(C1=C(C(=O)C3=CC(=C(C=C32)OC)O)O)C)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00729 | 9.69\_314.1514n | M+H-H2O, M+K, M+Na, M+NH4, M+H | C19H22O4 | 60.4 | 89 | -1.19 | Chalepin | 211.1118, 211.1472, 237.0907, 238.1348, 251.1423, 253.1584, 255.1014, 297.1476 | 297.1485 | 297.1481 | 9.69 | POS | 9700960.377 | 9711582.794 | 9980684.628 | 1.297874626 | 1.322389621 | 1.309877398 | 1.310047215 | JCDLLLXYAICSQV-UHFFFAOYSA-N | CC(C)(C=C)C1=CC2=CC3=C(C=C2OC1=O)OC(C3)C(C)(C)O |  | 67563 |  | C09267 | 119066 | 33054-89-6 |  |  |  |  |  |  |  | level2 |
| compound00730 | 8.39\_347.1499m/z | M-H | C19H24O6 | 51 | 0 | -0.43 | Chamissonin diacetate |  | 347.15 | 347.1499 | 8.39 | NEG | 17532.3287 | 17298.75124 | 18385.43065 | 0.00234562 | 0.002355506 | 0.002412927 | 0.002371351 | DEBBYPCBXVYUCZ-WZLFHOKTSA-N | CC1=CCC(C(=CC(C2C(C1)OC(=O)C2=C)OC(=O)C)C)OC(=O)C |  | 67628 |  | C09356 | 5281433 | 24112-95-6 |  |  |  |  |  |  |  | level2 |
| compound00731 | 10.22\_343.1538m/z | M+H | C20H22O5 | 41.3 | 0 | -0.68 | Chicanin |  | 343.154 | 343.1538 | 10.22 | POS | 3633.652353 | 3552.511869 | 4061.154523 | 0.00048614 | 0.000483732 | 0.000532991 | 0.000500954 | JPDORDSJPIKURD-OCBHBYCGSA-N | COc1cc([C@@H]2O[C@@H](c3ccc4c(c3)OCO4)[C@H](C)[C@@H]2C)ccc1O |  |  |  |  |  | 78919-28-5 | 襄五脂素 | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DX0051 | HPLC≥98% | level2 |
| compound00732 | 4.78\_474.0801n | M+NH4, M+Na | C22H18O12 | 47.9 | 0 | 0.61 | Chicoric acid |  | 497.069 | 497.0693 | 4.78 | POS | 35396.10309 | 32814.19127 | 33143.75364 | 0.004735583 | 0.004468185 | 0.004349827 | 0.004517865 | YDDGKXBLOXEEMN-IABMMNSOSA-N | OC(=O)[C@H](OC(=O)\C=C\C1=CC(O)=C(O)C=C1)[C@@H](OC(=O)\C=C\C1=CC(O)=C(O)C=C1)C(O)=O | HMDB0002375 | 58128 |  | C10437 | 5281764 | 70831-56-0 | 菊苣酸 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N0457 | HPLC≥98% | level2 |
| compound00733 | 4.80\_305.1030m/z | M-H | C16H18O6 | 40.3 | 0 | -0.26 | Cimifugin |  | 305.1031 | 305.103 | 4.8 | NEG | 12674.73462 | 13082.89391 | 12043.57708 | 0.001695731 | 0.001781448 | 0.001580614 | 0.001685931 | ATDBDSBKYKMRGZ-ZDUSSCGKSA-N | CC(C)(C1CC2=C(O1)C=C3C(=C2OC)C(=O)C=C(O3)CO)O |  | 67340 |  | C09000 | 441960 | 37921-38-3 | 升麻素 | 其他 |  | Others |  | HY-N0634 | HPLC≥98% | level2 |
| compound00734 | 5.21\_148.0755m/z | M+H | C9H9NO | 42.2 | 0 | -1.33 | Cinnamamide |  | 148.0757 | 148.0755 | 5.21 | POS | 1654.19549 | 1797.642839 | 1657.578411 | 0.000221312 | 0.000244778 | 0.000217543 | 0.000227878 | APEJMQOBVMLION-VOTSOKGWSA-N | C1=CC=C(C=C1)C=CC(=O)N |  | 339915 |  |  | 5273472 |  | 肉桂酰胺 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-W067479 | HPLC≥98% | level2 |
| compound00735 | 4.34\_619.1639m/z | M+Na | C27H32O15 | 50.7 | 0 | 0.89 | butrin |  | 619.1633 | 619.1639 | 4.34 | POS | 6289.326974 | 5400.328186 | 6204.958525 | 0.000841438 | 0.000735342 | 0.000814346 | 0.000797042 | QVCQYYYTMIZOGK-VQBAZXIRSA-N | C1(O[C@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)C=C2O[C@]([H])(C3C=C(O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)C(O)=CC=3)CC(=O)C2=CC=1 |  | 52555 | LMPK12140065 | C09616 | 164630 |  |  |  |  |  |  |  |  | level2 |
| compound00736 | 5.36\_273.0752m/z | M+H | C15H12O5 | 41.4 | 0 | -2.03 | Butin |  | 273.0758 | 273.0752 | 5.36 | POS | 4145.104133 | 3980.280794 | 3879.771282 | 0.000554566 | 0.00054198 | 0.000509186 | 0.000535244 | MJBPUQUGJNAPAZ-UHFFFAOYSA-N | OC1=CC2=C(C=C1)C(=O)CC(O2)C1=CC(O)=C(O)C=C1 | HMDB0249463 |  |  |  |  |  | 紫铆亭 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N6020B | HPLC≥98% | level2 |
| compound00737 | 6.47\_279.1931m/z | M+Na | C15H28O3 | 53.1 | 0 | -0.02 | bullatantriol | 149.0232, 279.1007, 279.1568, 279.1928 | 279.1931 | 279.1931 | 6.47 | POS | 23176.34324 | 22954.2699 | 21771.11703 | 0.003100723 | 0.003125596 | 0.002857268 | 0.003027862 | JQHTXZNYHSCIFE-FPVZYODXSA-N | C[C@@]12CC[C@@H]([C@H]1[C@@](CC[C@H]2O)(C)O)CC(C)(C)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00738 | 4.15\_412.1741n | M+NH4, M+Na | C20H28O9 | 40.6 | 0 | 1.89 | Bruceine E |  | 435.1625 | 435.1633 | 4.15 | POS | 23047.93846 | 21817.79766 | 21185.33062 | 0.003083544 | 0.002970847 | 0.002780389 | 0.002944927 | ZBXITHPYBBXZRG-UHFFFAOYSA-N | CC1=CC(O)C(O)C2(C)C1CC1OC(=O)C(O)C3(O)C4(C)OCC13C2C(O)C4O | HMDB0249403 |  |  |  | 14379939 |  | 鸦胆子素 E | 萜类 | 三萜类 | Terpenes | Triterpenes | B27056-20mg | HPLC≥95% | level2 |
