

## LIST OF STRESS MODULATED IDENTIFIED COMPOUNDS

**Lists of annotated significant  $m/z$  between fungus *Neofusicoccum parvum* and *Diplodia seriata* (Np or Ds) inoculated-grapevines and non-inoculated ones under abiotic stresses: none (NAS), water (WS), heat (HS) or both stresses (WSHS).** Comparisons were performed with Perseus software (Student T-test FDR < 0.05 and S0 = 0). Some lists are reduced to TOPs modulated compounds and the most specific ones selected by increasing the T-test stringency parameters (FDR and S0, specified in table legends) are highlighted in bold characters. Each compound is identified with an ID number. Measured  $m/z$  and calculated KEGG theoretical Mass and error (ppm) are indicated and the number of possible MassTrix identifications is indicated in the “n” column but only the first three ones are listed. Functional categories (Cat.) were manually determined according to KEGG annotations: Carbohydrates (Cb); Lipids (Lp); Phytochemicals (Ph); Peptides (Pp); Amino sugars (AmS); Nucleotides (Nu) and no match (NM). Functional categories counts are indicated in the table legends (Total and TOPs). Compounds are ranked according to their normalized value differences (up in green gradient and down in red gradient) between inoculated and non-inoculated samples. Identified isotopic compounds are indicated in italic characters.

### IDENTIFIED *Np* COMPOUNDS

**a) List of 33 identified “No abiotic stress” (NAS) *Np* vs NI (non-inoculated as control) from the significant 209  $m/z$  at time B** selected with T-test (FDR=0.05 and S0=0).

Total 33 functional category counts: Ph:15; Lp:5; Cb:6; Pp:1; AmS:2; Nu:2; NM:2.

| ID   | T-test<br><i>p-value</i> | NAS<br><i>Np-NI</i> | $m/z$      | Mass       | error<br>(ppm) | n | Cat. | Formula    | Identifications  |   |  |
|------|--------------------------|---------------------|------------|------------|----------------|---|------|------------|--|---|--|
| 7463 | 0.002902                 | -2.882              | 609.188462 | 610.195738 | 0.997565       | 1 | Ph   | C34H30N2O9 | Atalanine  |   |  |
| 5540 | 0.001066                 | -2.815              | 472.146076 | 473.153353 | 0.058057       | 1 | Ph   | C20H27NO12 | Proteacin  |   |  |
| 1590 | 0.016934                 | -2.706              | 299.113594 | 300.120870 | -0.109047      | 1 | Cb   | C14H20O7   | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside |   |  |
| 2931 | 0.031813                 | -2.544              | 351.127125 | 352.134401 | -0.124492      | 3 | Lp   | C18H24O5S  | Estradiol-17β 3-sulfate  | Estradiol-17β 3-sulfate (see KEGG C08357); (8S,9S,13S,14S,17S)-17-hydroxy-13-methyl-3-sulfooxy-6,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthrene [secondary alcohol] | Estradiol-17β 3-sulfate (see KEGG C08357); estra-1,3,5(10)-triene-3,17β-diol 3-sulfate [Sulfates [ST0502]] |
| 1194 | 0.006606                 | -2.456              | 274.056804 | 275.064080 | -0.131780      | 1 | Ph   | C10H13NO8  | 3-β-D-Glucopyranuronosyloxy-5-methylisoxazole                                |   |  |
| 2347 | 0.000273                 | -2.287              | 330.119400 | 331.126676 | -0.122722      | 1 | AmS  | C14H21NO8  | 5'-O-β-D-Glucosylpyridoxine  |   |  |
| 149  | 0.025849                 | -2.240              | 195.033221 | 196.040497 | -0.242029      | 2 | Cb   | C6H12O5S   | Thioglucoside  | Thiogalactoside   |  |
| 8451 | 0.018576                 | -2.217              | 721.416962 | 722.424238 | 0.153962       | 2 | Ph   | C39H62O12  | Yamogenin 3-O-neohesperidoside   | Ophiopogonin B  |  |
| 3153 | 0.033093                 | -2.118              | 359.134719 | 360.141996 | -0.102120      | 2 | Ph   | C16H24O9   | 7-Deoxyloganate  | 8-Epideoxyloganic acid  |  |
| 2999 | 0.011394                 | -2.076              | 353.124149 | 354.131425 | 0.362582       | 1 | Nu   | C16H20N2O7 | O18 isotope of Cotinineglucuronide; 3,4,5-                                   |   |  |

|      |          |        |            |            |           |   |     |              |   |  |   |
|------|----------|--------|------------|------------|-----------|---|-----|--------------|---|--|---|
| 5002 | 0.007963 | -1.848 | 441.189684 | 442.196960 | 0.399232  | 1 | Lp  | C18H35O10P   | trihydroxy-6-[5-(1-methyl-5-oxo-pyrrolidin-2-yl)pyridin-1-yl]-oxane-2-carboxylic acid [cation] PG(6:/6:); 1,2-dihexanoyl-sn-glycero-3-phospho-(1'-sn-glycerol) [Diacylglycerophosphoglycerols [GP0401]] |  |   |
| 3775 | 0.049025 | -1.846 | 382.100408 | 383.107685 | -0.072174 | 1 | Nu  | C14H17N5O8   | Succinyladenosine; (2S)-2-[[9-[(2S,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]purin-6-yl]amino]butanedioic acid [primary alcohol]   |  |   |
| 3454 | 0.022085 | -1.838 | 369.082692 | 370.089969 | -0.075560 | 1 | Ph  | C16H18O10    | Fraxin  |  |   |
| 2745 | 0.003371 | -1.828 | 345.119057 | 346.126333 | -0.142585 | 4 | Lp  | C15H22O9     | Aucubin   | Deutzioside  | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]                               |
| 1864 | 0.019281 | -1.826 | 311.098334 | 312.105610 | -0.117249 | 6 | Cb  | C11H20O10    | Vicianose; O- $\alpha$ -L-Arabinopyranosyl-(1-6)-D-glucopyranose  | Arabino-galactose  | 6-O- $\beta$ -D-Xylopyranosyl-D-glucose; Primeverose  |
| 1635 | 0.045664 | -1.784 | 301.056465 | 302.063741 | 0.451381  | 1 | NM  | C16H13ClN2O2 | Cl37 isotope of 3-(4-Chloro-benzyl)-5-(2-methoxy-phenyl)-[1,2,4]oxadiazole  |  |   |
| 3591 | 0.048769 | -1.771 | 375.129648 | 376.136925 | -0.059642 | 3 | Ph  | C16H24O10    | Loganate; Loganic acid  | 7-Epiloganic acid  |   |
| 2925 | 0.039102 | -1.713 | 351.085174 | 352.092450 | 0.281489  | 3 | Lp  | C18H23BrO2   | O18 isotope of 16 $\alpha$ -Bromo-17 $\beta$ -estradiol; 16 $\alpha$ -Bromo-1,3,5(10)-estratriene-3,17 $\beta$ -diol  | O18 isotope of 18-bromo-9E,17E-Octadecadiene-7,15-dienoic acid [Unsaturated fatty acids [FA0103]]  | O18 isotope of 18-bromo-9Z,17E-Octadecadiene-7,15-dienoic acid [Unsaturated fatty acids [FA0103]] |
| 5361 | 0.000000 | -1.692 | 461.202845 | 462.210121 | 0.020421  | 2 | Cb  | C21H34O11    | Patrinoside   | Valerosidatum; Valerosidate  |   |
| 2804 | 0.020608 | -1.688 | 347.116953 | 348.124230 | 0.459549  | 1 | NM  | C18H21ClN2O3 | Compound VII; 5-(5-(6-Chloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-methylisoxazole  |  |   |
| 1730 | 0.064316 | -1.542 | 305.087764 | 306.095041 | 0.422086  | 2 | Pp  | C11H16N2O8   | O18 isotope of N-Acetyl-aspartyl-glutamate; NAAG  | O18 isotope of N-Acetylasparylglutamic acid (see KEGG C12270); 2-[(2-acetamido-3-carboxy-propanoyl)amino]pentanedioic acid [carboxylic acid] |   |
| 4335 | 0.009150 | -1.527 | 405.119098 | 406.126375 | -0.018591 | 7 | Ph  | C20H22O9     | Astringin   | Trichocarpin   | Anadanthoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                               |
| 1197 | 0.060528 | -1.524 | 274.093187 | 275.100463 | -0.141722 | 2 | AmS | C11H17NO7    | Cardiospermin   | Sarmentosin; 2-Butenenitrile,4-( $\beta$ -D-glucopyranosyloxy)-2-(hydroxymethyl)-,(E)-   |   |
| 254  | 0.002153 | -1.485 | 215.032742 | 216.040018 | 0.600053  | 1 | Cb  | C5H13O7P     | 2-C-Methyl-D-erythritol 4-phosphate   |  |   |

|      |          |        |            |            |           |   |    |           |  |   |  |
|------|----------|--------|------------|------------|-----------|---|----|-----------|--|---|--|
| 3851 | 0.043273 | -1.480 | 385.077611 | 386.084888 | -0.061436 | 1 | Ph | C16H18O11 | O-Feruloylgalactarate; O-Feruloylgalactaric acid; 2'-(E)-O-Feruloylgalactaric acid   |   |  |
| 3918 | 0.019872 | -1.461 | 387.129645 | 388.136921 | -0.066108 | 5 | Cb | C17H24O10 | Secologanin; (-)-Secologanin   | Geniposide  | Verbenalin; Cornin (glycoside)   |
| 3972 | 0.063208 | -1.458 | 389.181684 | 390.188961 | -0.055764 | 1 | Lp | C18H30O9  | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11-β-D-glucoside; {(1R,2R)-2-[4-(β-D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]] |   |  |
| 199  | 0.009689 | -1.402 | 205.035328 | 206.042604 | -0.236504 | 7 | Ph | C7H10O7   | (R)-2-Hydroxybutane-1,2,4-tricarboxylate; Homocitrate; Homocitric acid; 3-Hydroxy-3-carboxyadipic acid; (R)-2-Hydroxy-1,2,4-butanetricarboxylic acid           | 2-Methylcitrate; 2-Hydroxybutane-1,2,3-tricarboxylate; (2R,3S)-2-Hydroxybutane-1,2,3-tricarboxylate | (2S,3R)-3-Hydroxybutane-1,2,3-tricarboxylate; Methylisocitrate; Methylisocitric acid |
| 631  | 0.027726 | -1.267 | 261.007409 | 262.014685 | -0.147911 | 1 | Ph | C9H10O7S  | Homovanillic acid sulfate (see KEGG C05582) [alkyl aryl ether]   |   |  |
| 3963 | 0.039111 | -1.216 | 389.108911 | 390.116188 | -0.061532 | 2 | Ph | C16H22O11 | Monotropein  | Monotropein (see KEGG C09788) [C10 isoprenoids (monoterpenes) [PR0102]]                             |  |
| 2668 | 0.037964 | -1.101 | 343.067029 | 344.074305 | -0.120136 | 1 | Ph | C14H16O10 | Theogallin   |   |  |
| 2127 | 0.067159 | -0.433 | 321.134320 | 322.141596 | -0.131584 | 2 | Ph | C17H22O6  | Tetraneurin A  | epi-Tulipinolide diepoxide  |  |
| 1219 | 0.042524 | -0.349 | 275.092466 | 276.099742 | -0.114667 | 5 | Ph | C15H16O5  | Lactucin   | Vernolepin  | Vernomenin   |

**b) List of 33 identified WS *Np* vs NI (non-inoculated as control) from the significant 157 *m/z* at time B** selected with T-test (FDR=0.05 and S0=0). Total 33 functional category counts: Ph:12; Lp:5; Cb:12; Pp:0; AmS:0; Nu:0; NM:4.

| ID   | T-test<br><i>p-value</i> | WS<br><i>Np-NI</i> | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula  | Identifications  |  |  |
|------|--------------------------|--------------------|------------|------------|----------------|----|------|----------|--|--|--|
| 9    | 0.012805                 | +1.811             | 159.029884 | 160.037160 | -0.082384      | 14 | Lp   | C6H8O5   | 2-Oxoadipate; 2-Oxoadipic acid   | 3-Oxoadipate; 3-Oxoadipic acid; 3-Keto-adipate   | 3D-(3,5/4)-Trihydroxycyclohexane-1,2-dione; D-2,3-Diketo-4-deoxy-epi-inositol; (3R,4S,5R)-3,4,5-Trihydroxy-1,2-cyclohexanedione; 3,5/4-Trihydroxycyclohexa-1,2-dione |
| 66   | 0.002355                 | +1.802             | 177.040444 | 178.047720 | -0.101633      | 28 | Cb   | C6H10O6  | D-Glucono-1,5-lactone; Gluconic lactone; Gluconic acid lactone; 1,5-Gluconolactone; delta-Gluconolactone; D-Gluconolactone; Gluconolactone | 2-Dehydro-3-deoxy-D-gluconate; 2-Keto-3-deoxy-D-gluconate                                      | 5-Dehydro-D-fructose   |
| 1191 | 0.000000                 | +1.674             | 273.170718 | 274.177995 | -0.106789      | 2  | Lp   | C14H26O5 | 3-Hydroxytetradecanedioic acid; 3-hydroxy-tetradecanedioic acid [secondary alcohol]  | 3-hydroxy-tetradecanedioic acid; 3-hydroxy-tetradecanedioic acid [Dicarboxylic acids [FA0117]] |  |