| compound00739 | 4.19\_459.1146m/z | M+FA-H | C18H22O11 | 40.5 | 0 | 0.38 | Asperuloside |  | 459.1144 | 459.1146 | 4.19 | NEG | 5526.465768 | 4986.462386 | 5164.692913 | 0.000739376 | 0.000678988 | 0.000677821 | 0.000698728 | IBIPGYWNOBGEMH-ANPUHXSGSA-N | CC(=O)OCC1=C[C@@H]2OC(=O)C3=COC(O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H]1[C@@H]32 |  |  |  |  |  | 14259-45-1 | 车叶草苷 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N1382 | HPLC≥98% | level2 |
| compound00740 | 4.05\_431.1193m/z | M-H | C18H24O12 | 43.7 | 0 | -0.36 | Asperulosidic Acid |  | 431.1195 | 431.1193 | 4.05 | NEG | 13646.89515 | 13921.2305 | 13169.79022 | 0.001825794 | 0.001895601 | 0.00172842 | 0.001816605 | DGDWCRWJRNMRKX-DILZHRMZSA-N | O=C(O)C1=COC(OC2OC(CO)C(O)C(O)C2O)C3C(=CC(O)C13)COC(=O)C |  |  |  |  |  | 25368-11-0 | 车叶草苷酸 | 萜类 | 单萜类 | Terpenes | Monoterpenes | HY-N6246 | HPLC≥98% | level2 |
| compound00741 | 9.64\_467.1933m/z | M+Na | C27H28N2O4 | 41 | 0 | -1.87 | Aurantiamide acetic acid |  | 467.1942 | 467.1933 | 9.64 | POS | 16815.48884 | 17757.35308 | 17793.63179 | 0.002249715 | 0.002417952 | 0.002335258 | 0.002334308 | VZPAURMDJZOGHU-SKCDSABHSA-N | O=C(OCC(N=C(O)C(N=C(O)C=1C=CC=CC1)CC=2C=CC=CC2)CC=3C=CC=CC3)C |  |  |  |  | 124319 | 56121-42-7 | 金色酰胺醇酯 | 氨基酸及多肽类 | 多肽类 | Amino Acids, Peptides and derivatives | Peptides | HY-N2905 | HPLC≥98% | level2 |
| compound00742 | 9.06\_309.2071m/z | M-H | C18H30O4 | 55.5 | 69.8 | -0.05 | Auxin b | 104.953, 171.102, 209.1175, 265.0867, 291.196, 308.997, 309.1693, 309.2069 | 309.2071 | 309.2071 | 9.06 | NEG | 426413.2172 | 423351.2687 | 427951.1699 | 0.057049083 | 0.057646146 | 0.056164841 | 0.056953357 | MQETZQLZTJUQHR-UHFFFAOYSA-N | CCC(C)C1CC(C(C)CC)C(=C1)C(O)CC(=O)CC(O)=O | HMDB0038484 | 93163 |  |  | 103739 |  |  |  |  |  |  |  |  | level2 |
| compound00743 | 10.20\_359.1123m/z | M+H | C19H18O7 | 53.3 | 0 | -0.73 | Averionol |  | 359.1125 | 359.1123 | 10.2 | POS | 18805.25956 | 19604.37329 | 20760.66066 | 0.002515923 | 0.002669454 | 0.002724655 | 0.002636677 | AAASNKNLMQBKFV-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=C(OC)C(OC)=CC=3)=C(O)C(=O)C=2C(OC)=C1 |  | 44016 | LMPK12112771 |  | 97142 | 1245-15-4 |  |  |  |  |  |  |  | level2 |
| compound00744 | 5.07\_505.2078m/z | M-H | C26H34O10 | 40.7 | 0 | -0.19 | Aviculin |  | 505.2079 | 505.2078 | 5.07 | NEG | 15157.46627 | 14777.6717 | 15738.51965 | 0.002027891 | 0.00201222 | 0.002065543 | 0.002035218 | FPJFPMQEUVMUKU-CDDCGRQRSA-N | COc1cc([C@H]2c3cc(O)c(OC)cc3C[C@@H](CO)[C@@H]2CO[C@@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)ccc1O |  |  |  |  |  | 156765-33-2 |  | 苯丙素类 | 木脂素类 | Phenylpropanoids | Lignans | DA0156 | HPLC≥98% | level2 |
| compound00745 | 4.13\_314.1391m/z | M+H-H2O | C18H21NO5 | 52.2 | 0 | 1.36 | AZWNRVNQMXFTSX-UHFFFAOYSA-N |  | 314.1387 | 314.1391 | 4.13 | POS | 16260.07644 | 15966.20373 | 16273.65155 | 0.002175407 | 0.002174058 | 0.002135774 | 0.002161746 | AZWNRVNQMXFTSX-UHFFFAOYSA-N | COC1=CC23CCC[N+]2(CCC4=CC5=C(C=C4C3C1O)OCO5)[O-] |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00746 | 1.85\_331.0674m/z | M-H | C13H16O10 | 60.7 | 77.1 | 0.95 | b-glucogallin | 125.0235, 168.0055, 331.0669 | 331.0671 | 331.0674 | 1.85 | NEG | 30685.32276 | 30705.10846 | 30720.30738 | 0.004105336 | 0.004180999 | 0.004031771 | 0.004106035 | GDVRUDXLQBVIKP-UHFFFAOYSA-N | OCC1OC(OC(=O)C2=CC(O)=C(O)C(O)=C2)C(O)C(O)C1O | HMDB0038728 | 93381 |  |  | 4628122 | 13405-60-2 |  |  |  |  |  |  |  | level2 |
| compound00747 | 8.39\_244.1097n | M+H, M+Na | C15H16O3 | 41.1 | 0.104 | -0.83 | Batatasin IV | 267.0991 | 267.0992 | 267.099 | 8.39 | POS | 54497.38489 | 54148.67 | 49494.28825 | 0.00729111 | 0.00737322 | 0.006495692 | 0.007053341 | IUMFLNFLJUUODE-UHFFFAOYSA-N | C1=C(OC)C=C(CCC2=C(O)C=CC=C2)C=C1O | HMDB0032641 | 53259 | LMPK13090032 | C10247 | 181271 | 60347-67-3 | 山药素IV | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | CFN95319 | HPLC≥98% | level2 |
| compound00748 | 6.94\_329.0667m/z | M-H | C17H14O7 | 50.7 | 45.4 | 0.12 | Cirsiliol | 241.1586, 261.1131, 285.1495, 299.0196, 314.0429, 328.2211, 329.0667 | 329.0667 | 329.0667 | 6.94 | NEG | 46932.76037 | 46082.31666 | 46841.90871 | 0.006279052 | 0.006274855 | 0.00614759 | 0.006233833 | IMEYGBIXGJLUIS-UHFFFAOYSA-N | C1(OC)=CC2OC(C3C=CC(O)=C(O)C=3)=CC(=O)C=2C(O)=C1OC | HMDB0250275 | 49652 | LMPK12111227 | C10033 | 160237 |  | 条叶蓟素 | 黄酮类 | 黄酮 | Flavonoids | Flavones | HY-110399 | HPLC≥98% | level2 |
| compound00749 | 9.15\_342.1696m/z | M+NH4 | C20H20O4 | 40.2 | 0 | -1.34 | Bavachin |  | 342.17 | 342.1696 | 9.15 | POS | 2760.373895 | 3002.319345 | 2440.28367 | 0.000369306 | 0.000408815 | 0.000320266 | 0.000366129 | OAUREGNZECGNQS-IBGZPJMESA-N | CC(=CCC1=CC2=C(C=C1O)OC(CC2=O)C3=CC=C(C=C3)O)C |  | 52529 |  |  | 14236566 |  | 补骨脂二氢黄酮 | 黄酮类 | 二氢黄酮类 | Flavonoids | Flavanones | HY-N0233 | HPLC≥98% | level2 |
| compound00750 | 10.40\_313.1805m/z | M-H | C20H26O3 | 41.6 | 0.00125 | -1.19 | beta-Estradiol 17-acetate | 283.1336, 313.1447, 313.1789 | 313.1809 | 313.1805 | 10.4 | NEG | 19049.73538 | 20788.79243 | 17117.85069 | 0.002548631 | 0.002830732 | 0.002246568 | 0.002541977 | QAHOQNJVHDHYRN-SLHNCBLASA-N | CC(=O)OC1CCC2C1(CCC3C2CCC4=C3C=CC(=C4)O)C |  | 70709 |  | C15228 | 6852404 |  | 17-乙酸-17-β-雌二酯 | 甾体类 | 其他甾体类 | Steroids | Other steroids | HY-B0708 | HPLC≥98% | level2 |
| compound00751 | 4.86\_595.1656m/z | M+H | C27H30O15 | 58 | 20.5 | -0.18 | Biorobin | 287.0547, 576.3871, 594.3976 | 595.1657 | 595.1656 | 4.86 | POS | 220018.8685 | 216434.2518 | 206762.5501 | 0.029435942 | 0.029471036 | 0.027135773 | 0.028680917 | RTATXGUCZHCSNG-KYGWAIEOSA-N | C1(O)=CC2OC(C3C=CC(O)=CC=3)=C(O[C@H]3[C@H](O)[C@@H](O)[C@@H](O)[C@@H](CO[C@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](C)O4)O3)C(=O)C=2C(O)=C1 |  |  | LMPK12111669 |  | 15944778 |  | 山奈酚 3-O-洋槐糖苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | DB0309-0010 | HPLC≥98% | level2 |
| compound00752 | 8.07\_210.1619n | M+H-H2O, M+NH4, M+H | C13H22O2 | 58.2 | 75.3 | -0.35 | Blumenol C | 151.1479, 175.1481, 186.9553, 187.0387, 193.1587, 211.0752, 211.1689, 228.1023, 228.1204, 228.1961 | 228.1958 | 228.1957 | 8.07 | POS | 140928.2312 | 139563.553 | 140280.3524 | 0.018854543 | 0.019003843 | 0.018410567 | 0.018756318 | UEEJDIUOCUCVHN-PWSUYJOCSA-N | CC1=CC(=O)CC([C@H]1CC[C@@H](C)O)(C)C |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00753 | 6.64\_311.0562m/z | M-H | C17H12O6 | 59.2 | 12.7 | 0.16 | boeravinoneB | 174.9551, 239.0712, 267.0664, 267.1016 | 311.0561 | 311.0562 | 6.64 | NEG | 17315.79491 | 16837.75033 | 16730.78466 | 0.00231665 | 0.002292733 | 0.002195769 | 0.002268384 | YVVDYYFGAWQOGB-UHFFFAOYSA-N | C1(O)=CC2OC3C(O)OC4C(=CC=CC=4)C=3C(=O)C=2C(O)=C1C |  | 48082 | LMPK12060073 |  | 14018348 |  |  |  |  |  |  |  |  | level2 |
| compound00754 | 12.45\_256.2631m/z | M+NH4 | C16H30O | 45.4 | 2.3 | -1.74 | Bombykol | 256.2631 | 256.2635 | 256.2631 | 12.45 | POS | 63110.5074 | 63356.48063 | 66030.31364 | 0.008443445 | 0.008627013 | 0.0086659 | 0.008578786 | CIVIWCVVOFNUST-SCFJQAPRSA-N | C(=C/C=C\CCC)\CCCCCCCCCO |  | 36465 | LMFA05000007 | C16873 | 445128 |  | 蚕蛾醇 | 其他 |  | Others |  | HY-N7145 | HPLC≥98% | level2 |
| compound00755 | 5.18\_479.1178m/z | M+H | C22H22O12 | 48.6 | 0 | -1.27 | Brassicin |  | 479.1184 | 479.1178 | 5.18 | POS | 8291.77641 | 7926.014084 | 7792.184952 | 0.001109342 | 0.001079255 | 0.001022656 | 0.001070418 | YCUNOXSUHVGZRI-UHFFFAOYSA-N | COC1=CC(=CC=C1O)C1=C(O)C(=O)C2=C(O)C=C(OC3OC(CO)C(O)C(O)C3O)C=C2O1 | HMDB0029479 |  |  |  | 12302035 | 6743-96-0 | 异鼠李素-7-O-β-D-葡萄糖苷 | 黄酮类 | 黄酮醇类 | Flavonoids | Flavonols | HY-N8193 | HPLC≥98% | level2 |
| compound00756 | 7.07\_319.1300m/z | M+K | C16H24O4 | 44.7 | 0 | -2.23 | Brefeldin A |  | 319.1307 | 319.13 | 7.07 | POS | 12878.43061 | 12397.52839 | 11056.73336 | 0.001722983 | 0.001688125 | 0.001451099 | 0.001620736 | KQNZDYYTLMIZCT-KQPMLPITSA-N | CC1CCCC=CC2CC(CC2C(C=CC(=O)O1)O)O |  | 85101 |  |  | 5287620 | 60132-23-2 | 布雷非德菌素 A | 其他 |  | Others |  | HY-16592 | HPLC≥98% | level2 |
| compound00757 | 4.91\_373.0924m/z | M-H2O-H | C19H20O9 | 60.4 | 91.3 | -1.31 | breynioside a | 72.992, 135.0441, 175.0392, 179.0342, 197.0449, 373.0927 | 373.0929 | 373.0924 | 4.91 | NEG | 149024.8675 | 145449.7213 | 145431.6899 | 0.019937778 | 0.01980534 | 0.019086635 | 0.019609918 | FTFZXPBVBBJTHV-OGJJZOIMSA-N | C1=CC(=CC=C1C(=O)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=CC=C(C=C3)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00758 | 3.89\_327.0722m/z | M-H | C14H16O9 | 42.8 | 6.81 | 0.04 | Bergenin | 99.0077, 125.0235, 143.0342, 161.0447, 165.0549, 190.9276, 191.0189, 205.0348, 209.0296, 327.0721 | 327.0722 | 327.0722 | 3.89 | NEG | 37303.26019 | 37432.89685 | 38092.01806 | 0.004990738 | 0.005097096 | 0.004999244 | 0.005029026 | YWJXCIXBAKGUKZ-HJJNZUOJSA-N | COC1=C(C=C2C(=C1O)C3C(C(C(C(O3)CO)O)O)OC2=O)O |  | 43945 |  | C09919 | 66065 | 477-90-7 | 岩白菜素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0017 | HPLC≥98% | level2 |