|      |          |        |            |            |           |    |    |              |  |  |   |
|------|----------|--------|------------|------------|-----------|----|----|--------------|--|--|---|
| 8272 | 0.054397 | +1.081 | 697.481468 | 698.488745 | 0.127128  | 14 | Lp | C39H71O8P    | PA(14:1(9Z)/22:2(13Z,16Z)); 1-(9Z-tetradecenoyl)-2-(13Z,16Z-docosadienoyl)-glycero-3-phosphate [Diacylglycerophosphates [GP1001]]                        | PA(16:1(9Z)/20:2(11Z,14Z)); 1-(9Z-hexadecenoyl)-2-(11Z,14Z-eicosadienoyl)-glycero-3-phosphate [Diacylglycerophosphates [GP1001]]                         | PA(17:2(9Z,12Z)/19:1(9Z)); 1-(9Z,12Z-heptadecadienoyl)-2-(9Z-nonadecenoyl)-glycero-3-phosphate [Diacylglycerophosphates [GP1001]] |
| 631  | 0.002411 | -2.932 | 261.007409 | 262.014685 | -0.147911 | 1  | Ph | C9H10O7S     | Homovanillic acid sulfate (see KEGG C05582) [alkyl aryl ether ]  |  |   |
| 2804 | 0.005229 | -2.512 | 347.116953 | 348.124230 | 0.459549  | 1  | NM | C18H21ClN2O3 | Compound VII; 5-(5-(6-Chloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-methylisoxazole   |  |   |
| 6424 | 0.013195 | -2.455 | 523.145770 | 524.153046 | 0.105903  | 1  | Ph | C24H28O13    | Barbatoflavan [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |  |   |
| 2668 | 0.047706 | -2.182 | 343.067029 | 344.074305 | -0.120136 | 1  | Ph | C14H16O10    | Theogallin   |  |   |
| 1635 | 0.000450 | -2.136 | 301.056465 | 302.063741 | 0.451381  | 1  | NM | C16H13ClN2O2 | Cl37 isotope of 3-(4-Chloro-benzyl)-5-(2-methoxy-phenyl)-[1,2,4]oxadiazole   |  |   |
| 3594 | 0.000056 | -2.029 | 375.166033 | 376.173310 | 0.410054  | 1  | NM | C21H27ClN2O2 | Cl37 isotope of Hydroxyzine  |  |   |
| 517  | 0.015029 | -1.987 | 249.080184 | 250.087460 | -0.138795 | 2  | Lp | C10H18O5S    | 2-(5'-Methylthio)pentylmalic acid; 2-(5'-Methylthio)pentylmalate   | 3-(5'-Methylthio)pentylmalic acid; 3-(5'-Methylthio)pentylmalate   |   |
| 1194 | 0.007014 | -1.939 | 274.056804 | 275.064080 | -0.131780 | 1  | Ph | C10H13NO8    | 3-β-D-Glucopyranuronosyloxy-5-methylisoxazole  |  |   |
| 7463 | 0.004680 | -1.736 | 609.188462 | 610.195738 | 0.997565  | 1  | Ph | C34H30N2O9   | Atalanine  |  |   |
| 3500 | 0.000835 | -1.727 | 371.134722 | 372.141998 | -0.092343 | 1  | Ph | C17H24O9     | Syringin; Eleutheroside B  |  |   |
| 3454 | 0.003527 | -1.708 | 369.082692 | 370.089969 | -0.075560 | 1  | Ph | C16H18O10    | Fraxin   |  |   |
| 2222 | 0.039798 | -1.654 | 325.113981 | 326.121258 | -0.120525 | 6  | Cb | C12H22O10    | α-L-Fucosyl-1,2-β-D-galactoside; Glycoprotein α-L-fucosyl-(1,2)-D-galactose; Glycolipid α-L-fucosyl-1,2-β-D-galactose; α-L-Fucosyl-(1->2)-D-galactosyl-R | 2-O-α-L-Rhamnopyranosyl-D-glucopyranose; Neohesperidose  | Robinobiose   |
| 3101 | 0.013537 | -1.646 | 357.119069 | 358.126345 | -0.103262 | 3  | Cb | C16H22O9     | Tarennoside  | 10-Deoxygeniposidic acid   | Sweroside   |
| 2389 | 0.052927 | -1.636 | 331.176183 | 332.183459 | -0.132727 | 2  | Lp | C16H28O7     | (2S,3S)-2-Hydroxytridecane-1,2,3-tricarboxylate  | (2S,3S)-2-hydroxytridecane-1,2,3-tricarboxylic acid (see KEGG C04655); (2S,3S)-2-hydroxytridecane-1,2,3-tricarboxylic acid [Dicarboxylic acids [FA0117]] |   |
| 2224 | 0.002050 | -1.630 | 325.129232 | 326.136508 | -0.138273 | 1  | NM | C16H22O7     | Hinokitiol glucoside; β-Thujaplicin 2-O-β-D-glucoside  |  |   |
| 2373 | 0.013486 | -1.628 | 331.067028 | 332.074304 | -0.128768 | 1  | Cb | C13H16O10    | 1-O-Galloyl-β-D-glucose; 1-Galloyl-β-glucose; β-Glucogallin; 1-Galloyl-β-D-glucose   |  |   |
| 2074 | 0.027394 | -1.610 | 319.139804 | 320.147080 | -0.116812 | 2  | Cb | C14H24O8     | Valproic acid glucuronide (see KEGG C03033); 3,4,5-trihydroxy-6-(2-  | Octanoylglucuronide (see KEGG C03033) [secondary alcohol]  |   |

|      |          |        |            |            |           |    |    |           |   |   |   |
|------|----------|--------|------------|------------|-----------|----|----|-----------|---|---|---|
| 4335 | 0.004527 | -1.559 | 405.119098 | 406.126375 | -0.018591 | 7  | Ph | C20H22O9  | propylpentanoyloxy)oxane-2-carboxylic acid [secondary alcohol]<br>Astringin                                       | Trichocarpin  | Anadanthoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                               |
| 3591 | 0.010757 | -1.521 | 375.129648 | 376.136925 | -0.059642 | 3  | Ph | C16H24O10 | Loganate; Loganic acid  | 7-Epiloganic acid   |   |
| 5934 | 0.013027 | -1.485 | 493.098797 | 494.106073 | 0.065861  | 31 | Ph | C22H22O13 | Pleurostimin 7-glucoside; 5,6,7,3',4'-Pentahydroxy-8-methoxyflavone 7-glucoside [Flavones and Flavanols [PK1211]] | Laricitrin 3-galactoside [Flavones and Flavanols [PK1211]]  | Laricitrin 3-glucoside [Flavones and Flavanols [PK1211]]  |
| 2920 | 0.008095 | -1.456 | 351.056857 | 352.064133 | -0.122128 | 2  | Cb | C12H16O12 | 4-(4-Deoxy-β-D-gluc-4-enuronosyl)-D-galacturonate   | 4-(4-Deoxy-α-D-gluc-4-enuronosyl)-D-galacturonate; 4-(4-Deoxy-α-D-galact-4-enuronosyl)-D-galacturonate; Unsaturated digalacturonate |   |
| 3977 | 0.001828 | -1.236 | 389.218068 | 390.225344 | -0.061128 | 2  | Cb | C19H34O8  | Rehmaionoside A   | Rehmaionoside B   |   |
| 7699 | 0.012660 | -1.208 | 633.073451 | 634.080728 | 0.180016  | 1  | Ph | C27H22O18 | Corilagin   |   |   |
| 3540 | 0.039047 | -1.067 | 373.113993 | 374.121269 | -0.074217 | 4  | Ph | C16H22O10 | Secologanate  | Swertiamarin  | Geniposidic acid  |
| 1864 | 0.039079 | -1.066 | 311.098334 | 312.105610 | -0.117249 | 6  | Cb | C11H20O10 | Vicianose; O-α-L-Arabinopyranosyl-(1-6)-D-glucopyranose   | Arabino-galactose   | 6-O-β-D-Xylopyranosyl-D-glucose; Primeverose  |
| 5732 | 0.053416 | -1.039 | 483.078040 | 484.085316 | 0.022519  | 1  | Cb | C20H20O14 | 1-O,6-O-Digalloyl-β-D-glucose   |   |   |
| 2811 | 0.043362 | -1.020 | 347.171101 | 348.178377 | -0.116791 | 1  | Cb | C16H28O8  | Schizonepetoside E  |   |   |
| 3926 | 0.002504 | -0.928 | 387.202414 | 388.209691 | -0.070880 | 5  | Cb | C19H32O8  | Rehmaionoside C   | methyl 9-hydroperoxy-10,12,13,15-bisepidioxy-16E-octadecenoate [Hydroperoxy fatty acids [FA0104]]                                   | methyl 10,12,13,15-bisepidioxy-16-hydroperoxy-8E-octadecenoate [Hydroperoxy fatty acids [FA0104]] |
| 1590 | 0.028032 | -0.798 | 299.113594 | 300.120870 | -0.109047 | 1  | Cb | C14H20O7  | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside                                      |   |   |

**c) List of TOP 41 compounds identified HS *Np* vs NI (non-inoculated as control) from the significant 583 *m/z* at time A** selected with T-test (FDR=0.01 and S0=1). Total: 131 annotated compounds (128-/3+): Total 131 structure category counts: Ph:16; Lp:20; Cb:2; Pp:0; AmS:1; Nu:0; NM:2. The most specific compounds selected with higher stringency (FDR=0.08 and S0=1) are indicated in bolded lines. TOPs 41 functional category counts: Ph:66; Lp:18; Cb:33; Pp:3; AmS:3; Nu:1; NM:7.

| ID   | T-test<br><i>p-value</i> | HS<br><i>Np-NI</i> | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula   | Identifications   |   |  |
|------|--------------------------|--------------------|------------|------------|----------------|----|------|-----------|---|---|--|
| 93   | 0.000183                 | +1.920             | 181.050603 | 182.057880 | -0.160171      | 17 | Ph   | C9H10O4   | 3-(4-Hydroxyphenyl)lactate; 4-Hydroxyphenyllactate; p-Hydroxyphenyllactate; 2-Hydroxy-3-(4-hydroxyphenyl)propanoate | (R)-3-(4-Hydroxyphenyl)lactate                      | 3-(2,3-Dihydroxyphenyl)propanoate; 2,3-Dihydroxyphenylpropanoate |
| 8177 | 0.010349                 | +1.845             | 685.481404 | 686.488680 | 0.035433       | 14 | Lp   | C38H71O8P | PA(13:0/22:2(13Z,16Z)); 1-tridecanoyl-2-(13Z,16Z-   | PA(15:0/20:2(11Z,14Z)); 1-pentadecanoyl-2-(11Z,14Z- | PA(15:1(9Z)/20:1(11Z)); 1-(9Z-pentadecenoyl)-2-(11Z-             |

|      |          |        |            |            |           |    |     |              |   |  |   |
|------|----------|--------|------------|------------|-----------|----|-----|--------------|---|--|---|
|      |          |        |            |            |           |    |     |              | docosadienoyl)-glycero-3-phosphate<br>[Diacylglycerophosphates<br>[GP1001]]                                       | eicosadienoyl)-glycero-3-phosphate<br>[Diacylglycerophosphates<br>[GP1001]]        | eicosenoyl)-glycero-3-phosphate<br>[Diacylglycerophosphates<br>[GP1001]]                  |
| 2579 | 0.001213 | -2.455 | 339.129643 | 340.136919 | -0.081507 | 1  | Cb  | C13H24O10    | Methyl-2- $\alpha$ -L-fucopyranosyl- $\beta$ -D-galactoside   |  |   |
| 1677 | 0.002185 | -2.438 | 303.050993 | 304.058270 | -0.108829 | 7  | Ph  | C15H12O7     | Taxifolin; Dihydroquercetin; (+)-Dihydroquercetin; (+)-Taxifolin; <i>trans</i> -Dihydroquercetin                  | Pentahydroxyflavanone; Dihydrotricetin   | <i>cis</i> -Dihydroquercetin  |
| 2347 | 0.044133 | -2.354 | 330.119400 | 331.126676 | -0.122722 | 1  | AmS | C14H21NO8    | 5'-O- $\beta$ -D-Glucosylpyridoxine   |  |   |
| 5361 | 0.034364 | -2.318 | 461.202845 | 462.210121 | 0.020421  | 2  | Cb  | C21H34O11    | Patrinoside   | Valerosidatum; Valerosidate  |   |
| 1158 | 0.011871 | -2.272 | 271.061181 | 272.068458 | -0.058348 | 37 | Ph  | C15H12O5     | Naringenin; 4',5,7-Trihydroxyflavanone  | (6aS,11aS)-3,6a,9-Trihydroxypterocarpan; 3,6,9-Trihydroxypterocarpan; (-)-Glycinol | Licodione   |
| 4814 | 0.004251 | -2.258 | 431.155905 | 432.163181 | 0.044900  | 1  | Cb  | C19H28O11    | Zizybeoside I   |  |   |
| 11   | 0.007951 | -2.180 | 161.045532 | 162.052809 | -0.091525 | 30 | Cb  | C6H10O5      | Lichenin; Lichenan  | (R)-3,3-Dimethylmalate   | 3-Ethylmalate   |
| 65   | 0.013675 | -2.147 | 177.019326 | 178.026603 | -0.033633 | 4  | Ph  | C9H6O4       | 7,8-Dihydroxycoumarin; Daphnetin  | 5,7-Dihydroxychromone  | Esculetin; Aesculetin   |
| 5431 | 0.008132 | -2.144 | 465.103882 | 466.111159 | 0.069908  | 6  | Ph  | C21H22O12    | Quercetin 7-O-glucoside   | Plantagoside   | 3,4,5,2',4',6'-Hexahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]] |
| 51   | 0.011332 | -2.107 | 173.009145 | 174.016422 | -0.092226 | 6  | Ph  | C6H6O6       | <i>cis</i> -Aconitate; <i>cis</i> -Aconitic acid  | <i>trans</i> -Aconitate; <i>trans</i> -Aconitic acid                               | Dehydroascorbate; Dehydroascorbic acid; L-Dehydroascorbate; L-Dehydroascorbic acid        |
| 2893 | 0.000054 | -2.104 | 350.306446 | 351.313723 | -0.019531 | 1  | Lp  | C22H41NO2    | Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids) [FA0804]] |  |   |
| 928  | 0.013838 | -2.092 | 263.128852 | 264.136128 | -0.116493 | 33 | Ph  | C15H20O4     | Abcisate; Absciscic acid; (+)-Absciscic acid  | Amaralin   | Artemisiifolin  |
| 4627 | 0.002328 | -2.091 | 421.114055 | 422.121331 | 0.081091  | 7  | Ph  | C20H22O10    | Catechin 7-O- $\beta$ -D-xyloside   | Plicatic acid  | Catechin 7-O- $\beta$ -D-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 4027 | 0.005346 | -2.088 | 391.160971 | 392.168248 | 0.453424  | 1  | NM  | C21H27ClN2O3 | Cl37 isotope of Compound II(R/S); 5-(7-(6-Chloro-4-(5-  |  |   |

|             |          |               |                   |                   |                  |           |           |                  |  |  |   |
|-------------|----------|---------------|-------------------|-------------------|------------------|-----------|-----------|------------------|--|--|---|
| 3049        | 0.023822 | -2.081        | 355.103413        | 356.110690        | -0.119119        | 3         | Ph        | C16H20O9         | <i>hydro-4-methyl-2-oxazolyl)phenoxy)heptyl)-3-methylisoxazole</i><br>Gentiopicrin; Gentiopicroside  | 1-O-Feruloyl-β-D-glucose; 1-Feruloyl-D-glucose   | Gentiopicrin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]  |
| 2277        | 0.020385 | -2.081        | 327.163515        | 328.170791        | -0.119791        | 1         | Lp        | C17H28O4S        | Steryl sulfate   |  |   |
| 4847        | 0.021465 | -2.075        | 433.114041        | 434.121318        | 0.048061         | 32        | Ph        | C21H22O10        | Naringenin 7-O-β-D-glucoside; Prunin   | Phlorizin chalcone; Chalcone 2'-O-glucoside  | 2',4,4',6'-Tetrahydrochalcone 4'-O-glucoside; THC 4'-glucoside  |
| 2506        | 0.012550 | -2.069        | 336.129968        | 337.137244        | -0.110462        | 3         | AmS       | C13H23NO9        | Streptobiosamine   |  |   |
| 3153        | 0.016177 | -2.052        | 359.134719        | 360.141996        | -0.102120        | 2         | Ph        | C16H24O9         | 7-Deoxyloganate  | 8-Epideoxyloganic acid   |   |
| <b>5064</b> | 0.001825 | <b>-2.048</b> | <b>445.190118</b> | <b>446.197394</b> | <b>-0.100135</b> | <b>1</b>  | <b>Lp</b> | <b>C21H34O8S</b> | <b>Ptilosteroid A; 5α-pregn-20-en-2β,3β,4β,15β,16β-pentol 2-sulfate [C21 steroids (gluco/mineralocorticoids, progestogens) and derivatives [ST0203]]</b> |  |   |
| 3922        | 0.003605 | -2.042        | 387.166034        | 388.173310        | -0.057526        | 2         | Lp        | C18H28O9         | Tuberonic acid glucoside   | Tuberonic acid glucoside (see KEGG C08558); (1R,2S)-3-oxo-2-(5'-O-β-D-glucopyranosyloxy-2''Z-pentenyl)-cyclopentaneacetic acid [Fatty acyl glycosides of mono- and disaccharides [FA1301]] |   |
| 5133        | 0.007019 | -2.027        | 449.108952        | 450.116229        | 0.038519         | 25        | Ph        | C21H22O11        | Neoastilbin; (2S,3S)-Taxifolin 3-rhamnoside  | 2',3,4,4',6'-Peptahydrochalcone 4'-O-glucoside; PHC 4'-O-glucoside   | Astilbin  |
| <b>80</b>   | 0.000435 | <b>-1.984</b> | <b>179.056091</b> | <b>180.063368</b> | <b>-0.114407</b> | <b>69</b> | <b>Cb</b> | <b>C6H12O6</b>   | <b>D-Glucose; Grape sugar; Dextrose</b>  | <b>D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose</b>   | <b>D-Galactose</b>  |
| 4511        | 0.005081 | -1.967        | 413.218120        | 414.225397        | 0.069673         | 3         | Lp        | C21H34O8         | methyl 5-hydroperoxy-6,8,9,11-bisepidioxy-12,14-eicosadienoate [Hydroperoxy fatty acids [FA0104]]  | methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]]   | methyl 6,8-epidioxy-5,15-dihydroperoxy-9,11,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]]                 |
| 8870        | 0.005483 | -1.918        | 833.518322        | 834.525598        | -0.277170        | 23        | Lp        | C43H79O13P       | PI(16:0/18:2(9Z,12Z)) (see KEGG C00626); 1-hexadecanoyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoinositol [secondary alcohol]                      | PI(16:1(9Z)/18:1(11Z)) (see KEGG C00626); 1-(9Z-hexadecenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphoinositol [secondary alcohol]  | PI(16:1(9Z)/18:1(9Z)) (see KEGG C00626); 1-(9Z-hexadecenoyl)-2-(9Z-octadecenoyl)-sn-glycero-3-phosphoinositol [secondary alcohol] |
| <b>7603</b> | 0.000011 | <b>-1.906</b> | <b>623.255794</b> | <b>624.263070</b> | <b>0.216834</b>  | <b>1</b>  | <b>Cb</b> | <b>C27H44O16</b> | <b>Kanokoside D</b>  |  |   |