| compound00759 | 5.04\_473.1084m/z | M-H2O-H | C23H24O12 | 52.2 | 0 | -1.15 | cirsiliol-4'-monoglucoside |  | 473.1089 | 473.1084 | 5.04 | NEG | 33803.95503 | 37058.60788 | 38399.09754 | 0.004522572 | 0.005046131 | 0.005039545 | 0.004869416 | GLTCTFBPNQJRQT-UHFFFAOYSA-N | COC1=C(C(=C2C(=C1)OC(=CC2=O)C3=CC(=C(C=C3)OC4C(C(C(C(O4)CO)O)O)O)O)O)OC |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00760 | 5.82\_475.1246m/z | M-H | C23H24O11 | 44.7 | 0 | 0.02 | Cirsimarin |  | 475.1246 | 475.1246 | 5.82 | NEG | 12965.24231 | 13085.40578 | 12786.24786 | 0.001734597 | 0.00178179 | 0.001678083 | 0.00173149 | RETJLKUBHXTIGH-FZFRBNDOSA-N | C1(OC)=CC2OC(C3C=CC(O[C@H]4[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O4)=CC=3)=CC(=O)C=2C(O)=C1OC |  |  | LMPK12111122 |  | 159460 |  | 滨蓟黄苷 | 黄酮类 | 黄酮 | Flavonoids | Flavones | DB0201-0020 | HPLC≥98% | level2 |
| compound00761 | 4.20\_355.1033m/z | M-H | C16H20O9 | 49.2 | 36 | -0.33 | Cis-Ferulic acid 4-O-beta-D-glucopyranoside | 178.0264, 191.0191, 191.0716, 193.0496, 209.0297, 217.0499, 235.0607, 311.0558, 355.0456, 355.1031 | 355.1035 | 355.1033 | 4.2 | NEG | 39007.76534 | 42195.36351 | 39074.81695 | 0.005218781 | 0.005745584 | 0.005128227 | 0.005364197 | IEMIRSXOYFWPFD-QEQKPWIDSA-N | COc1cc(/C=C\C(=O)O)ccc1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 94942-20-8 | (Z)-阿魏酸-4-O-葡萄糖苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DA0145-0005 | HPLC≥98% | level2 |
| compound00762 | 4.40\_241.1191m/z | M+FA-H | C10H16N2O2 | 59.5 | 92.9 | -1.19 | Cyclo(Pro-Val) | 197.1289, 241.119 | 241.1194 | 241.1191 | 4.4 | NEG | 51905.43669 | 51268.1895 | 50292.49468 | 0.006944338 | 0.006980996 | 0.006600449 | 0.006841928 | XLUAWXQORJEMBD-UHFFFAOYSA-N | O=C1N2CCCC2C(O)=NC1C(C)C |  |  |  |  |  | 2854-40-2 |  |  |  |  |  |  |  | level2 |
| compound00763 | 7.11\_413.1237m/z | M+FA-H | C21H20O6 | 44 | 2.78 | -1.23 | Cyclocurcumin | 61.9874, 119.0493, 134.0363, 163.039, 193.05, 329.1396, 329.2316, 345.0624, 413.1236 | 413.1242 | 413.1237 | 7.11 | NEG | 57188.98919 | 59764.73536 | 58764.34972 | 0.007651215 | 0.008137939 | 0.007712306 | 0.00783382 | IZLBLUIBVMGMIY-ZZXKWVIFSA-N | COC1=C(O)C=CC(\C=C\C2=CC(=O)CC(O2)C2=CC(OC)=C(O)C=C2)=C1 | HMDB0033086 | 88978 |  |  | 69879809 | 153127-42-5 | 环姜黄素 | 酚类 | 多酚类 | Phenols | Polyphenols | DH0303-0010 | HPLC≥98% | level2 |
| compound00764 | 4.89\_399.1413m/z | M+Na | C20H24O7 | 40.5 | 0 | -0.37 | Cycloolivil |  | 399.1414 | 399.1413 | 4.89 | POS | 59172.13894 | 60615.24581 | 59043.81466 | 0.007916538 | 0.00825375 | 0.007748983 | 0.00797309 | KCIQZCNOUZCRGH-VOBQZIQPSA-N | OC1=CC=C(C=C1OC)C2C3=CC(O)=C(OC)C=C3CC(O)(CO)C2CO |  |  |  |  |  |  | 异橄榄树脂素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DY0153 | HPLC≥98% | level2 |
| compound00765 | 9.86\_331.1551m/z | M+FA-H | C18H22O3 | 54.9 | 59.5 | -0.16 | Cyclopiloselloidone | 287.1653, 290.9825, 301.1810, 303.1964, 310.9912, 313.1439, 330.1783, 330.9804, 330.9898, 331.1525 | 331.1551 | 331.1551 | 9.86 | NEG | 35200.95573 | 35686.92924 | 36671.97643 | 0.004709475 | 0.004859355 | 0.004812876 | 0.004793902 | DUPPHCJMEGRLRP-UHFFFAOYSA-N | CC(C)CC(=O)C1=CC(=CC2=C1OC(C=C2)(C)C)C(=O)C |  |  |  |  | 5316266 | 54963-37-0 |  |  |  |  |  |  |  | level2 |
| compound00766 | 0.77\_209.0659m/z | M-H | C7H14O7 | 48.4 | 47 | -3.8 | D-altrofurano-heptulose-3 | 57.0335, 59.0128, 85.0285, 87.0077, 129.0184, 159.0289, 209.0294, 209.0661 | 209.0667 | 209.0659 | 0.77 | NEG | 225834.1227 | 227020.1706 | 222697.9198 | 0.030213955 | 0.030912481 | 0.029227151 | 0.030117862 | NSQDEHXIGIPNHO-GKHCUFPYSA-N | OC[C@H]1O[C@@](O)([C@H](O)CO)[C@H](O)[C@@H]1O |  |  |  |  |  | 25545-06-6 | 景天庚酮糖 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | DJ0358 | HPLC≥98% | level2 |
| compound00767 | 5.01\_501.1031m/z | M-H | C24H22O12 | 41.4 | 0 | -1.42 | Daidzin 6′′-O-malonate |  | 501.1038 | 501.1031 | 5.01 | NEG | 10241.38055 | 9062.841811 | 12176.391 | 0.001370177 | 0.001234053 | 0.001598045 | 0.001400758 | MTXMHWSVSZKYBT-UHFFFAOYSA-N | OC1C(O)C(COC(=O)CC(O)=O)OC(OC2=CC3=C(C=C2)C(=O)C(=CO3)C2=CC=C(O)C=C2)C1O | HMDB0041263 |  |  | C16191 | 14500869 | 124590-31-4 | 6''-O-丙二酰基大豆苷 | 黄酮类 | 异黄酮类 | Flavonoids | Isoflavones | ST83810205 | HPLC≥95% | level2 |
| compound00768 | 10.48\_268.1097n | M+H-H2O, M+H | C17H16O3 | 57.2 | 70.8 | -1.01 | Danshinspiroketallactone | 195.1167, 223.1115, 233.0957, 251.1064, 269.1171 | 269.1172 | 269.117 | 10.48 | POS | 117265.2767 | 116164.0771 | 120617.32 | 0.015688718 | 0.015817625 | 0.015829966 | 0.015778769 | DNLNYCCHXAULQA-UHFFFAOYSA-N | CC1CC2(C3=C(C4=CC=CC(=C4C=C3)C)C(=O)O2)OC1 |  |  |  |  | 127567 |  |  |  |  |  |  |  |  | level2 |