|      |          |        |            |            |           |    |    |           |  |  |   |
|------|----------|--------|------------|------------|-----------|----|----|-----------|--|--|---|
| 6367 | 0.010584 | -1.879 | 519.187226 | 520.194503 | 0.078545  | 2  | Ph | C26H32O11 | Brusatol   | (-)-Pinoresinol glucoside  |   |
| 1303 | 0.006311 | -1.835 | 281.139425 | 282.146702 | -0.078970 | 6  | Ph | C15H22O5  | Hymenoxon  | Qing Hau Sau; Artemisinin  | Dihydrophaseic acid; (-)-Dihydrophaseic acid  |
| 3972 | 0.001427 | -1.830 | 389.181684 | 390.188961 | -0.055764 |    | Lp | C18H30O9  | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11-β-D-glucoside; {(1R,2R)-2-[4-(β-D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]] |  |   |
| 4021 | 0.007441 | -1.828 | 391.124562 | 392.131838 | -0.059958 | 1  | Ph | C16H24O11 | Shanzhiside  |  |   |
| 2745 | 0.009898 | -1.822 | 345.119057 | 346.126333 | -0.142585 | 4  | Lp | C15H22O9  | Aucubin  | Deutzioside  | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]                                     |
| 449  | 0.009663 | -1.808 | 243.066250 | 244.073527 | -0.131492 | 10 | Ph | C14H12O4  | 3,3',4'5-Tetrahydroxystilbene; Piceatannol   | Wyerone acid   | Eriobofuran   |
| 6042 | 0.000000 | -1.751 | 499.291301 | 500.298577 | 0.088261  | 1  | NM | C26H44O9  | Mupirocin  |  |   |
| 3508 | 0.001932 | -1.751 | 371.243903 | 372.251179 | -0.025932 | 5  | Lp | C20H36O6  | 8,8a-Deoxyoleandolide  | 19(R)-hydroxy-PGF1α; 9S,11R,15S,19R-tetrahydroxy-13E-prostaenoic acid [Prostaglandins [FA0301]]          | 13,14-dihydro-19(R)-hydroxyPGE1; 9-oxo-11R,15S,19R-trihydroxy-prostanoic acid [Prostaglandins [FA0301]] |
| 4022 | 0.007294 | -1.742 | 391.128449 | 392.135726 | 0.030165  | 5  | Ph | C20H22O8  | O18 isotope of Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside   | O18 isotope of Populin   | O18 isotope of Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]         |
| 5691 | 0.006981 | -1.739 | 481.098785 | 482.106061 | 0.042399  | 1  | Ph | C21H22O13 | 3,4,2',3',4',6',α-Heptahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]]  |  |   |
| 4329 | 0.001465 | -1.712 | 405.082709 | 406.089985 | -0.028041 | 7  | Ph | C19H18O10 | Lancerin; 4-C-Glucosyl-1,3,7-trihydroxyxanthone  | 5,7,3',5'-Tetrahydroxy-3,6,8,4'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]                    | 5,7,3',4'-Tetrahydroxy-3,6,8,5'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]                   |
| 4594 | 0.004359 | -1.690 | 419.134784 | 420.142061 | 0.067492  | 10 | Ph | C21H24O9  | Melampodin A   | Glycyphyllin; Phloretin 2'-O-rhamnoside  | Isorhapontin  |
| 2276 | 0.002669 | -1.688 | 327.144911 | 328.152188 | -0.047159 | 3  | Ph | C16H24O7  | Rhododendrin   | Tetranor-PGEM; 11R-hydroxy-9,15-dioxo-2,3,4,5-tetranor-prostan-1,20-dioic acid [Prostaglandins [FA0301]] | Prostaglandin M; 7R-hydroxy-5,11-dioxotetranorprostane-1,16-dioic acid [Prostaglandins [FA0301]]        |



**d) List of TOP 39 identified WSHS *Np* vs NI (non-inoculated as control) from the significant 882 *m/z* at time A** selected with T-test (FDR=0.0001 and S0=3). Total: 187 annotated compounds (181-/6+): Total 187 functional category counts: Ph:102; Lp:25; Cb:37; Pp:6; AmS:6; Nu:1; NM:10. TOPs 39 functional category counts: Ph:19; Lp:5; Cb:9; Pp:2; AmS:0; Nu:0; NM:4.

| ID   | T-test<br><i>p-value</i> | WSHS<br><i>Np-NI</i> | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula    | Identifications  |   |   |
|------|--------------------------|----------------------|------------|------------|----------------|----|------|------------|--|---|---|
| 502  | 0.00252                  | +3.023               | 247.047368 | 248.054644 | -0.228030      | 1  | Lp   | C6H15O8P   | O18 isotope of<br>Glycerophosphoglycerol   |   |   |
| 2474 | 0.008504                 | +2.930               | 335.063417 | 336.070694 | -0.151416      | 5  | Cb   | C9H19O11P  | O18 isotope of <i>sn</i> -glycero-3-<br>Phospho-1-inositol; 1-( <i>sn</i> -<br>glycero-3-Phospho)-1D-myo-<br>inositol  | O18 isotope of 2-( $\alpha$ -D-<br>Galactosyl)- <i>sn</i> -glycerol 3-<br>phosphate                           | O18 isotope of $\alpha$ -D-Galactosyl-<br>(1,1')- <i>sn</i> -glycerol 3-phosphate; 1-<br>O- $\alpha$ -D-Galactosyl- <i>sn</i> -glycerol 3-<br>phosphate |
| 7699 | 0.000388                 | -2.997               | 633.073451 | 634.080728 | 0.180016       | 1  | Ph   | C27H22O18  | Corilagin  |   |   |
| 5781 | 0.001096                 | -2.818               | 485.108961 | 486.116238 | 0.054370       | 2  | Ph   | C24H22O11  | Flavonol 3-O-(6-O-malonyl- $\beta$ -D-<br>glucoside)   | Epigallocatechin 3-O-(3,5-di-O-<br>methylgallate) [Flavans,<br>Flavanols and<br>Leucoanthocyanidins [PK1202]] |   |
| 4393 | 0.014393                 | -2.795               | 407.171139 | 408.178415 | -0.005805      | 2  | Ph   | C21H28O8   | Vernoflexuoside  |   |   |
| 4717 | 0.032512                 | -2.791               | 425.087827 | 426.095103 | 0.049636       | 2  | Ph   | C22H18O9   | Epiafzelechin 3-O-gallate<br>[Flavans, Flavanols and<br>Leucoanthocyanidins [PK1202]]  | Epigallocatechin 3-O-(4-<br>hydroxybenzoate) [Flavans,<br>Flavanols and<br>Leucoanthocyanidins [PK1202]]      |   |
| 1087 | 0.000557                 | -2.766               | 265.144542 | 266.151818 | 0.677275       | 6  | Pp   | C14H20N2O3 | O18 isotope of Subaphyllin;<br><i>Feruloylputrescine</i>   | <i>Mukaadial</i>  | <i>Rugosal</i>  |
| 4985 | 0.015744                 | -2.728               | 441.082837 | 442.090114 | 0.264769       | 10 | Ph   | C22H18O10  | Robinetinidol 3-O-gallate<br>[Flavans, Flavanols and<br>Leucoanthocyanidins [PK1202]]  | ent-Robinetinidol 3-O-gallate<br>[Flavans, Flavanols and<br>Leucoanthocyanidins [PK1202]]                     | Catechin 3-O-gallate [Flavans,<br>Flavanols and<br>Leucoanthocyanidins [PK1202]]  |
| 5457 | 0.022641                 | -2.645               | 467.098394 | 468.105671 | 0.051411       | 2  | Ph   | C24H20O10  | Epigallocatechin 3-O-caffeate<br>[Flavans, Flavanols and<br>Leucoanthocyanidins [PK1202]]  | Apocynin A [Flavans, Flavanols<br>and Leucoanthocyanidins<br>[PK1202]]  |   |
| 291  | 0.007195                 | -2.619               | 221.066628 | 222.073904 | -0.220142      | 4  | Cb   | C8H14O7    | 6-Acetyl-D-glucose   | 6-Acetyl- $\beta$ -D-galactoside  | Ethyl glucuronide;<br>(2S,3S,4S,5R)-6-ethoxy-3,4,5-<br>trihydroxyoxane-2-carboxylic<br>acid [acetal]<br>Robinobiose                                     |
| 2222 | 0.002763                 | -2.601               | 325.113981 | 326.121258 | -0.120525      | 6  | Cb   | C12H22O10  | $\alpha$ -L-Fucosyl-1,2- $\beta$ -D-galactoside;<br>Glycoprotein $\alpha$ -L-fucosyl-(1,2)-<br>D-galactose; Glycolipid $\alpha$ -L-<br>fucosyl-1,2- $\beta$ -D-galactose; $\alpha$ -L-<br>Fucosyl-(1 $\rightarrow$ 2)-D-galactosyl-R | 2-O- $\alpha$ -L-Rhamnopyranosyl-D-<br>glucopyranose; Neohesperidose  |   |
| 1130 | 0.000774                 | -2.584               | 269.045564 | 270.052841 | 0.064429       | 42 | Ph   | C15H10O5   | Apigenin; 4',5,7-<br>Trihydroxyflavone; 5,7,4'-<br>Trihydroxyflavone   | 2'-Hydroxydaidzein  | Genistein; 5,7,4'-<br>Trihydroxyisoflavone  |
| 1622 | 0.011095                 | -2.589               | 300.998953 | 302.006230 | -0.124868      | 2  | Ph   | C14H6O8    | Ellagic acid   | Ellagic acid (see KEGG C10788)<br>[phenol or hydroxyhetarene]   |   |
| 1135 | 0.002842                 | -2.546               | 269.081904 | 270.089181 | -0.104475      | 35 | Lp   | C16H14O4   | (+)-Medicarpin; 3-Hydroxy-9-<br>methoxypterocarpan   | Vignafuran  | Alloimperatorin   |
| 4289 | 0.007513                 | -2.539               | 403.124570 | 404.131847 | -0.036646      | 2  | Ph   | C17H24O11  | Gardenoside  | Scandoside methyl ester   |   |

|      |          |        |            |            |           |    |    |              |   |   |  |
|------|----------|--------|------------|------------|-----------|----|----|--------------|---|---|--|
| 233  | 0.008054 | -2.480 | 211.133944 | 212.141220 | -0.115861 | 15 | Lp | C12H20O3     | Cucurbic acid   | Putaminoxin   | Traumatin; (10E)-12-Oxododecenoic acid   |
| 1843 | 0.000007 | -2.474 | 310.093192 | 311.100468 | -0.108516 | 4  | Ph | C14H17NO7    | Taxiphyllin; (R)-4-Hydroxymandelonitrile $\beta$ -D-glucoside   | Dhurrin; (S)-4-Hydroxymandelonitrile $\beta$ -D-glucoside   | p-Glucosyloxymandelonitrile  |
| 5778 | 0.000002 | -2.458 | 485.082492 | 486.089768 | 0.446498  | 1  | Cb | C20H20O14    | O18 isotope of 1-O,6-O-Digalloyl- $\beta$ -D-glucose  |   |  |
| 3121 | 0.005300 | -2.451 | 358.114330 | 359.121606 | -0.070431 | 1  | Pp | C15H21NO9    | Epinephrine glucuronide (see KEGG C03033); (2S,3S,4S,6S)-3,4,5,5-tetrahydroxy-3-[(1R)-1-hydroxy-2-methylaminoethyl]-6-(phenoxy)oxane-2-carboxylic acid [acetal] |   |  |
| 4441 | 0.001599 | -2.412 | 409.150412 | 410.157688 | 0.014166  | 2  | Ph | C20H26O9     | Bruceine D  | C20H26O9  |  |
| 132  | 0.000032 | -2.410 | 191.034952 | 192.042228 | -0.159394 | 10 | Ph | C10H8O4      | Scopoletin  | Naphthazarin; 5,8-Dihydroxy-1,4-naphthoquinone  | 3,4-Dehydro-6-hydroxymellein   |
| 2684 | 0.000005 | -2.383 | 343.124543 | 344.131820 | -0.121434 | 4  | Cb | C12H24O11    | Melibiiitol; 6-O- $\alpha$ -D-Galactosyl-D-glucitol   | Clusianose  | Maltitol; 4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol [acetal] |
| 3969 | 0.007159 | -2.378 | 389.145306 | 390.152582 | 0.415595  | 4  | NM | C21H25ClN2O3 | Cl37 isotope of Cetirizine  | Cl37 isotope of Cetirizine (see KEGG C07778); 2-[2-[4-[(4-chlorophenyl)-phenyl-methyl]piperazin-1-yl]ethoxy]acetic acid [dialkyl ether] | Loganin  |
| 3099 | 0.000347 | -2.369 | 357.107697 | 358.114974 | -0.013607 | 4  | Ph | C16H20O9     | O18 isotope of Gentiopicrocin; Gentiopicroside  | O18 isotope of 1-O-Feruloyl- $\beta$ -D-glucose; 1-Feruloyl-D-glucose   | O18 isotope of Gentiopicrocin (see KEGG C09782) [C10 isoprenoids (monoterpenes)] [PR0102]]   |
| 6042 | 0.000214 | -2.337 | 499.291301 | 500.298577 | 0.088261  | 1  | NM | C26H44O9     | Mupirocin   |   |  |
| 4635 | 0.002498 | -2.320 | 421.186827 | 422.194104 | 0.084740  | 4  | Ph | C22H30O8     | Valtratum; Valtrate   | Isovaltrate   | Picrasin F   |
| 3088 | 0.001545 | -2.319 | 357.061579 | 358.068856 | -0.032332 | 10 | Ph | C18H14O8     | 5,3'-Dihydroxy-4',5'-dimethoxy-6,7-methylenedioxyisoflavone [Isoflavonoids [PK1205]]  | Dalpalatin [Isoflavonoids [PK1205]]   | Luteolin 7-lactate [Flavones and Flavonols [PK1211]]   |
| 6216 | 0.003172 | -2.313 | 511.218562 | 512.225838 | 0.149097  | 1  | Ph | C25H36O11    | gibberellin A2 O- $\beta$ -D-glucoside [C20 isoprenoids (diterpenes)] [PR0104]]   |   |  |
| 1138 | 0.001137 | -2.284 | 269.175813 | 270.183090 | -0.072009 | 1  | Lp | C15H26O4     | (10S)-Juvenile hormone III acid diol  |   |  |
| 2893 | 0.001210 | -2.258 | 350.306446 | 351.313723 | -0.019531 | 1  | Lp | C22H41NO2    | Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids)] [FA0804]]  |   |  |
| 4730 | 0.000106 | -2.237 | 425.181737 | 426.189014 | 0.073384  | 2  | Ph | C21H30O9     | Abscisic acid glucose ester; abscisic acid- $\beta$ -D-glucopyranosyl ester   | $\gamma$ -CEHC Glc; $\gamma$ -carboxyethyl-hydroxychroman $\beta$ -D-glucoside [Vitamin E [PR0202]]                                     |  |
| 11   | 0.000069 | -2.234 | 161.045532 | 162.052809 | -0.091525 | 30 | Cb | C6H10O5      | Lichenin; Lichenan  | (R)-3,3-Dimethylmalate  | 3-Ethylmalate  |
| 3918 | 0.000909 | -2.229 | 387.129645 | 388.136921 | -0.066108 | 5  | Cb | C17H24O10    | Secologanin; (-)-Secologanin  | Geniposide  | Verbenalin; Cornin (glycoside)   |

|      |          |        |            |            |           |   |    |            |  |  |  |
|------|----------|--------|------------|------------|-----------|---|----|------------|--|--|--|
| 306  | 0.000004 | -2.204 | 223.133928 | 224.141204 | -0.180408 | 8 | Ph | C13H20O3   | Vomifolioside; (6S,9R)-6-hydroxy-3-oxo- $\alpha$ -ionol              | (+/-)-6-Hydroxy-3-oxo- $\alpha$ -ionol   | Methyl jasmonate; (-)-Methyl jasmonate |
| 6299 | 0.000011 | -2.172 | 515.286219 | 516.293495 | 0.092665  | 2 | Lp | C26H44O10  | L-Olivosyl-oleandolide   | L-Olivosyl-oleandolide (see KEGG C11991) [Macrolides and lactone polyketides [PK04]] |  |
| 1869 | 0.000018 | -2.162 | 313.147866 | 314.155142 | 0.528679  | 1 | NM | C19H23ClN2 | Clomipramine   |  |  |
| 1252 | 0.000042 | -2.153 | 277.144506 | 278.151783 | -0.095744 | 7 | NM | C16H22O4   | 2-Ethylhexyl phthalate   | Dibutyl phthalate; Di-n-butyl phthalate; Dibutyl 1,2-benzenedicarboxylate            | Diisobutyl phthalate; DIBP             |
| 4597 | 0.000028 | -2.126 | 419.155889 | 420.163166 | 0.009385  | 2 | Ph | C18H28O11  | Lamioside  | Lamioside (see KEGG C11645) [C10 isoprenoids (monoterpenes) [PR0102]]                |  |
| 3598 | 0.000034 | -2.111 | 375.202440 | 376.209716 | -0.005151 | 1 | Cb | C18H32O8   | 2,3-di--hexanoyl- $\alpha$ -glucopyranose [Other acyl sugars [SL05]] |  |  |

## TABLES IDENTIFIED *Ds* COMPOUNDS

e) List of 25 identified “No abiotic stress” (NAS) *Ds* vs NI (non-inoculated as control) from the significant 135 *m/z* at time B selected with T-test (FDR=0.05 and S0=0).

Total 25 functional category counts: Ph:12; Lp:4; Cb:7; Pp:0; AmS:1; Nu:1; NM:0.

| ID   | T-test<br><i>p-value</i> | NAS<br><i>Ds-NI</i> | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula    | Identifications  |   |   |
|------|--------------------------|---------------------|------------|------------|----------------|----|------|------------|--|---|---|
| 7463 | 0.004622                 | -2.686              | 609.188462 | 610.195738 | 0.997565       | 1  | Ph   | C34H30N2O9 | Atalanine  |   |   |
| 3591 | 0.022328                 | -2.367              | 375.129648 | 376.136925 | -0.059642      | 3  | Ph   | C16H24O10  | Loganate; Loganic acid   | 7-Epiloganic acid   |   |
| 5540 | 0.019670                 | -2.302              | 472.146076 | 473.153353 | 0.058057       | 1  | Ph   | C20H27NO12 | Proteacin  |   |   |
| 3851 | 0.001480                 | -2.301              | 385.077611 | 386.084888 | -0.061436      | 1  | Ph   | C16H18O11  | O-Feruloylgalactarate; O-Feruloylgalactaric acid; 2'-(E)-O-Feruloylgalactaric acid                           |   |   |
| 2347 | 0.000273                 | -2.287              | 330.119400 | 331.126676 | -0.122722      | 1  | AmS  | C14H21NO8  | 5'-O- $\beta$ -D-Glucosylpyridoxine  |   |   |
| 3153 | 0.022575                 | -2.279              | 359.134719 | 360.141996 | -0.102120      | 2  | Ph   | C16H24O9   | 7-Deoxyloganate  | 8-Epideoxyloganic acid  |   |
| 1590 | 0.035859                 | -2.233              | 299.113594 | 300.120870 | -0.109047      | 1  | Cb   | C14H20O7   | Salidroside; p-Hydroxyphenethyl alcohol 1-O- $\beta$ -D-glucoside; Tyrosol glucoside                         |   |   |
| 2681 | 0.042487                 | -2.173              | 343.113128 | 344.120404 | -0.156273      | 45 | Cb   | C12H22O11  | O18 isotope of Sucrose; Cane sugar; Saccharose; 1- $\alpha$ -D-Glucopyranosyl-2- $\beta$ -D-fructofuranoside | O18 isotope of Cellobiose; 1- $\beta$ -D-Glucopyranosyl-4-D-glucopyranose | O18 isotope of Maltose; Malt sugar; $\alpha$ -D-Glucopyranosyl-(1->4)-D-glucopyranose |
| 2745 | 0.004061                 | -2.156              | 345.119057 | 346.126333 | -0.142585      | 4  | Lp   | C15H22O9   | Aucubin  | Deutzioside   | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]                   |
| 2614 | 0.027651                 | -1.971              | 341.108884 | 342.116161 | -0.149462      | 45 | Cb   | C12H22O11  | Sucrose; Cane sugar; Saccharose; 1- $\alpha$ -D-Glucopyranosyl-2- $\beta$ -D-fructofuranoside                | Cellobiose; 1- $\beta$ -D-Glucopyranosyl-4-D-glucopyranose                | Maltose; Malt sugar; $\alpha$ -D-Glucopyranosyl-(1->4)-D-glucopyranose                |

|      |          |        |            |            |           |    |    |            |   |  |   |
|------|----------|--------|------------|------------|-----------|----|----|------------|---|--|---|
| 3775 | 0.045960 | -1.871 | 382.100408 | 383.107685 | -0.072174 | 1  | Nu | C14H17N5O8 | Succinyladenosine; (2S)-2-[[9-<br>[(2S,3R,4S,5R)-3,4-dihydroxy-5-<br>(hydroxymethyl)oxolan-2-<br>yl]purin-6-yl]amino]butanedioic<br>acid [primary alcohol]  |  |   |
| 1864 | 0.018181 | -1.860 | 311.098334 | 312.105610 | -0.117249 | 6  | Cb | C11H20O10  | Vicianose; O- $\alpha$ -L-<br>Arabinopyranosyl-(1-6)-D-<br>glucopyranose  | Arabino-galactose  | 6-O- $\beta$ -D-Xylopyranosyl-D-<br>glucose; Primeverose  |
| 8272 | 0.003918 | -1.639 | 697.481468 | 698.488745 | 0.127128  | 14 | Lp | C39H71O8P  | PA(14:1(9Z)/22:2(13Z,16Z)); 1-<br>(9Z-tetradecenoyl)-2-(13Z,16Z-<br>docosadienoyl)-glycero-3-<br>phosphate<br>[Diacylglycerophosphates<br>[GP1001]]   | PA(16:1(9Z)/20:2(11Z,14Z)); 1-<br>(9Z-hexadecenoyl)-2-(11Z,14Z-<br>eicosadienoyl)-glycero-3-<br>phosphate<br>[Diacylglycerophosphates<br>[GP1001]]             | PA(17:2(9Z,12Z)/19:1(9Z)); 1-<br>(9Z,12Z-heptadecadienoyl)-2-<br>(9Z-nonadecenoyl)-glycero-3-<br>phosphate<br>[Diacylglycerophosphates<br>[GP1001]]       |
| 8293 | 0.021010 | -1.567 | 699.497125 | 700.504401 | 0.135904  | 20 | Lp | C39H73O8P  | PA(18:1(18:2(9Z,12Z)) (see<br>KEGG C00416); 1-octadecanoyl-<br>2-(9Z,12Z-octadecadienoyl)-sn-<br>glycero-3-phosphate [carboxylic<br>acid ester]   | PA(18:1(11Z)/18:1(11Z)) (see<br>KEGG C00416); 1,2-di(11Z-<br>octadecenoyl)-rac-glycero-3-<br>phosphate [carboxylic acid ester]                                 | PA(18:1(11Z)/18:1(9Z)) (see<br>KEGG C00416); 1-(11Z-<br>octadecenoyl)-2-(9Z-<br>octadecenoyl)-sn-glycero-3-<br>phosphate [carboxylic acid ester]          |
| 1194 | 0.036655 | -1.551 | 274.056804 | 275.064080 | -0.131780 | 1  | Ph | C10H13NO8  | 3- $\beta$ -D-Glucopyranuronosyloxy-5-<br>methylisoxazole   |  |   |
| 3101 | 0.018617 | -1.520 | 357.119069 | 358.126345 | -0.103262 | 3  | Cb | C16H22O9   | Tarennoside   | 10-Deoxygeniposidic acid   | Sweroside   |
| 414  | 0.005905 | -1.488 | 239.056069 | 240.063345 | -0.178947 | 1  | Ph | C11H12O6   | (1R,6R)-6-Hydroxy-2-<br>succinylcyclohexa-2,4-diene-1-<br>carboxylate; (1R,6R)-2-Succinyl-<br>6-hydroxy-2,4-cyclohexadiene-1-<br>carboxylate; SHCHC   |  |   |
| 3454 | 0.001419 | -1.415 | 369.082692 | 370.089969 | -0.075560 | 1  | Ph | C16H18O10  | Fraxin  |  |   |
| 5069 | 0.000031 | -1.191 | 445.368738 | 446.376015 | 0.043363  | 4  | Lp | C29H50O3   | 13'-hydroxy- $\alpha$ -tocopherol<br>[primary alcohol]  | Nebrosteroid M; 4 $\alpha$ -methyl-24-<br>methylene-cholestan-3 $\beta$ ,8 $\beta$ ,11 $\beta$ -<br>triol [Ergosterols and C24-methyl<br>derivatives [ST0103]] | 24-hydroperoxy-24-<br>vinylcholesterol; 24-<br>hydroperoxy-24-vinyl-cholest-5-<br>en-3 $\beta$ -ol [Stigmasterols and C24-<br>ethyl derivatives [ST0104]] |
| 2373 | 0.027657 | -0.876 | 331.067028 | 332.074304 | -0.128768 | 1  | Cb | C13H16O10  | 1-O-Galloyl- $\beta$ -D-glucose; 1-<br>Galloyl- $\beta$ -glucose; $\beta$ -Glucogallin;<br>1-Galloyl- $\beta$ -D-glucose  |  |   |
| 2668 | 0.040378 | -0.818 | 343.067029 | 344.074305 | -0.120136 | 1  | Ph | C14H16O10  | Theogallin  |  |   |
| 2222 | 0.036017 | -0.753 | 325.113981 | 326.121258 | -0.120525 | 6  | Cb | C12H22O10  | $\alpha$ -L-Fucosyl-1,2- $\beta$ -D-<br>galactoside; Glycoprotein $\alpha$ -L-<br>fucosyl-(1,2)-D-galactose;<br>Glycolipid $\alpha$ -L-fucosyl-1,2- $\beta$ -D-<br>galactose; $\alpha$ -L-Fucosyl-(1->2)-D-<br>galactosyl-R | 2-O- $\alpha$ -L-Rhamnopyranosyl-D-<br>glucopyranose; Neohesperidose   | Robinobiose   |
| 1219 | 0.024786 | -0.494 | 275.092466 | 276.099742 | -0.114667 | 5  | Ph | C15H16O5   | Lactucin  | Vernolepin   | Vernomenin  |
| 4380 | 0.034810 | -0.351 | 407.098363 | 408.105640 | -0.017139 | 1  | Ph | C19H20O10  | Khellol glucoside; Khelloside   |  |   |
| 2127 | 0.023288 | -0.294 | 321.134320 | 322.141596 | -0.131584 | 2  | Ph | C17H22O6   | Tetraneurin A   | epi-Tulipinolide diepoxide   |   |

**f) List of TOP 80 identified HS Ds vs NI (non-inoculated ascontrol) from the significant 538 m/z at time A** selected with T-test (FDR=0.01 and S0=1). Total: 128 annotated compounds (121-/7+): Total 128 functional category counts: Ph:52; Lp:9; Cb:14; Pp:0; AmS:1; Nu:1; NM:3. The most specific compounds selected with higher stringency (FDR=0.005 and S0=1) are indicated in bolded lines. TOPs 80 functional category counts: Ph:73; Lp:15; Cb:29; Pp:2; AmS:3; Nu:1; NM:5.