| compound00769 | 7.81\_271.1326m/z | M+H | C17H18O3 | 51.4 | 0 | -0.94 | daphneolon |  | 271.1329 | 271.1326 | 7.81 | POS | 10676.80129 | 10414.81686 | 10770.09702 | 0.001428431 | 0.001418146 | 0.001413481 | 0.001420019 | NNPDNNXUSPXBRO-UHFFFAOYSA-N | C1=CC=C(C=C1)CCC(CC(=O)C2=CC=C(C=C2)O)O |  |  |  |  | 5316300 |  |  |  |  |  |  |  |  | level2 |
| compound00770 | 0.81\_204.0866m/z | M+H-H2O | C8H15NO6 | 45.8 | 34.1 | -0.35 | Cyclic N-Acetyl-D-mannosamine | 168.0652, 170.0813, 175.1189, 186.0731, 187.1075, 203.0526, 203.1153, 203.1494, 204.0561, 204.0868 | 204.0866 | 204.0866 | 0.81 | POS | 61744.85741 | 68490.26084 | 76109.22291 | 0.008260737 | 0.009326061 | 0.009988669 | 0.009191822 | OVRNDRQMDRJTHS-OZRXBMAMSA-N | CC(=O)N[C@@H]1[C@H](O)O[C@H](CO)[C@@H](O)[C@@H]1O | HMDB0001129 | 6024 |  | C00645 | 11096158 | 7772-94-3 | N-乙酰-D-甘露糖胺 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-W040154 | HPLC≥98% | level2 |
| compound00771 | 4.51\_355.0459m/z | 2M-H | C9H6O4 | 43.4 | 0 | -0.23 | Daphnetin |  | 355.0459 | 355.0459 | 4.51 | NEG | 7354.426841 | 7275.937369 | 7378.422232 | 0.000983936 | 0.000990737 | 0.000968353 | 0.000981009 | ATEFPOUAMCWAQS-UHFFFAOYSA-N | C1=CC(=C(C2=C1C=CC(=O)O2)O)O |  | 65905 |  | C03093 | 5280569 | 486-35-1 | 瑞香素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N0281 | HPLC≥98% | level2 |
| compound00772 | 4.14\_457.1718m/z | M-H2O-H | C21H32O12 | 52.8 | 0.516 | 0.58 | darendoside B | 231.1027, 267.0875, 305.1234, 321.0942, 389.0848, 411.1875, 456.2927, 457.1275, 457.1751, 457.1836 | 457.1715 | 457.1718 | 4.14 | NEG | 22867.02935 | 24460.71092 | 23061.59093 | 0.00305934 | 0.003330723 | 0.003026632 | 0.003138898 | ZLPXZRZUFKQINJ-DDPVKAFRSA-N | CCO[C@H]1[C@]([C@H]([C@@H]([C@H](O1)CO)O)O[C@H]2[C@@H]([C@@H]([C@H]([C@@H](O2)C)O)O)O)(C3=CC(=C(C=C3)OC)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00773 | 10.50\_325.2147m/z | M+H-H2O | C22H30O3 | 50.6 | 0 | -4.5 | daurichromene b |  | 325.2161 | 325.2147 | 10.5 | POS | 2103.626407 | 2181.309158 | 2064.250209 | 0.000281441 | 0.000297021 | 0.000270915 | 0.000283125 | RXKAJVPBSTXEAH-BPARTEKVSA-N | CC1=CC(=C2C=C[C@@](OC2=C1)(C)CCC(C(=C)CCC=C(C)C)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00774 | 9.59\_343.2235m/z | M+Na | C20H32O3 | 52.3 | 0 | -2.81 | Dayecrystal A |  | 343.2244 | 343.2235 | 9.59 | POS | 13358.77253 | 14316.76392 | 13457.01181 | 0.001787247 | 0.00194946 | 0.001766115 | 0.001834274 | HGSLTWCHZKTSMQ-UHFFFAOYSA-N | CC1(CCCC2(C1CCC34C2CCC(C3O)C(C4)(C)O)C=O)C |  |  |  |  | 102004538 |  |  |  |  |  |  |  |  | level2 |
| compound00775 | 5.33\_362.1359n | M+H-H2O, M+Na | C19H22O7 | 53.5 | 0 | -1.9 | Deacetylorientalide |  | 345.1332 | 345.1326 | 5.33 | POS | 25800.05252 | 24642.86736 | 23285.63709 | 0.003451744 | 0.003355526 | 0.003056036 | 0.003287769 | HQPSNGXRJBMMAL-WHZRINGVSA-N | O=CC1=CCCC(=CC2OC(=O)C(=C)C2C(OC(=O)C(=C)C)C1O)CO |  |  |  |  |  |  |  | 萜类 | 倍半萜类 | Terpenes | Sesquiterpenes | DD0367 | HPLC≥95% | level2 |
| compound00776 | 4.89\_469.1351m/z | M+FA-H | C20H24O10 | 42.1 | 0 | -0.15 | Decuroside V |  | 469.1352 | 469.1351 | 4.89 | NEG | 5264.542298 | 6028.846278 | 4300.721726 | 0.000704334 | 0.000820925 | 0.000564432 | 0.000696564 | KLPNFWKZLQAVTH-CWMWYVAESA-N | CC(C)(O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H]1Oc2cc3oc(=O)ccc3cc2[C@H]1O |  |  |  |  |  | 96648-59-8 | 前胡苷V | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | DQ0217 | HPLC≥98% | level2 |
| compound00777 | 8.41\_331.1914m/z | M-H | C20H28O4 | 44.5 | 14.7 | -0.38 | Dehydroandrographolide | 283.17, 287.1652, 330.2366, 331.1524, 331.1912 | 331.1915 | 331.1914 | 8.41 | NEG | 184690.253 | 184515.6331 | 197352.8055 | 0.024709388 | 0.025124798 | 0.025900826 | 0.025245004 | YIIRVUDGRKEWBV-CZUXAOBFSA-N | C=C1CC[C@H]2[C@@](C)(CC[C@@H](O)[C@@]2(C)CO)[C@H]1C/C=C1\C=COC1=O |  |  |  |  |  | 134418-28-3 | 脱水穿心莲内酯 | 萜类 | 二萜类 | Terpenes | Diterpenes | HY-N0676 | HPLC≥98% | level2 |
| compound00778 | 1.06\_173.0083m/z | M-H | C6H6O6 | 51.1 | 53.7 | -4.69 | dehydroascorbates | 85.0284, 111.0077, 129.0184 | 173.0092 | 173.0083 | 1.06 | NEG | 1089705.816 | 1058051.017 | 1071258.738 | 0.145789847 | 0.144070819 | 0.140593322 | 0.143484663 | SBJKKFFYIZUCET-UHFFFAOYSA-N | C(C(C1C(=O)C(=O)C(=O)O1)O)O |  |  |  |  | 440667 |  |  |  |  |  |  |  |  | level2 |
| compound00779 | 8.30\_251.1064m/z | M+H | C17H14O2 | 41.9 | 0 | -1.06 | Dehydroeffusol |  | 251.1067 | 251.1064 | 8.3 | POS | 4673.571639 | 4919.582428 | 4763.013548 | 0.000625269 | 0.000669881 | 0.000625104 | 0.000640085 | GSSPKCPIRDPBQE-UHFFFAOYSA-N | C=Cc1cc(O)cc2ccc3c(C)c(O)ccc3c12 |  |  |  |  |  | 137319-34-7 | 去氢厄弗酚 | 酚类 | 多酚类 | Phenols | Polyphenols | HY-N5058 | HPLC≥98% | level2 |
| compound00780 | 9.39\_229.1221m/z | M+H | C15H16O2 | 50.9 | 0 | -0.81 | Dehydroshizukanolide |  | 229.1223 | 229.1221 | 9.39 | POS | 10286.48917 | 9894.849373 | 10436.3851 | 0.001376212 | 0.001347344 | 0.001369684 | 0.001364413 | OVEQSZKTJIUNHZ-UHFFFAOYSA-N | CC1=C2CC3C(=C)C4CC4C3(C=C2OC1=O)C |  |  |  |  | 333361 | 66395-02-6 |  |  |  |  |  |  |  | level2 |
| compound00781 | 5.70\_267.1234m/z | M+FA-H | C13H18O3 | 53.2 | 54.1 | -1.59 | Dehydrovomifoliol | 59.0128, 223.1334, 226.994, 247.0003, 266.9848, 267.0656, 267.1015 | 267.1239 | 267.1234 | 5.7 | NEG | 15175.47884 | 15275.8803 | 15370.86758 | 0.002030301 | 0.002080059 | 0.002017292 | 0.002042551 | JJRYPZMXNLLZFH-URWSZGRFSA-N | C1(CC(C)(C)[C@](O)(C(C)=C1)/C=C/C(C)=O)=O | HMDB0302822 | 53371 | LMPR0103050009 | C02533 | 688492 |  |  |  |  |  |  |  |  | level2 |
| compound00782 | 4.01\_385.0775m/z | M+FA-H | C15H16O9 | 48.5 | 0.0102 | -0.35 | Daphnin | 57.0335, 85.0284, 129.0183, 147.029, 191.019, 209.0296, 385.0775 | 385.0777 | 385.0775 | 4.01 | NEG | 4083872.297 | 4168080.135 | 4092507.529 | 0.546374176 | 0.56755176 | 0.537105751 | 0.550343896 | HOIXTKAYCMNVMY-PVOAASPHSA-N | C1=CC(=C(C2=C1C=CC(=O)O2)O)OC3C(C(C(C(O3)CO)O)O)O |  | 65594 |  | C01421 | 439499 | 486-55-5 | 祖师麻乙素 | 苯丙素类 | 香豆素类 | Phenylpropanoids | Coumarins | HY-N7252 | HPLC≥98% | level2 |
| compound00783 | 9.66\_317.1755m/z | M+FA-H | C18H24O2 | 47.1 | 17 | -1.32 | Delta3,2-Hydroxylbakuchiol | 112.9845, 180.9723, 248.9601, 273.1858, 316.9881, 317.1759 | 317.1759 | 317.1755 | 9.66 | NEG | 16729.68021 | 16937.34968 | 17424.28804 | 0.002238235 | 0.002306295 | 0.002286785 | 0.002277105 | KGYDEXUROYEYFL-UHFFFAOYSA-N | C=CC(C)(C=Cc1ccc(O)cc1)CC=CC(C)(C)O |  |  |  |  |  | 178765-49-6 | 13-羟基补骨脂酚 | 酚类 | 单酚类 | Phenols | Monophenols | ST81450205 | HPLC≥95% | level2 |
| compound00784 | 4.84\_287.0549m/z | M+ | C15H11O6+ | 43.2 | 0 | -2.46 | Cyanidin |  | 287.0556 | 287.0549 | 4.84 | POS | 12596.29538 | 13139.95139 | 11969.01079 | 0.001685236 | 0.001789218 | 0.001570828 | 0.001681761 | VEVZSMAEJFVWIL-UHFFFAOYSA-O | C1(O)C=C2[O+]=C(C3=CC=C(O)C(O)=C3)C(O)=CC2=C(O)C=1 | HMDB0002708 | 419517 | LMPK12010002 | C05905 | 128861 | 13306-05-3 | 氯化花青素 | 黄酮类 | 花青素类 | Flavonoids | Anthocyanins | HY-N0499 | HPLC≥98% | level2 |
| compound00785 | 2.80\_359.0981m/z | M+FA-H | C14H18O8 | 58.8 | 87.4 | -0.72 | cuneataside a | 72.992, 179.0342, 197.0447, 359.0982 | 359.0984 | 359.0981 | 2.8 | NEG | 156479.0182 | 153249.3848 | 155580.7445 | 0.020935056 | 0.020867391 | 0.020418609 | 0.020740352 | CTVFMNLFBWRHJH-UHFFFAOYSA-N | C1C(OC2C(C(C(OC2O1)CO)O)O)C3=CC(=C(C=C3)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00786 | 3.85\_471.1480m/z | M+H-H2O | C21H28O13 | 40.7 | 0 | -3.48 | Cistanoside F |  | 471.1496 | 471.148 | 3.85 | POS | 11935.37229 | 12801.62325 | 11612.1194 | 0.001596813 | 0.001743149 | 0.001523989 | 0.001621317 | KARNWFDIYRKBOE-BHSPTIPFSA-N | C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@H]([C@H](C=O)O)[C@@H]([C@@H](CO)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O)O |  |  |  |  |  | 97411-47-7 | 肉苁蓉苷F | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | DR0044 | HPLC≥98% | level2 |
| compound00787 | 4.95\_567.2076m/z | M-H | C27H36O13 | 53.9 | 20.4 | -1.21 | Citrusin B | 179.0552, 197.0443, 281.0819, 311.0915, 325.0708, 326.1154, 341.1396, 521.1988, 566.3401, 567.1166 | 567.2083 | 567.2076 | 4.95 | NEG | 34275.1701 | 26517.2879 | 34266.61586 | 0.004585615 | 0.003610759 | 0.004497193 | 0.004231189 | XMGKCJUCYBLMBY-OGVRJPSHSA-N | COC1=CC(=CC(=C1O[C@H](CO)[C@H](C2=CC(=C(C=C2)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)OC)O)OC)/C=C/CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00788 | 5.51\_457.1467m/z | M+Na | C22H26O9 | 53.3 | 0 | -0.47 | ciwujiatone |  | 457.1469 | 457.1467 | 5.51 | POS | 10028.41062 | 10244.46319 | 10934.85756 | 0.001341684 | 0.00139495 | 0.001435104 | 0.001390579 | ANCVHDRNDJRUOT-FBJOKTGGSA-N | COC1=CC(=CC(=C1O)OC)[C@@H]2[C@H]([C@H](CO2)C(=O)C3=CC(=C(C(=C3)OC)O)OC)CO |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00789 | 4.72\_358.0929m/z | M-H | C18H17NO7 | 41.2 | 0 | -0.85 | Clovamide |  | 358.0932 | 358.0929 | 4.72 | NEG | 4336.414718 | 4255.278527 | 4135.268178 | 0.000580161 | 0.000579425 | 0.000542718 | 0.000567435 | GPZFXSWMDFBRGS-UXONFWTHSA-N | O=C(O)C(N=C(O)C=CC1=CC=C(O)C(O)=C1)CC2=CC=C(O)C(O)=C2 |  |  |  |  |  | 53755-02-5 |  | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-122267 | HPLC≥98% | level2 |