| ID   | T-test<br><i>p-value</i> | HS<br><i>Ds-NI</i> | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula    | Identifications  |  |  |
|------|--------------------------|--------------------|------------|------------|----------------|----|------|------------|--|--|--|
| 4953 | 0.024454                 | +2.652             | 439.124589 | 440.131866 | 0.009877       | 2  | Ph   | C20H24O11  | Ginkgolide C; BN 52022   | Ginkgolide C (see KEGG C07603) [C20 isoprenoids (diterpenes) [PR0104]] |  |
| 4380 | 0.038096                 | +2.449             | 407.098363 | 408.105640 | -0.017139      | 1  | Ph   | C19H20O10  | Khellol glucoside; Khelloside  |  |  |
| 1219 | 0.030303                 | +2.380             | 275.092466 | 276.099742 | -0.114667      | 5  | Ph   | C15H16O5   | Lactucin   | Vernolepin   | Vernomenin   |
| 1788 | 0.027959                 | +2.052             | 307.118678 | 308.125954 | -0.110488      | 3  | Ph   | C16H20O6   | 14-Dihydroxycornestin; Cornexistin   | Monocerin  |  |
| 2467 | 0.001702                 | +2.033             | 335.040834 | 336.048111 | -0.990151      | 1  | Nu   | C11H15NO9P | Nicotinate D-ribonucleotide; β-Nicotinate D-ribonucleotide; Nicotinate ribonucleotide; Nicotinic acid ribonucleotide |  |  |
| 1918 | 0.058023                 | -2.620             | 313.147866 | 314.155142 | 0.528679       | 1  | NM   | C19H23ClN2 | Clomipramine   |  |  |
| 1677 | 0.071333                 | -2.589             | 303.050993 | 304.058270 | -0.108829      | 7  | Ph   | C15H12O7   | Taxifolin; Dihydroquercetin; (+)-Dihydroquercetin; (+)-Taxifolin; trans-Dihydroquercetin                             | Pentahydroxyflavanone; Dihydrotricetin                                 | cis-Dihydroquercetin   |
| 5431 | 0.039450                 | -2.508             | 465.103882 | 466.111159 | 0.069908       | 6  | Ph   | C21H22O12  | Quercetin 7-O-glucoside  | Plantagoside   | 3,4,5,2',4',6'-Hexahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]]  |
| 1590 | 0.031800                 | -2.490             | 299.113594 | 300.120870 | -0.109047      | 1  | Cb   | C14H20O7   | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside   |  |  |
| 2057 | 0.046867                 | -2.427             | 319.045905 | 320.053181 | -0.113324      | 3  | Ph   | C15H12O8   | Dihydromyricetin; Ampelopsin; (+)-Dihydromyricetin; (+)-Ampelopsin   | 2,3-Dihydrogossypetin  | Amaranol A; (+)- 2,4,6-Trihydroxy-2-[(3,4,5-trihydroxyphenyl)methyl]-3(2H)-benzofuranone [Aurone flavonoids [PK1213]]  |
| 478  | 0.006533                 | -2.395             | 245.081895 | 246.089171 | -0.153334      | 6  | Ph   | C14H14O4   | Columbianetin  | Decursinol   | Marmesin; (+)-Marmesin   |
| 1409 | 0.065922                 | -2.383             | 289.071731 | 290.079007 | -0.106598      | 35 | Ph   | C15H14O6   | cis-3,4-Leucopelargonidin  | Luteoforol; 3-Deoxy-leucocyanidin                                      | (+)-Catechin; D-Catechin; Cyanidanol; (2R-trans)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-Benzopyran-3,5,7-triol; (2R,3S)-Catechin; (2R,3S)-(+)-Catechin; Cianidanol |
| 5133 | 0.069413                 | -2.371             | 449.108952 | 450.116229 | 0.038519       | 25 | Ph   | C21H22O11  | Neoastilbin; (2S,3S)-Taxifolin 3-rhamnoside  | 2',3,4,4',6'-Peptahydroxychalcone 4'-O-glucoside; PHC 4'-O-glucoside   | Astilbin   |
| 4847 | 0.088631                 | -2.358             | 433.114041 | 434.121318 | 0.048061       | 32 | Ph   | C21H22O10  | Naringenin 7-O-β-D-glucoside; Prunin   | Phlorizin chalcone; Chalcone 2'-O-glucoside                            | 2',4,4',6'-Tetrahydroxychalcone 4'-O-glucoside; THC 4'-glucoside   |
| 1186 | 0.069386                 | -2.356             | 273.076829 | 274.084105 | -0.067655      | 26 | Ph   | C15H14O5   | Phloretin  | α-Pyrufuluran  | β-Pyrufuluran  |
| 5493 | 0.031666                 | -2.297             | 469.135176 | 470.142452 | 0.055729       | 1  | Ph   | C21H26O12  | Plumieride   |  |  |

|      |          |        |            |            |           |    |     |           |   |   |   |
|------|----------|--------|------------|------------|-----------|----|-----|-----------|---|---|---|
| 2347 | 0.016412 | -2.288 | 330.119400 | 331.126676 | -0.122722 | 1  | AmS | C14H21NO8 | 5'-O-β-D-Glucosylpyridoxine   |   |   |
| 2277 | 0.070602 | -2.285 | 327.163515 | 328.170791 | -0.119791 | 1  | Lp  | C17H28O4S | Steryl sulfate  |   |   |
| 1158 | 0.039929 | -2.272 | 271.061181 | 272.068458 | -0.058348 | 37 | Ph  | C15H12O5  | Naringenin; 4',5,7-Trihydroxyflavanone  | (6aS,11aS)-3,6a,9-Trihydroxypterocarpan; 3,6,9-Trihydroxypterocarpan; (-)-Glycinol  | Licodione   |
| 1346 | 0.05955  | -2.212 | 285.040436 | 286.047712 | -0.089823 | 34 | Ph  | C15H10O6  | Luteolin; 3',4',5,7-Tetrahydroxyflavone; 5,7,3',4'-Tetrahydroxyflavone  | Kaempferol; 3,4',5,7-Tetrahydroxyflavone; 4H-1-Benzopyran-4-one,3,5,7-trihydroxy-2-(4-hydroxyphenyl)-5,7,4'-Trihydroxyflavonol; C.I. 75640; Indigo yellow; Kaempferol; Kempferol; Nimbecetin; Pelargidenolon; Populnetin; Rhamnolutein; Rhamnolutin; Robigenin; Swartziol; Trifolitin | Aureusidin  |
| 7597 | 0.053253 | -2.207 | 623.161749 | 624.169025 | -0.015889 | 60 | Ph  | C28H32O16 | Tectorigenin 7-O-gentiobioside [Isoflavonoids [PK1205]]   | Isorhamnetin 3-neohesperidoside [Flavones and Flavonols [PK1211]]   | Narcissin [Flavones and Flavonols [PK1211]]                                     |
| 3049 | 0.030753 | -2.183 | 355.103413 | 356.110690 | -0.119119 | 3  | Ph  | C16H20O9  | Gentiopicrin; Gentiopicroside   | 1-O-Feruloyl-β-D-glucose; 1-Feruloyl-D-glucose  | Gentiopicrin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]        |
| 4887 | 0.064083 | -2.146 | 435.129686 | 436.136963 | 0.036110  | 16 | Ph  | C21H24O10 | Phlorizin; Phlorhizin; Phloridzin   | Epiafzelechin 3-O-β-D-allopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Arthromerin B [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]             |
| 1376 | 0.049557 | -2.130 | 287.056089 | 288.063365 | -0.079954 | 33 | Ph  | C15H12O6  | Dihydrokaempferol; Aromadendrin; (+)-Dihydrokaempferol; (+)-Aromadendrin  | Fustin; 2,3-Dihydrofisetin  | Eriodictyol   |
| 5691 | 0.065446 | -2.127 | 481.098785 | 482.106061 | 0.042399  | 1  | Ph  | C21H22O13 | 3,4,2',3',4',6',α-Heptahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]]                     |   |   |
| 2893 | 0.055781 | -2.104 | 350.306446 | 351.313723 | -0.019531 | 1  | Lp  | C22H41NO2 | Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids) [FA0804]] |   |   |
| 4627 | 0.000164 | -2.091 | 421.114055 | 422.121331 | 0.081091  | 7  | Ph  | C20H22O10 | Catechin 7-O-β-D-xyloside   | Plicatic acid   | Catechin 7-O-β-D-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] |
| 2745 | 0.004778 | -2.084 | 345.119057 | 346.126333 | -0.142585 | 4  | Lp  | C15H22O9  | Aucubin   | Deutzioside   | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]             |
| 3088 | 0.046723 | -2.079 | 357.061579 | 358.068856 | -0.032332 | 10 | Ph  | C18H14O8  | 5,3'-Dihydroxy-4',5'-dimethoxy-6,7-methylenedioxyisoflavone [Isoflavonoids [PK1205]]                              | Dalpalatin [Isoflavonoids [PK1205]]   | Luteolin 7-lactate [Flavones and Flavonols [PK1211]]                            |

|      |          |        |            |            |           |    |    |           |  |   |  |
|------|----------|--------|------------|------------|-----------|----|----|-----------|--|---|--|
| 5064 | 0.032395 | -2.048 | 445.190118 | 446.197394 | -0.100135 | 1  | Lp | C21H34O8S | Ptilosteroid A; 5 $\alpha$ -pregn-20-en-2 $\beta$ ,3 $\beta$ ,4 $\beta$ ,15 $\beta$ ,16 $\beta$ -pentol 2-sulfate [C21 steroids (gluco/mineralocorticoids, progestogens) and derivatives [ST0203]]   |   |  |
| 3153 | 0.075825 | -2.043 | 359.134719 | 360.141996 | -0.102120 | 2  | Ph | C16H24O9  | 7-Deoxyloganate  | 8-Epideoxyloganic acid  |  |
| 2579 | 0.067408 | -2.037 | 339.129643 | 340.136919 | -0.081507 | 1  | Cb | C13H24O10 | Methyl-2- $\alpha$ -L-fucopyranosyl- $\beta$ -D-galactoside  |   |  |
| 3154 | 0.025590 | -2.025 | 359.149987 | 360.157263 | -0.070751 | 11 | Ph | C20H24O6  | Antheridiogen-An   | Triptolide  | Euponin  |
| 2111 | 0.002536 | -2.019 | 321.061550 | 322.068827 | -0.126928 | 3  | Ph | C15H14O8  | Leucodelphinidin   | Elephantorrhizol [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Galocatechin-4 $\beta$ -ol [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]         |
| 3857 | 0.048409 | -1.998 | 385.113996 | 386.121273 | -0.063172 | 2  | Ph | C17H22O10 | 1-O-Sinapoyl- $\beta$ -D-glucose; 1-O-Sinapoyl $\beta$ -D-glucoside  | 4-O- $\beta$ -D-Glucosyl-sinapate   |  |
| 328  | 0.000022 | -1.992 | 227.071321 | 228.078597 | -0.205916 | 10 | Ph | C14H12O3  | 3,4',5-Trihydroxystilbene; Resveratrol   | Seselin   | Trioxsalen; Trioxysalen; 4,8,5'-Trimethylpsoralen  |
| 1722 | 0.003721 | -1.980 | 305.066640 | 306.073916 | -0.120233 | 11 | Ph | C15H14O7  | Leucocyanidin; 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol; 3,3',4,4',5,7-Flavanhexol; 3,4-Cyanidiol; Leucoanthocyanidol; Leucocianidol; Leucocyanidol; Leukocyanidine; Procyanidol; Resivit; 2,3- <i>trans</i> -3,4- <i>cis</i> -Leucocyanidin | (+)-Galocatechin; Gallocatechol   | (-)-Epigallocatechin   |
| 1255 | 0.000667 | -1.977 | 277.217271 | 278.224548 | -0.117541 | 62 | Lp | C18H30O2  | (6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; $\gamma$ -Linolenic acid; Gamolenic acid  | (9Z,12Z,15Z)-Octadecatrienoic acid; $\alpha$ -Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; $\alpha$ -Linolenate                                 | Crepenynate; (9Z)-Octadec-9-en-12-ynoate; (Z)-9-Octadecen-12-ynoic acid; Crepenynic acid |
| 5457 | 0.052513 | -1.967 | 467.098394 | 468.105671 | 0.051411  | 2  | Ph | C24H20O10 | Epigallocatechin 3-O-cafeate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Apocynin A [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |  |
| 51   | 0.002089 | -1.967 | 173.009145 | 174.016422 | -0.092226 | 6  | Ph | C6H6O6    | <i>cis</i> -Aconitate; <i>cis</i> -Aconitic acid   | <i>trans</i> -Aconitate; <i>trans</i> -Aconitic acid  | Dehydroascorbate; Dehydroascorbic acid; L-Dehydroascorbate; L-Dehydroascorbic acid       |
| 3101 | 0.051993 | -1.932 | 357.119069 | 358.126345 | -0.103262 | 3  | Cb | C16H22O9  | Tarennoside  | 10-Deoxygeniposidic acid  | Sweroside  |
| 1247 | 0.071058 | -1.922 | 277.092868 | 278.100145 | -0.082506 | 5  | Ph | C11H18O8  | Tuliposide A   | Isovalerylglucuronide (see KEGG C03033); (2S,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(3-methylbutanoyloxy)oxane-2-carboxylic acid [secondary alcohol]                 |  |
| 7603 | 0.048851 | -1.906 | 623.255794 | 624.263070 | 0.216834  | 1  | Cb | C27H44O16 | Kanokoside D   | (9E)-Octadecenoic acid; 9-Octadecenoic acid, (E)-; (E)-Oleic acid; D9- <i>trans</i> -Octadecenoic acid; 9- <i>trans</i> -Octadecenoic acid; <i>trans</i> -D9- | (6Z)-Octadecenoic acid; Petroselinic acid; <i>cis</i> -6-Octadecenoic acid               |
| 1304 | 0.040718 | -1.898 | 281.248574 | 282.255850 | -0.106353 | 58 | Lp | C18H34O2  | (9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; Oleate; Oleic acid   |   |  |



|      |          |        |            |            |           |    |    |              |  |  |   |
|------|----------|--------|------------|------------|-----------|----|----|--------------|--|--|---|
| 8583 | 0.004363 | -1.884 | 743.486985 | 744.494261 | 0.169877  | 18 | Lp | C40H73O10P   | PG(16:/18:3(6Z,9Z,12Z)); 1-hexadecanoyl-2-(6Z,9Z,12Z-octadecatrienoyl)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol]   | Octadecenoic acid; <i>trans</i> -9-Octadecenoic acid; <i>trans</i> -Elaidic acid; Acide elaidique; Elaidinsaure                |   |
| 4814 | 0.052664 | -1.857 | 431.155905 | 432.163181 | 0.044900  | 1  | Cb | C19H28O11    | Zizybeoside I  | PG(16:/18:3(9Z,12Z,15Z)); 1-hexadecanoyl-2-(9Z,12Z,15Z-octadetrienoil)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol] | PG(16:1(9Z)/18:2(9Z,12Z)); 1-(9Z-hexadecenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol] |
| 5036 | 0.080100 | -1.831 | 443.192275 | 444.199552 | 0.009678  | 1  | Cb | C21H32O10    | dihydrophaseic acid 4-O-β-D-glucoside; (2Z,4E)-5-[(1R,3S,5R,8S)-3-(β-D-glucopyranosyloxy)-8-hydroxy-1,5-dimethyl-6-oxabicyclo[3.2.1]oct-8-yl]-3-methylpenta-2,4-dienoic acid [C15 isoprenoids (sesquiterpenes) [PR0103]] |  |   |
| 4021 | 0.027272 | -1.828 | 391.124562 | 392.131838 | -0.059958 | 1  | Ph | C16H24O11    | Shanzhiside  |  |   |
| 449  | 0.023042 | -1.808 | 243.066250 | 244.073527 | -0.131492 | 10 | Ph | C14H12O4     | 3,3',4'5-Tetrahydroxystilbene; Piceatannol   | Wyerone acid   | Eriobofuran   |
| 5171 | 0.056776 | -1.806 | 451.103475 | 452.110751 | 0.041592  | 6  | Ph | C24H20O9     | Cinchonain 1a  | 9,10-Dihydro-10-(3,4-dihydroxyphenyl)-pyrano[2,3-h]catechin-8-one [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]        | Cinchonain Ib [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 4027 | 0.047126 | -1.795 | 391.160971 | 392.168248 | 0.453424  | 1  | NM | C21H27ClN2O3 | Cl37 isotope of Compound II(R/S); 5-(7-(6-Chloro-4-(5-hydro-4-methyl-2-oxazolyl)phenoxy)heptyl)-3-methylisoxazole  |  |   |
| 2219 | 0.012638 | -1.754 | 325.092849 | 326.100126 | -0.128228 | 8  | Ph | C15H18O8     | 4-O-β-D-Glucosyl-4-hydroxycinnamate  | <i>trans</i> -β-D-Glucosyl-2-hydroxycinnamate; β-D-Glucosyl-2-coumarate  | <i>cis</i> -β-D-Glucosyl-2-hydroxycinnamate; β-D-Glucosyl-2-coumarinate   |
| 6042 | 0.001942 | -1.751 | 499.291301 | 500.298577 | 0.088261  | 1  | NM | C26H44O9     | Mupirocin  |  |   |
| 4022 | 0.001195 | -1.742 | 391.128449 | 392.135726 | 0.030165  | 5  | Ph | C20H22O8     | O18 isotope of Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside   | O18 isotope of Populin   | O18 isotope of Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                   |
| 2179 | 0.049689 | -1.738 | 323.098329 | 324.105606 | -0.127735 | 2  | Cb | C12H20O10    | Bis-D-fructose 2',1:2,1'-dianhydride; Difructose anhydride I; Di-D-fructose 1,2'; 2,1' dianhydride   | D-Fructofuranose 1,2':2,3'-dianhydride   |   |
| 4636 | 0.050494 | -1.720 | 421.207924 | 422.215201 | 0.008100  | 1  | Cb | C19H34O10    | 1-Octen-3-ol-3-o-β-D-xylopyranosyl(1->6)-β-D-glucopyranoside   |  |   |
| 6367 | 0.048713 | -1.714 | 519.187226 | 520.194503 | 0.078545  | 2  | Ph | C26H32O11    | Brusatol   | (-)-Pinoresinol glucoside  |   |
| 11   | 0.079341 | -1.706 | 161.045532 | 162.052809 | -0.091525 | 30 | Cb | C6H10O5      | Lichenin; Lichenan   | (R)-3,3-Dimethylmalate   | 3-Ethylmalate   |