| compound00790 | 7.88\_315.1225m/z | M+H-H2O | C18H20O6 | 44.5 | 0 | -0.53 | Colutehydroquinone |  | 315.1227 | 315.1225 | 7.88 | POS | 14757.14295 | 14564.47798 | 15044.25284 | 0.001974333 | 0.00198319 | 0.001974426 | 0.001977316 | RRVWIPPRKMQDAO-NSHDSACASA-N | COc1ccc2c(c1)OC[C@@H](c1cc(O)c(OC)c(OC)c1O)C2 |  |  |  |  |  | 181311-16-0 | 鱼鳔槐氢醌 | 黄酮类 | 其他黄酮类 | Flavonoids | Other flavonoids | HY-N8026 | HPLC≥98% | level2 |
| compound00791 | 9.64\_297.1129m/z | M-H2O-H | C18H20O5 | 42.3 | 0.0217 | -1.12 | Combretastatin A4 | 229.1806, 267.1016, 296.105, 296.997, 297.1131 | 297.1132 | 297.1129 | 9.64 | NEG | 160460.9721 | 156268.4707 | 155811.1887 | 0.021467795 | 0.021278489 | 0.020448853 | 0.021065045 | HVXBOLULGPECHP-WAYWQWQTSA-N | COC1=C(C=C(C=C1)C=CC2=CC(=C(C(=C2)OC)OC)OC)O |  | 45060 |  |  | 5351344 | 117048-59-6 | 康普瑞汀A4 | 苯丙素类 | 二苯乙烯苷类 | Phenylpropanoids | Stilbenoids | HY-N2146 | HPLC≥98% | level2 |
| compound00792 | 4.29\_624.1692n | M+H, M+Na | C28H32O16 | 51.3 | 49.5 | 0.2 | Complanatuside A | 409.0906, 421.0905, 433.0893, 439.1022, 457.1125, 487.1228, 606.3629, 607.1650, 624.3730, 625.1806 | 625.1763 | 625.1764 | 4.29 | POS | 530884.5527 | 517150.3186 | 520149.2087 | 0.071026121 | 0.070418409 | 0.068265026 | 0.069903186 | KKPKUPKKMALLKG-UHFFFAOYSA-N | COC1=CC(=C2C(=C1)OC(=C(C2=O)OC3C(C(C(C(O3)CO)O)O)O)C4=CC=C(C=C4)OC5C(C(C(C(O5)CO)O)O)O)O |  |  |  |  | 5492406 | 116183-66-5 |  |  |  |  |  |  |  | level2 |
| compound00793 | 3.88\_342.1319n | M+Na, M+K, M+NH4 | C16H22O8 | 42.1 | 2.72 | 1.28 | Coniferin | 204.1016, 284.155, 364.1353, 365.119 | 365.1207 | 365.1211 | 3.88 | POS | 106000.1298 | 105561.3221 | 108085.0775 | 0.014181573 | 0.014373887 | 0.014185219 | 0.014246893 | SFLMUHDGSQZDOW-FAOXUISGSA-N | COC1=C(O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C=CC(\C=C\CO)=C1 | HMDB0013682 | 64182 |  | C00761 | 5280372 | 124151-33-3 | 松柏苷 | 糖及糖苷类 | 糖苷类 | Carbohydrates and Glycosides | Glycosides | HY-N3617 | HPLC≥98% | level2 |
| compound00794 | 5.43\_357.1326m/z | M+H | C20H20O6 | 42.4 | 0 | -1.99 | Coniferyl ferulic acid |  | 357.1333 | 357.1326 | 5.43 | POS | 14976.63965 | 15181.90638 | 13791.96771 | 0.002003699 | 0.002067263 | 0.001810075 | 0.001960345 | PGLIMMMHQDNVRS-YZQQHVNFSA-N | COC1=C(C=CC(=C1)C=CCOC(=O)C=CC2=CC(=C(C=C2)O)OC)O |  |  |  | C17855 | 6441913 |  | 阿魏酸松柏酯 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N1916 | HPLC≥98% | level2 |
| compound00795 | 5.27\_505.1128m/z | M+K | C22H26O11 | 43.8 | 0 | 4.59 | Curculigoside |  | 505.1105 | 505.1128 | 5.27 | POS | 8217.273527 | 6776.081257 | 7717.506702 | 0.001099375 | 0.000922673 | 0.001012855 | 0.001011634 | SJJRKHVKAXVFJQ-QKYBYQKWSA-N | COc1cccc(OC)c1C(=O)OCc1cc(O)ccc1O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 85643-19-2 | 仙茅苷 | 苯丙素类 | 简单苯丙素类 | Phenylpropanoids | Simple phenylpropanoids | HY-N0705 | HPLC≥98% | level2 |
| compound00796 | 5.53\_343.0808m/z | M+Na | C19H14NO4+ | 48 | 0 | -2.23 | Coptisine |  | 343.0816 | 343.0808 | 5.53 | POS | 3436.907235 | 3026.84446 | 3165.201748 | 0.000459818 | 0.000412154 | 0.000415405 | 0.000429126 | XYHOBCMEDLZUMP-UHFFFAOYSA-N | O1C=2C=CC3=CC=4C5=CC=6OCOC6C=C5CC[N+]4C=C3C2OC1 |  |  |  |  | 72322 | 3486-66-6 | 盐酸黄连碱 | 生物碱 |  | Alkaloids |  | HY-N0736 | HPLC≥98% | level2 |
| compound00797 | 1.38\_252.1093m/z | M+H | C10H13N5O3 | 52.7 | 49.3 | 0.58 | Cordycepin | 85.0288, 136.0614, 136.075, 252.084, 252.1082 | 252.1091 | 252.1093 | 1.38 | POS | 272472.7681 | 268097.4427 | 253750.6511 | 0.036453658 | 0.036505818 | 0.033302549 | 0.035420675 | OFEZSBMBBKLLBJ-BAJZRUMYSA-N | C1C(OC(C1O)N2C=NC3=C(N=CN=C32)N)CO |  | 66970 |  | C08431 | 6303 | 73-03-0 | 虫草素 | 糖及糖苷类 | 糖类 | Carbohydrates and Glycosides | Carbohydrates | HY-N0262 | HPLC≥98% | level2 |
| compound00798 | 6.88\_273.1131m/z | M-H2O-H | C16H20O5 | 57.8 | 79 | -0.32 | Coriandrone B | 211.1122, 227.1073, 229.1234, 232.9821, 252.9906, 255.1026, 272.9952, 273.1133 | 273.1132 | 273.1131 | 6.88 | NEG | 14919.38529 | 14535.22193 | 15144.75189 | 0.001996039 | 0.001979206 | 0.001987616 | 0.00198762 | BWHXOOBBSCGLBC-UHFFFAOYSA-N | COC1=C2CC(O)C(C)(C)OC2=C2C(=O)OC(C)CC2=C1 | HMDB0037775 | 92590 |  |  | 131752232 | 139906-04-0 |  |  |  |  |  |  |  | level2 |