|      |          |        |            |            |           |    |    |            |  |  |  |
|------|----------|--------|------------|------------|-----------|----|----|------------|--|--|--|
| 4393 | 0.077835 | -1.694 | 407.171139 | 408.178415 | -0.005805 | 2  | Ph | C21H28O8   | Vernoflexuoside  |  |  |
| 4594 | 0.003211 | -1.690 | 419.134784 | 420.142061 | 0.067492  | 10 | Ph | C21H24O9   | Melampodin A   | Glycyphyllin; Phloretin 2'-O-rhamnoside  | Isorhapontin   |
| 2276 | 0.028060 | -1.688 | 327.144911 | 328.152188 | -0.047159 | 3  | Ph | C16H24O7   | Rhododendrin   | Tetranor-PGEM; 11R-hydroxy-9,15-dioxo-2,3,4,5-tetranor-prostan-1,20-dioic acid [Prostaglandins [FA0301]]   | Prostaglandin M; 7R-hydroxy-5,11-dioxotetranorprostane-1,16-dioic acid [Prostaglandins [FA0301]] |
| 4292 | 0.052111 | -1.672 | 403.139861 | 404.147137 | 0.048967  | 4  | Ph | C21H24O8   | Mallotophenone   | Koaburanin [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Orientanol A [Pterocarpans [PK1207]]   |
| 6989 | 0.000813 | -1.658 | 563.140743 | 564.148019 | 0.201658  | 52 | Ph | C26H28O14  | Apigenin 7-O-[β-D-apiosyl-(1->2)-β-D-glucoside]; 7-O-(β-D-Apiofuranosyl-1,2-β-D-glucosyl)-5,7,4'-trihydroxyflavone; Apiin; 7-[(2-O-D-Apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxy-phenyl)-4H-1-benzopyran-4-one; Apioside | Neoschaftoside   | Schaftoside  |
| 3591 | 0.049406 | -1.657 | 375.129648 | 376.136925 | -0.059642 | 3  | Ph | C16H24O10  | Loganate; Loganic acid   | 7-Epiloganic acid  |  |
| 2539 | 0.038221 | -1.650 | 337.113983 | 338.121259 | 0.392818  | 1  | Ph | C12H20N2O9 | <i>O18 isotope of 3-Epihydroxymugineic acid</i>  |  |  |
| 3972 | 0.000701 | -1.622 | 389.181684 | 390.188961 | -0.055764 | 1  | Lp | C18H30O9   | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11-β-D-glucoside; {(1R,2R)-2-[4-(β-D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]]   |  |  |
| 7153 | 0.006694 | -1.619 | 577.135234 | 578.142510 | 0.145859  | 12 | Ph | C30H26O12  | Epicatechin-(4β->8)-ent-epicatechin  | Procyanidin B4; Catechin-(4α->8)-epicatechin   | Procyanidin B2; Procyanidol B2   |
| 3967 | 0.00036  | -1.597 | 389.124168 | 390.131444 | -0.060382 | 5  | Ph | C20H22O8   | Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside  | Populin  | Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                 |
| 1480 | 0.046372 | -1.569 | 293.030257 | 294.037533 | -0.115504 | 1  | Ph | C13H10O8   | Tricrozarin A  |  |  |
| 1303 | 0.050254 | -1.544 | 281.139425 | 282.146702 | -0.078970 | 6  | Ph | C15H22O5   | Hymenoxon  | Qing Hau Sau; Artemisinin  | Dihydrophaseic acid; (-)-Dihydrophaseic acid   |
| 80   | 0.006086 | -1.538 | 179.056091 | 180.063368 | -0.114407 | 69 | Cb | C6H12O6    | D-Glucose; Grape sugar; Dextrose   | D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose  | D-Galactose  |
| 1351 | 0.000212 | -1.532 | 285.097947 | 286.105223 | -0.104355 | 4  | Cb | C13H18O7   | Salicin; Salicoside  | Gastrodin; 4-(Hydroxymethyl)phenyl-β-D-glucopyranoside   | Methylarbutin  |
| 5778 | 7.93E-08 | -1.528 | 485.082492 | 486.089768 | 0.446498  | 1  | Cb | C20H20O14  | <i>O18 isotope of 1-O,6-O-Digalloyl-β-D-glucose</i>  |  |  |
| 3922 | 0.035977 | -1.497 | 387.166034 | 388.173310 | -0.057526 | 2  | Lp | C18H28O9   | Tuberonic acid glucoside   | Tuberonic acid glucoside (see KEGG C08558); (1R,2S)-3-oxo-2-(5'-O-β-D-glucopyranosyloxy-2''Z-pentenyl)-cyclopentaneacetic acid [Fatty acyl glycosides of |  |

|      |          |        |            |            |           |    |    |           |  |                                   |   |
|------|----------|--------|------------|------------|-----------|----|----|-----------|--|-----------------------------------|---|
| 6824 | 0.011486 | -1.451 | 549.182543 | 550.189820 | 0.089857  | 1  | Ph | C23H34O15 | Genipin 1-β-gentiobioside  | mono- and disaccharides [FA1301]] |   |
| 6097 | 0.005081 | -1.407 | 503.161797 | 504.169074 | 0.077257  | 21 | Cb | C18H32O16 | Raffinose; Melitose; Melitriose; Gossypose; 6G-α-D-galactosylsucrose | Panose                            | Galactomannan; Galactomannoglycan                                   |
| 7699 | 0.011577 | -1.389 | 633.073451 | 634.080728 | 0.180016  | 1  | Ph | C27H22O18 | Corilagin  |                                   |   |
| 1586 | 0.023494 | -1.363 | 299.077209 | 300.084485 | -0.108396 | 1  | Ph | C13H16O8  | 4-(β-D-Glucosyloxy)benzoate  |                                   |   |
| 4335 | 0.082859 | -1.358 | 405.119098 | 406.126375 | -0.018591 | 7  | Ph | C20H22O9  | Astringin  | Trichocarpin                      | Anadanthoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] |
| 5732 | 0.068787 | -1.325 | 483.078040 | 484.085316 | 0.022519  | 1  | Cb | C20H20O14 | 1-O,6-O-Digalloyl-β-D-glucose  |                                   |   |

**g) List of TOP 51 identified WSHS *Ds* vs NI (non-inoculated as control) from the significant 802 *m/z* at time A** selected with T-test (FDR=0.005 and S0=2). Total: 174 annotated compounds (173-/1+); Total 174 functional category counts: Ph:31; Lp:8; Cb:8; Pp:1; AmS:2; Nu:0; NM:1. The most specific compounds selected with higher stringency (FDR=0.001 and S0=2) are indicated in bolded lines. TOPs 51 functional category counts: Ph:91; Lp:26; Cb:37; Pp:6; AmS:4; Nu:0; NM:10.

| ID   | T-test<br><i>p-value</i> | WSHS<br><i>Ds</i> -NI | <i>m/z</i> | Mass       | error<br>(ppm) | n  | Cat. | Formula    | Identifications  |   |   |
|------|--------------------------|-----------------------|------------|------------|----------------|----|------|------------|--|---|---|
| 5781 | 0.023383                 | -2.818                | 485.108961 | 486.116238 | 0.054370       | 2  | Ph   | C24H22O11  | Flavonol 3-O-(6-O-malonyl-β-D-glucoside)   | Epigallocatechin 3-O-(3,5-di-O-methylgallate) [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] |   |
| 1087 | 0.116299                 | -2.766                | 265.144542 | 266.151818 | 0.677275       | 6  | Pp   | C14H20N2O3 | O18 isotope of Subaphyllin; Feruloylputrescine                                     | Mukaadial   | Rugosal   |
| 5566 | 0.021056                 | -2.662                | 473.363676 | 474.370953 | 0.090535       | 15 | Ph   | C30H50O4   | Sapelin A  | Bryodulcosigenin  | Soyasapogenol A   |
| 4717 | 0.000313                 | -2.655                | 425.087827 | 426.095103 | 0.049636       | 2  | Ph   | C22H18O9   | Epiafzelechin 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]    | Epigallocatechin 3-O-(4-hydroxybenzoate) [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]      |   |
| 1130 | 0.038652                 | -2.584                | 269.045564 | 270.052841 | 0.064429       | 42 | Ph   | C15H10O5   | Apigenin; 4',5,7-Trihydroxyflavone; 5,7,4'-Trihydroxyflavone                       | 2'-Hydroxydaidzein  | Genistein; 5,7,4'-Trihydroxyisoflavone  |
| 7699 | 0.068581                 | -2.575                | 633.073451 | 634.080728 | 0.180016       | 1  | Ph   | C27H22O18  | Corilagin  |   |   |
| 5278 | 0.081839                 | -2.563                | 457.077691 | 458.084967 | 0.122575       | 7  | Ph   | C22H18O11  | Epigallocatechin 3-gallate   | 8-Demethyltetracenomycin C  | Epigallocatechin gallate (see KEGG C09731); [(2R,3R)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)chroman-3-yl] 3,4,5-trihydroxybenzoate [phenol or hydroxyhetarene] |
| 233  | 0.034641                 | -2.480                | 211.133944 | 212.141220 | -0.115861      | 15 | Lp   | C12H20O3   | Cucurbic acid  | Putaminoxin   | Traumatins; (10E)-12-Oxododecenoic acid   |
| 5457 | 0.036977                 | -2.465                | 467.098394 | 468.105671 | 0.051411       | 2  | Ph   | C24H20O10  | Epigallocatechin 3-O-cafeate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] | Apocynin A [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                    |   |
| 3970 | 0.029056                 | -2.462                | 389.160552 | 390.167829 | -0.062778      | 2  | Ph   | C21H26O7   | Erioflorin acetate   |   |   |

|      |          |        |            |            |           |    |    |           |   |  |  |
|------|----------|--------|------------|------------|-----------|----|----|-----------|---|--|--|
| 5778 | 0.056400 | -2.458 | 485.082492 | 486.089768 | 0.446498  | 1  | Cb | C20H20O14 | O18 isotope of 1-O,6-O-Digalloyl- $\beta$ -D-glucose  |  |  |
| 132  | 0.116164 | -2.410 | 191.034952 | 192.042228 | -0.159394 | 10 | Ph | C10H8O4   | Scopoletin  | Naphthazarin; 5,8-Dihydroxy-1,4-naphthoquinone   | 3,4-Dehydro-6-hydroxymellein   |
| 3099 | 0.000109 | -2.369 | 357.107697 | 358.114974 | -0.013607 | 4  | Ph | C16H20O9  | O18 isotope of Gentiopicrin; Gentiopicroside  | O18 isotope of 1-O-Feruloyl- $\beta$ -D-glucose; 1-Feruloyl-D-glucose  | O18 isotope of Gentiopicrin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]  |
| 3831 | 0.000344 | -2.353 | 384.145333 | 385.152609 | 0.187448  | 1  | Ph | C21H23NO6 | Polycarpine   |  |  |
| 6042 | 0.076656 | -2.337 | 499.291301 | 500.298577 | 0.088261  | 1  | NM | C26H44O9  | Mupirocin   |  |  |
| 1843 | 0.058426 | -2.335 | 310.093192 | 311.100468 | -0.108516 | 4  | Ph | C14H17NO7 | Taxiphyllin; (R)-4-Hydroxymandelonitrile $\beta$ -D-glucoside   | Dhurrin; (S)-4-Hydroxymandelonitrile $\beta$ -D-glucoside  | p-Glucosyloxymandelonitrile  |
| 4635 | 0.018222 | -2.320 | 421.186827 | 422.194104 | 0.084740  | 4  | Ph | C22H30O8  | Valtratum; Valtrate   | Isovaltrate  | Picrasin F   |
| 3088 | 0.022141 | -2.319 | 357.061579 | 358.068856 | -0.032332 | 10 | Ph | C18H14O8  | 5,3'-Dihydroxy-4',5'-dimethoxy-6,7-methylenedioxyisoflavone [Isoflavonoids [PK1205]]                              | Dalpalatin [Isoflavonoids [PK1205]]  | Luteolin 7-lactate [Flavones and Flavonols [PK1211]]   |
| 5262 | 0.023223 | -2.317 | 455.353108 | 456.360385 | 0.086530  | 20 | Ph | C30H48O3  | Betulinic acid  | $\alpha$ -Elemolic acid  | Ursolic acid   |
| 4511 | 0.029686 | -2.304 | 413.218120 | 414.225397 | 0.069673  | 3  | Lp | C21H34O8  | methyl 5-hydroperoxy-6,8,9,11-bisepidioxy-12,14-eicosadienoate [Hydroperoxy fatty acids [FA0104]]                 | methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]] | methyl 6,8-epidioxy-5,15-dihydroperoxy-9,11,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]]  |
| 4985 | 0.045130 | -2.295 | 441.082837 | 442.090114 | 0.264769  | 10 | Ph | C22H18O10 | Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                   | ent-Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                | Catechin 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 2893 | 0.072813 | -2.258 | 350.306446 | 351.313723 | -0.019531 | 1  | Lp | C22H41NO2 | Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids) [FA0804]] |  |  |
| 3591 | 0.076360 | -2.248 | 375.129648 | 376.136925 | -0.059642 | 3  | Ph | C16H24O10 | Loganate; Loganic acid  | 7-Epiloganic acid  |  |
| 4688 | 0.013266 | -2.246 | 423.326893 | 424.334170 | 0.092124  | 4  | Lp | C29H44O2  | $\alpha$ -Tocotrienol   | 4,4'-Methylenebis(2,6-di-tert-butylphenol)   | $\alpha$ -Tocotrienol (see KEGG C14153); (2R)-2,5,7,8-tetramethyl-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trienyl]chroman-6-ol [phenol or hydroxyhetarene] |
| 4730 | 0.023538 | -2.237 | 425.181737 | 426.189014 | 0.073384  | 2  | Ph | C21H30O9  | Abscisic acid glucose ester; abscisic acid- $\beta$ -D-glucopyranosyl ester                                       | $\gamma$ -CEHC Glc; $\gamma$ -carboxyethyl-hydroxychroman $\beta$ -D-glucoside [Vitamin E [PR0202]]                |  |
| 2684 | 0.022418 | -2.216 | 343.124543 | 344.131820 | -0.121434 | 4  | Cb | C12H24O11 | Melibiiitol; 6-O- $\alpha$ -D-Galactosyl-D-glucitol   | Clusianose   | Maltitol; 4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol [acetal]   |
| 5171 | 0.006168 | -2.211 | 451.103475 | 452.110751 | 0.041592  | 6  | Ph | C24H20O9  | Cinchonain 1a   | 9,10-Dihydro-10-(3,4-dihydroxyphenyl)-pyrano[2,3-h]catechin-8-one [Flavans,  | Cinchonain Ib [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |

|             |                 |               |                   |                   |                  |          |            |                   |   |  |  |
|-------------|-----------------|---------------|-------------------|-------------------|------------------|----------|------------|-------------------|---|--|--|
| 4636        | 0.008933        | -2.209        | 421.207924        | 422.215201        | 0.008100         | 1        | Cb         | C19H34O10         | 1-Octen-3-ol-3-o-β-D-xylopyranosyl(1->6)-β-D-glucopyranoside                                  | Flavanols and Leucoanthocyanidins [PK1202]]  |  |
| <b>306</b>  | <b>0.033012</b> | <b>-2.204</b> | <b>223.133928</b> | <b>224.141204</b> | <b>-0.180408</b> | <b>8</b> | <b>Ph</b>  | <b>C13H20O3</b>   | <b>Vomifoliol; (6S,9R)-6-hydroxy-3-oxo-α-ionol</b>  | <b>(+/-)-6-Hydroxy-3-oxo-α-ionol</b>   | <b>Methyl jasmonate; (-)-Methyl jasmonate</b>  |
| 928         | 0.084980        | -2.200        | 263.128852        | 264.136128        | -0.116493        | 33       | Ph         | C15H20O4          | Abscisate; Absciscic acid; (+)-Absciscic acid   | Amaralin   | Artemisiifolin   |
| 1583        | 0.055928        | -2.176        | 299.056112        | 300.063389        | 0.002400         | 77       | Ph         | C16H12O6          | 5,7,4'-Trihydroxy-3'-methoxyflavone; 3'-O-Methyluteolin; Chrysoeriol                          | 3-Methoxyapigenin; 3-O-Methylkaempferol  | Leptosidin   |
| <b>6299</b> | <b>0.003170</b> | <b>-2.172</b> | <b>515.286219</b> | <b>516.293495</b> | <b>0.092665</b>  | <b>2</b> | <b>Lp</b>  | <b>C26H44O10</b>  | <b>L-Olivosyl-oleandolide</b>   | <b>L-Olivosyl-oleandolide (see KEGG C11991) [Macrolides and lactone polyketides [PK04]]</b>  |  |
| <b>1247</b> | <b>0.008038</b> | <b>-2.143</b> | <b>277.092868</b> | <b>278.100145</b> | <b>-0.082506</b> | <b>5</b> | <b>Ph</b>  | <b>C11H18O8</b>   | <b>Tuliposide A</b>   | <b>Isovalerylglucuronide (see KEGG C03033); (2S,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(3-methylbutanoyloxy)oxane-2-carboxylic acid [secondary alcohol]</b> |  |
| 2506        | 0.010083        | -2.134        | 336.129968        | 337.137244        | -0.110462        | 3        | AmS        | C13H23NO9         | Streptobiosamine  |  |  |
| 5460        | 0.026091        | -2.126        | 467.119547        | 468.126824        | 0.101485         | 3        | Ph         | C21H24O12         | Catechin-4-ol 3-O-β-D-galactopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] | Catechin-4-ol 3-O-β-D-glycopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Leucodelphinidin 3-O-α-L-rhamnopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 6097        | 0.002255        | -2.126        | 503.161797        | 504.169074        | 0.077257         | 21       | Cb         | C18H32O16         | Raffinose; Melitose; Melitriose; Gossypose; 6G-α-D-galactosylsucrose                          | Panose   | Galactomannan; Galactomannoglycan  |
| <b>1303</b> | <b>0.013100</b> | <b>-2.121</b> | <b>281.139425</b> | <b>282.146702</b> | <b>-0.078970</b> | <b>6</b> | <b>Ph</b>  | <b>C15H22O5</b>   | <b>Hymenoxon</b>  | <b>Qing Hau Sau; Artemisinin</b>   | <b>Dihydrophaseic acid; (-)-Dihydrophaseic acid</b>  |
| 3153        | 0.069033        | -2.095        | 359.134719        | 360.141996        | -0.102120        | 2        | Ph         | C16H24O9          | 7-Deoxyloganate   | 8-Epideoxyloganic acid   |  |
| 3540        | 0.038126        | -2.086        | 373.113993        | 374.121269        | -0.074217        | 4        | Ph         | C16H22O10         | Secologanate  | Swertiamarin   | Geniposidic acid   |
| <b>4590</b> | <b>0.022306</b> | <b>-2.077</b> | <b>419.098382</b> | <b>420.105659</b> | <b>0.027948</b>  | <b>7</b> | <b>Ph</b>  | <b>C20H20O10</b>  | <b>5,3',5'-Trihydroxy-3,6,7,8,4'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]</b>    | <b>5,7,4'-Trihydroxy-3,6,8,3',5'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]</b>   | <b>5,7,3'-Trihydroxy-3,6,8,4',5'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]</b>   |
| <b>3355</b> | <b>0.001644</b> | <b>-2.075</b> | <b>366.140542</b> | <b>367.147819</b> | <b>-0.074144</b> | <b>3</b> | <b>AmS</b> | <b>C14H25NO10</b> | <b>N-Acetyl-6-O-L-fucosyl-D-glucosamine [aldehyde]</b>  | <b>2-Acetamido-2-deoxy-6-O-a-L-fucopyranosyl-D-glucose [aldehyde]</b>  | <b>3-O-fucopyranosyl-2-acetamido-2-deoxyglucopyranose; N-[(2R,3R,4R,5R)-4,5,6-trihydroxy-1-oxo-3-[(2R,3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyl-oxan-2-yl]oxy-hexan-2-yl]acetamide [aldehyde]</b> |
| 5493        | 0.050417        | -2.050        | 469.135176        | 470.142452        | 0.055729         | 1        | Ph         | C21H26O12         | Plumieride  |  |  |
| 80          | 0.028026        | -2.026        | 179.056091        | 180.063368        | -0.114407        | 69       | Cb         | C6H12O6           | D-Glucose; Grape sugar; Dextrose  | D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose  | D-Galactose  |

|      |          |        |            |            |           |    |    |           |  |  |  |
|------|----------|--------|------------|------------|-----------|----|----|-----------|--|--|--|
| 2222 | 0.013499 | -2.026 | 325.113981 | 326.121258 | -0.120525 | 6  | Cb | C12H22O10 | $\alpha$ -L-Fucosyl-1,2- $\beta$ -D-galactoside; Glycoprotein $\alpha$ -L-fucosyl-(1,2)-D-galactose; Glycolipid $\alpha$ -L-fucosyl-1,2- $\beta$ -D-galactose; $\alpha$ -L-Fucosyl-(1->2)-D-galactosyl-R | 2-O- $\alpha$ -L-Rhamnopyranosyl-D-glucopyranose; Neohesperidose     | Robinobiose  |
| 4022 | 0.003224 | -2.017 | 391.128449 | 392.135726 | 0.030165  | 5  | Ph | C20H22O8  | <i>018 isotope of Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-<math>\beta</math>-monoglucoside</i>   | <i>018 isotope of Populin</i>  | <i>018 isotope of Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]</i> |
| 3544 | 0.008113 | -2.003 | 373.150383 | 374.157659 | -0.062393 | 4  | Ph | C17H26O9  | Deoxyloganin; 7-Deoxyloganin   | 8-Epideoxyloganin  | Deoxyloganin (see KEGG C06071) [C10 isoprenoids (monoterpenes) [PR0102]]                               |
| 3927 | 0.049133 | -1.972 | 387.238811 | 388.246087 | -0.041617 | 1  | Lp | C20H36O7  | 5,6-Dihydroxyprostaglandin F1a (see KEGG C06475) [secondary alcohol]   |  |  |
| 2179 | 0.008813 | -1.911 | 323.098329 | 324.105606 | -0.127735 | 2  | Cb | C12H20O10 | Bis-D-fructose 2',1:2,1'-dianhydride; Difructose anhydride I; Di-D-fructose 1,2'; 2,1' dianhydride   | D-Fructofuranose 1,2':2,3'-dianhydride                               |  |
| 1864 | 0.088433 | -1.896 | 311.098334 | 312.105610 | -0.117249 | 6  | Cb | C11H20O10 | Vicianose; O- $\alpha$ -L-Arabinopyranosyl-(1-6)-D-glucopyranose   | Arabino-galactose  | 6-O- $\beta$ -D-Xylopyranosyl-D-glucose; Primeverose   |
| 3972 | 0.029020 | -1.878 | 389.181684 | 390.188961 | -0.055764 | 1  | Lp | C18H30O9  | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11- $\beta$ -D-glucoside; {(1R,2R)-2-[4-( $\beta$ -D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]]                           |  |  |
| 170  | 0.004956 | -1.761 | 199.170322 | 200.177598 | -0.159280 | 13 | Lp | C12H24O2  | Dodecanoic acid; Dodecanoate; Dodecylcarboxylate; Lauric acid  | Dodecanoic acid (see KEGG C02679); Dodecanoic acid [carboxylic acid] | Lauric acid (see KEGG C02679); dodecanoic acid [Straight chain fatty acids [FA0101]]                   |

### TABLES of COMMON *Ds* and *Np* DOWN-ACCUMULATED COMPOUNDS

Table lists of common annotated down-accumulated significant *m/z* between fungus *Neofusicoccum parvum* and *Diplodia seriata* (*Np* or *Ds*) inoculated-vines and non-inoculated ones under abiotic stresses: none (NAS), water (WS), heat (HS) or both stresses (WSHS). Lists of down-accumulated significant *m/z* in inoculated vines were compared per stress at Time-points A or B. Each compound is identified with an ID number and level of down-regulation is expressed by the difference versus non-infected samples by Perseus software (Student T-test FDR < 0.05, S0=0). Measured *m/z* and calculated KEGG theoretical Mass and error (ppm) are indicated and the number of possible MassTrix identifications is indicated in the “n” column but only the first three ones are listed. Functional categories (Cat.) were determined according to KEGG annotations: Carbohydrates (Cb); Lipids (Lp); Phytochemicals (Ph); Peptides (Pp); Amino sugars (AmS); Nucleotides (Nu) and no match (NM). Down-accumulated (-) compounds are colored in red gradient. Identified isotopic compounds are indicated in italic characters.

**h) List of the 15 identified compounds from the 105 common significant *m/z* of no abiotic stress (NAS) samples at time B.** Functional category counts: Ph:10; Lp:1; Cb:2; Pp:0; AmS:1; Nu:1; NM:0.

| ID   | NAS<br><i>Ds</i> - NI | NAS<br><i>Np</i> - NI | Cat. | <i>m/z</i> | Mass       | error<br>(ppm) | Formula    | n | Identification  |                            |   |
|------|-----------------------|-----------------------|------|------------|------------|----------------|------------|---|---|----------------------------|---|
| 7463 | -2.686                | -2.882                | Ph   | 609.188462 | 610.195738 | 0.997565       | C34H30N2O9 | 1 | Atalanine   |                            |   |
| 3591 | -2.367                | -1.771                | Ph   | 375.129648 | 376.136925 | -0.059642      | C16H24O10  | 3 | Loganate; Loganic acid  | 7-Epiloganic acid          |   |
| 5540 | -2.302                | -2.815                | Ph   | 472.146076 | 473.153353 | 0.058057       | C20H27NO12 | 1 | Proteacin   |                            |   |
| 3851 | -2.301                | -1.480                | Ph   | 385.077611 | 386.084888 | -0.061436      | C16H18O11  | 1 | O-Feruloylgalactarate; O-Feruloylgalactaric acid; 2'-(E)-O-Feruloylgalactaric acid  |                            |   |
| 2347 | -2.287                | -2.287                | AmS  | 330.119400 | 331.126676 | -0.122722      | C14H21NO8  | 1 | 5'-O-β-D-Glucosylpyridoxine   |                            |   |
| 3153 | -2.279                | -2.118                | Ph   | 359.134719 | 360.141996 | -0.102120      | C16H24O9   | 2 | 7-Deoxyloganate   | 8-Epideoxyloganic acid     |   |
| 1590 | -2.233                | -2.706                | Cb   | 299.113594 | 300.120870 | -0.109047      | C14H20O7   | 1 | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside  |                            |   |
| 2745 | -2.156                | -1.828                | Lp   | 345.119057 | 346.126333 | -0.142585      | C15H22O9   | 4 | Aucubin   | Deutzioside                | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]] |
| 3775 | -1.871                | -1.846                | Nu   | 382.100408 | 383.107685 | -0.072174      | C14H17N5O8 | 1 | Succinyladenosine; (2S)-2-[[9-[(2S,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]purin-6-yl]amino]butanedioic acid [primary alcohol] |                            |   |
| 1864 | -1.860                | -1.826                | Cb   | 311.098334 | 312.105610 | -0.117249      | C11H20O10  | 6 | Vicianose; O-α-L-Arabinopyranosyl-(1-6)-D-glucopyranose   | Arabino-galactose          | 6-O-β-D-Xylopyranosyl-D-glucose; Primeverose                        |
| 1194 | -1.551                | -2.456                | Ph   | 274.056804 | 275.064080 | -0.131780      | C10H13NO8  | 1 | 3-β-D-Glucopyranuronosyloxy-5-methylisoxazole   |                            |   |
| 3454 | -1.415                | -1.838                | Ph   | 369.082692 | 370.089969 | -0.075560      | C16H18O10  | 1 | Fraxin  |                            |   |
| 2668 | -0.818                | -1.101                | Ph   | 343.067029 | 344.074305 | -0.120136      | C14H16O10  | 1 | Theogallin  |                            |   |
| 1219 | -0.494                | -0.349                | Ph   | 275.092466 | 276.099742 | -0.114667      | C15H16O5   | 5 | Lactucin  | Vernolepin                 | Vernomenin  |
| 2127 | -0.294                | -0.433                | Ph   | 321.134320 | 322.141596 | -0.131584      | C17H22O6   | 2 | Tetraneurin A   | epi-Tulipinolide diepoxide |   |