| compound00799 | 10.69\_315.1965m/z | M-H2O-H | C20H30O4 | 51.6 | 35.4 | -0.23 | Coronarin B | 271.1701, 314.9825, 315.1532, 315.1956 | 315.1966 | 315.1965 | 10.69 | NEG | 263229.1878 | 267006.5721 | 250100.7714 | 0.035216975 | 0.036357278 | 0.032823535 | 0.034799263 | FTQNGEYQJGYGFY-UHFFFAOYSA-N | CC1(CCCC2(C1CCC(=C)C2C3C=C(CC(OO3)O)C=O)C)C |  |  |  |  | 129316571 |  |  |  |  |  |  |  |  | level2 |
| compound00800 | 7.84\_455.3517m/z | M+H-H2O | C30H48O4 | 43.2 | 0 | -0.58 | Corosolic acid |  | 455.352 | 455.3517 | 7.84 | POS | 20032.00693 | 19953.78378 | 21663.56281 | 0.002680047 | 0.002717032 | 0.002843153 | 0.002746744 | HFGSQOYIOKBQOW-ZSDYHTTISA-N | C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@@H](O)[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]2[C@H]1C)C(O)=O | HMDB0304746 |  |  |  |  |  | 科罗索酸 | 萜类 | 三萜类 | Terpenes | Triterpenes | HY-N0280 | HPLC≥98% | level2 |
| compound00801 | 5.81\_357.0970m/z | M+Na | C20H16NO4+ | 40.8 | 0 | -0.42 | Corysamine |  | 357.0972 | 357.097 | 5.81 | POS | 4141.868509 | 2854.332523 | 2991.73196 | 0.000554133 | 0.000388664 | 0.000392639 | 0.000445145 | YESPQCLKTIRGLU-UHFFFAOYSA-N | Cc1c2[n+](cc3c4c(ccc13)OCO4)CCc1cc3c(cc1-2)OCO3 |  |  |  |  |  | 11028-77-6 | 紫堇沙明碱 | 生物碱 |  | Alkaloids |  | DZ0188 | HPLC≥98% | level2 |
| compound00802 | 5.74\_662.1820n | M-H, M+FA-H | C31H34O16 | 50.9 | 0 | -4.05 | crassirhizomoside c | 285.0766, 353.0638, 593.1873, 615.1696, 661.1746 | 661.1774 | 661.1747 | 5.74 | NEG | 508733.8592 | 505016.6356 | 505816.476 | 0.068062619 | 0.068766212 | 0.06638398 | 0.067737603 | FRCCTBPYYAMKIB-PVVPWINYSA-N | CC1C(C(C(C(O1)OC2=CC(=C3C(=C2)OC(=C(C3=O)OC4C(C(C(C(O4)C)O)OC(=O)C)OC(=O)C)C5=CC=C(C=C5)O)O)O)O)O |  | 50374 |  |  | 44259028 |  |  |  |  |  |  |  |  | level2 |
| compound00803 | 4.02\_271.1154m/z | M+Na | C11H20O6 | 54.9 | 10.3 | 0.7 | Crenulatin | 271.1142 | 271.1152 | 271.1154 | 4.02 | POS | 31120.00615 | 30316.52052 | 32289.35302 | 0.004163492 | 0.004128086 | 0.004237695 | 0.004176424 | ZEGGZNOPAPRAIG-SPFKKGSWSA-N | C=CC(C)(C)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O |  |  |  |  |  | 63026-02-8 | 大花红天素 | 萜类 | 单萜类 | Terpenes | Monoterpenes | DD0302 | HPLC≥98% | level2 |
| compound00804 | 10.70\_316.2030n | M+H-H2O, M+H | C20H28O3 | 51.3 | 0 | -2.71 | crotohalimaneicacid | 191.1066, 205.1217, 215.1065, 243.137, 281.1903, 287.2002, 299.1999, 317.1145, 317.1736, 317.2094 | 317.2111 | 317.2103 | 10.7 | POS | 125858.8124 | 126402.6073 | 133552.7737 | 0.016838432 | 0.017211767 | 0.017527631 | 0.01719261 | QSCGVVYGWUHJIU-UHFFFAOYSA-N | CC1CCC2=C(C1(C)CCC3=COC=C3)CCCC2(C)C(=O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00805 | 10.77\_296.1409n | M+H, M+Na | C19H20O3 | 42.9 | 1.91 | -1.21 | Cryptotanshinone | 251.1427, 279.1377, 297.1482 | 297.1485 | 297.1482 | 10.77 | POS | 23666222.92 | 24329914.96 | 24890070.61 | 3.166262825 | 3.312912808 | 3.26660366 | 3.248593098 | GVKKJJOMQCNPGB-JTQLQIEISA-N | O=C1C(=O)C2=C(OCC2C)C=3C=CC4=C(C13)CCCC4(C)C |  |  |  |  | 160254 | 35825-57-1 | 隐丹参酮 | 醌类 | 萘醌类 | Quinones | Naphthoquinones | HY-N0174 | HPLC≥98% | level2 |
| compound00806 | 4.11\_477.1611m/z | M+FA-H | C19H28O11 | 60.3 | 32.2 | -0.61 | cuchiloside | 153.0549, 197.045, 239.058, 477.161 | 477.1614 | 477.1611 | 4.11 | NEG | 26229.16598 | 25157.56135 | 25021.7985 | 0.003509155 | 0.00342561 | 0.003283892 | 0.003406219 | COATVAWKNHHMEI-UHFFFAOYSA-N | C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCCC3=CC=C(C=C3)O)O)O)O)O)O)O |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |
| compound00807 | 6.33\_279.1235m/z | M-H | C15H20O5 | 56.5 | 75.6 | -0.9 | Cordilin | 205.1225, 235.0003, 235.1335, 278.9905, 279.1239 | 279.1238 | 279.1235 | 6.33 | NEG | 11339.66508 | 11228.73861 | 12145.97191 | 0.001517114 | 0.001528975 | 0.001594052 | 0.001546714 | IRPFOXRBPHCCTG-UHFFFAOYSA-N | CC1CCC2C(OC(=O)C2=C)C(C)(O)C11CCC(=O)O1 | HMDB0302335 |  |  |  | 98331 |  |  |  |  |  |  |  |  | level2 |
| compound00808 | 1.93\_247.1292m/z | M+H | C10H18N2O5 | 54.8 | 74.4 | 1.31 | γ-glutamyl-valine | 70.0657, 72.0813, 84.0448, 118.0863, 130.0498, 184.0966, 230.1023, 247.0704, 247.1311 | 247.1288 | 247.1292 | 1.93 | POS | 29195.13531 | 29836.05474 | 28689.00568 | 0.003905966 | 0.004062663 | 0.003765181 | 0.00391127 | AQAKHZVPOOGUCK-UHFFFAOYSA-N | CC(C)C(C(=O)O)NC(=O)CCC(C(=O)O)N |  |  |  |  |  |  |  |  |  |  |  |  |  | level2 |