**i) List of the 106 identified compounds from the 486 common significant *m/z* of HS stress samples at time A.** Structure category counts: Ph:56; Lp:13; Cb:28; Pp:2; AmS:3; Nu:0; NM:4

| ID   | HS<br><i>Ds</i> -NI | HS<br><i>Np</i> -NI | Cat. | <i>m/z</i> | Mass       | error<br>(ppm) | Formula    | n | Identification   |  |   |
|------|---------------------|---------------------|------|------------|------------|----------------|------------|---|--|--|---|
| 1918 | -2.620              | -2.307              | NM   | 313.147866 | 314.155142 | 0.528679       | C19H23ClN2 | 1 | Clomipramine   |  |   |
| 1677 | -2.589              | -2.438              | Ph   | 303.050993 | 304.058270 | -0.108829      | C15H12O7   | 7 | Taxifolin; Dihydroquercetin; (+)-Dihydroquercetin; (+)-Taxifolin; <i>trans</i> -Dihydroquercetin | Pentahydroxyflavanone; Dihydrotricetin | <i>cis</i> -Dihydroquercetin  |
| 5431 | -2.508              | -2.144              | Ph   | 465.103882 | 466.111159 | 0.069908       | C21H22O12  | 6 | Quercetin 7-O-glucoside  | Plantagoside                           | 3,4,5,2',4',6'-Hexahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]] |
| 1590 | -2.490              | -2.126              | Cb   | 299.113594 | 300.120870 | -0.109047      | C14H20O7   | 1 | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside                     |  |   |



|      |        |        |     |            |            |           |           |    |  |   |   |
|------|--------|--------|-----|------------|------------|-----------|-----------|----|--|---|---|
| 2057 | -2.427 | -1.793 | Ph  | 319.045905 | 320.053181 | -0.113324 | C15H12O8  | 3  | Dihydromyricetin; Ampelopsin; (+)-Dihydromyricetin; (+)-Ampelopsin       | 2,3-Dihydrogossypetin   | Amaranol A; (+)- 2,4,6-Trihydroxy-2-[(3,4,5-trihydroxyphenyl)methyl]-3(2H)-benzofuranone [Aurone flavonoids [PK1213]]   |
| 1409 | -2.383 | -1.745 | Ph  | 289.071731 | 290.079007 | -0.106598 | C15H14O6  | 35 | cis-3,4-Leucopelargonidin  | Luteoforol; 3-Deoxyleucocyanidin  | (+)-Catechin; D-Catechin; Cyanidanol; (2R- <i>trans</i> )-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-Benzopyran-3,5,7-triol; (2R,3S)-Catechin; (2R,3S)-(+)-Catechin; Cianidanol |
| 5133 | -2.371 | -2.027 | Ph  | 449.108952 | 450.116229 | 0.038519  | C21H22O11 | 25 | Neoastilbin; (2S,3S)-Taxifolin 3-rhamnoside                              | 2',3,4,4',6'-Peptahydroxychalcone 4'-O-glucoside; PHC 4'-O-glucoside  | Astilbin  |
| 4847 | -2.358 | -2.075 | Ph  | 433.114041 | 434.121318 | 0.048061  | C21H22O10 | 32 | Naringenin 7-O-β-D-glucoside; Prunin                                     | Phlorizin chalcone; Chalcone 2'-O-glucoside   | 2',4,4',6'-Tetrahydroxychalcone 4'-O-glucoside; THC 4'-glucoside  |
| 2347 | -2.288 | -2.354 | AmS | 330.119400 | 331.126676 | -0.122722 | C14H21NO8 | 1  | 5'-O-β-D-Glucosylpyridoxine  |   |   |
| 2277 | -2.285 | -2.081 | Lp  | 327.163515 | 328.170791 | -0.119791 | C17H28O4S | 1  | Steryl sulfate   |   |   |
| 1158 | -2.272 | -2.272 | Ph  | 271.061181 | 272.068458 | -0.058348 | C15H12O5  | 37 | Naringenin; 4',5,7-Trihydroxyflavanone                                   | (6aS,11aS)-3,6a,9-Trihydroxypterocarpan; 3,6,9-Trihydroxypterocarpan; (-)-Glycinol  | Licodione   |
| 1346 | -2.212 | -2.212 | Ph  | 285.040436 | 286.047712 | -0.089823 | C15H10O6  | 34 | Luteolin; 3',4',5,7-Tetrahydroxyflavone; 5,7,3',4'-Tetrahydroxyflavone   | Kaempferol; 3,4',5,7-Tetrahydroxyflavone; 4H-1-Benzopyran-4-one,3,5,7-trihydroxy-2-(4-hydroxyphenyl)-5,7,4'-Trihydroxyflavonol; C,I, 75640; Indigo yellow; Kaempferol; Kempferol; Nimbecetin; Pelargidenolon; Populnetin; Rhamnolutein; Rhamnolutin; Robigenin; Swartziol; Trifolitin | Aureusidin  |
| 7597 | -2.207 | -2.207 | Ph  | 623.161749 | 624.169025 | -0.015889 | C28H32O16 | 60 | Tectorigenin 7-O-gentiobioside [Isoflavonoids [PK1205]]                  | Isorhamnetin 3-neohesperidoside [Flavones and Flavonols [PK1211]]   | Narcissin [Flavones and Flavonols [PK1211]]   |
| 3049 | -2.183 | -2.081 | Ph  | 355.103413 | 356.110690 | -0.119119 | C16H20O9  | 3  | Gentiopicrin; Gentiopicroside  | 1-O-Feruloyl-β-D-glucose; 1-Feruloyl-D-glucose  | Gentiopicrin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]  |
| 4887 | -2.146 | -2.028 | Ph  | 435.129686 | 436.136963 | 0.036110  | C21H24O10 | 16 | Phlorizin; Phlorhizin; Phloridzin  | Epiafzelechin 3-O-β-D-allopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Arthromerin B [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 1376 | -2.130 | -1.998 | Ph  | 287.056089 | 288.063365 | -0.079954 | C15H12O6  | 33 | Dihydrokaempferol; Aromadendrin; (+)-Dihydrokaempferol; (+)-Aromadendrin | Fustin; 2,3-Dihydrofisetin  | Eriodictyol   |
| 5691 | -2.127 | -1.739 | Ph  | 481.098785 | 482.106061 | 0.042399  | C21H22O13 | 1  | 3,4,2',3',4',6',α-Heptahydroxychalcone 2'-                               |   |   |

|      |        |        |    |            |            |           |           |    |  |   |  |
|------|--------|--------|----|------------|------------|-----------|-----------|----|--|---|--|
| 2893 | -2.104 | -2.104 | Lp | 350.306446 | 351.313723 | -0.019531 | C22H41NO2 | 1  | glucoside [Chalcones and dihydrochalcones [PK1212]]<br>Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids) [FA0804]] |   |  |
| 4627 | -2.091 | -2.091 | Ph | 421.114055 | 422.121331 | 0.081091  | C20H22O10 | 7  | Catechin 7-O-β-D-xyloside  | Plicatic acid   | Catechin 7-O-β-D-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]          |
| 2745 | -2.084 | -1.822 | Lp | 345.119057 | 346.126333 | -0.142585 | C15H22O9  | 4  | Aucubin  | Deutzioside   | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]                      |
| 3088 | -2.079 | -2.079 | Ph | 357.061579 | 358.068856 | -0.032332 | C18H14O8  | 10 | 5,3'-Dihydroxy-4',5'-dimethoxy-6,7-methylenedioxyisoflavone [Isoflavonoids [PK1205]]   | Dalpalatin [Isoflavonoids [PK1205]]   | Luteolin 7-lactate [Flavones and Flavanols [PK1211]]                                     |
| 5064 | -2.048 | -2.048 | Lp | 445.190118 | 446.197394 | -0.100135 | C21H34O8S | 1  | Ptilosteroid A; 5α-pregn-20-en-2β,3β,4β,15β,16β-pentol 2-sulfate [C21 steroids (gluco/mineralocorticoids, progestogens) and derivatives [ST0203]]                        |   |  |
| 3153 | -2.043 | -2.052 | Ph | 359.134719 | 360.141996 | -0.102120 | C16H24O9  | 2  | 7-Deoxyloganate  | 8-Epideoxyloganic acid  |  |
| 2579 | -2.037 | -2.455 | Cb | 339.129643 | 340.136919 | -0.081507 | C13H24O10 | 1  | Methyl-2-α-L-fucopyranosyl-β-D-galactoside   |   |  |
| 3154 | -2.025 | -1.682 | Ph | 359.149987 | 360.157263 | -0.070751 | C20H24O6  | 11 | Antheridiogen-An   | Triptolide  | Euponin  |
| 3857 | -1.998 | -1.469 | Ph | 385.113996 | 386.121273 | -0.063172 | C17H22O10 | 2  | 1-O-Sinapoyl-β-D-glucose; 1-O-Sinapoyl β-D-glucoside   | 4-O-β-D-Glucosyl-sinapate   |  |
| 328  | -1.992 | -1.482 | Ph | 227.071321 | 228.078597 | -0.205916 | C14H12O3  | 10 | 3,4',5'-Trihydroxystilbene; Resveratrol  | Seselin   | Trioxsalen; Trioxysalen; 4,8,5'-Trimethylpsoralen  |
| 1255 | -1.977 | -2.051 | Lp | 277.217271 | 278.224548 | -0.117541 | C18H30O2  | 62 | (6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; γ-Linolenic acid; Gamolenic acid  | (9Z,12Z,15Z)-Octadecatrienoic acid; α-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; α-Linolenate                                 | Crepenynate; (9Z)-Octadec-9-en-12-ynoate; (Z)-9-Octadecen-12-ynoic acid; Crepenynic acid |
| 5457 | -1.967 | -1.760 | Ph | 467.098394 | 468.105671 | 0.051411  | C24H20O10 | 2  | Epigallocatechin 3-O-cafeate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Apocynin A [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |  |
| 51   | -1.967 | -2.107 | Ph | 173.009145 | 174.016422 | -0.092226 | C6H6O6    | 6  | cis-Aconitate; cis-Aconitic acid   | trans-Aconitate; trans-Aconitic acid  | Dehydroascorbate; Dehydroascorbic acid; L-Dehydroascorbate; L-Dehydroascorbic acid       |
| 3101 | -1.932 | -1.938 | Cb | 357.119069 | 358.126345 | -0.103262 | C16H22O9  | 3  | Tarennoside  | 10-Deoxygeniposidic acid  | Sweroside  |
| 1247 | -1.922 | -1.922 | Ph | 277.092868 | 278.100145 | -0.082506 | C11H18O8  | 5  | Tuliposide A   | Isovalerylglucuronide (see KEGG C03033); (2S,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(3-methylbutanoyloxy)oxane-2-carboxylic acid [secondary alcohol] |  |
| 7603 | -1.906 | -1.906 | Cb | 623.255794 | 624.263070 | 0.216834  | C27H44O16 | 1  | Kanokoside D   |   |  |

|      |        |        |    |            |            |           |              |    |  |   |   |
|------|--------|--------|----|------------|------------|-----------|--------------|----|--|---|---|
| 1304 | -1.898 | -2.205 | Lp | 281.248574 | 282.255850 | -0.106353 | C18H34O2     | 58 | (9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; Oleate; Oleic acid   | (9E)-Octadecenoic acid; 9-Octadecenoic acid, (E)-; (E)-Oleic acid; D9- <i>trans</i> -Octadecenoic acid; 9- <i>trans</i> -Octadecenoic acid; <i>trans</i> -D9-Octadecenoic acid; <i>trans</i> -9-Octadecenoic acid; <i>trans</i> -Elaidic acid; <i>trans</i> -Oleic acid; Elaidic acid; Acide elaidique; Elaidinsauure | (6Z)-Octadecenoic acid; Petroselinic acid; <i>cis</i> -6-Octadecenoic acid  |
| 8583 | -1.884 | -1.348 | Lp | 743.486985 | 744.494261 | 0.169877  | C40H73O10P   | 18 | PG(16:0/18:3(6Z,9Z,12Z)); 1-hexadecanoyl-2-(6Z,9Z,12Z-octadecatrienoyl)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol]  | PG(16:0/18:3(9Z,12Z,15Z)); 1-hexadecanoyl-2-(9Z,12Z,15Z-octadecatrienoyl)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol]   | PG(16:1(9Z)/18:2(9Z,12Z)); 1-(9Z-hexadecenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phospho-(1'-sn-glycerol) [primary alcohol] |
| 4814 | -1.857 | -2.258 | Cb | 431.155905 | 432.163181 | 0.044900  | C19H28O11    | 1  | Zizybeoside I  |   |   |
| 5036 | -1.831 | -2.007 | Cb | 443.192275 | 444.199552 | 0.009678  | C21H32O10    | 1  | dihydrophaseic acid 4-O-β-D-glucoside; (2Z,4E)-5-[(1R,3S,5R,8S)-3-(β-D-glucopyranosyloxy)-8-hydroxy-1,5-dimethyl-6-oxabicyclo[3,2,1]oct-8-yl]-3-methylpenta-2,4-dienoic acid [C15 isoprenoids (sesquiterpenes) [PR0103]] |   |   |
| 4021 | -1.828 | -1.828 | Ph | 391.124562 | 392.131838 | -0.059958 | C16H24O11    | 1  | Shanzhiside  |   |   |
| 449  | -1.808 | -1.808 | Ph | 243.066250 | 244.073527 | -0.131492 | C14H12O4     | 10 | 3,3',4'5-Tetrahydroxystilbene; Piceatannol   | Wyerone acid  | Eriobofuran   |
| 5171 | -1.806 | -1.648 | Ph | 451.103475 | 452.110751 | 0.041592  | C24H20O9     | 6  | Cinchonain 1a  | 9,10-Dihydro-10-(3,4-dihydroxyphenyl)-pyrano[2,3-h]catechin-8-one [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Cinchonain Ib [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 4599 | -1.804 | -1.804 | Ph | 419.171164 | 420.178440 | 0.053946  | C22H28O8     | 6  | Eupacunolin  | Eupacunoxin   | Eupaformosanin  |
| 4027 | -1.795 | -2.088 | NM | 391.160971 | 392.168248 | 0.453424  | C21H27ClN2O3 | 1  | <i>Cl37 isotope of Compound II(R/S); 5-(7-(6-Chloro-4-(5-hydro-4-methyl-2-oxazolyl)phenoxy)heptyl)-3-methylisoxazole</i>   |   |   |
| 6042 | -1.751 | -1.751 | NM | 499.291301 | 500.298577 | 0.088261  | C26H44O9     | 1  | Mupirocin  |   |   |
| 4022 | -1.742 | -1.742 | Ph | 391.128449 | 392.135726 | 0.030165  | C20H22O8     | 5  | <i>O18 isotope of Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside</i>  | <i>O18 isotope of Populin</i>   | <i>O18 isotope of Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]</i>                            |
| 2179 | -1.738 | -1.506 | Cb | 323.098329 | 324.105606 | -0.127735 | C12H20O10    | 2  | Bis-D-fructose 2',1:2,1'-dianhydride; Difructose anhydride I; Di-D-fructose 1,2'; 2,1' dianhydride   | D-Fructofuranose 1,2':2,3'-dianhydride  |   |

|      |        |        |     |            |            |           |              |    |  |   |  |
|------|--------|--------|-----|------------|------------|-----------|--------------|----|--|---|--|
| 4636 | -1.720 | -1.525 | Cb  | 421.207924 | 422.215201 | 0.008100  | C19H34O10    | 1  | 1-Octen-3-ol-3-o-β-D-xylopyranosyl(1->6)-β-D-glucopyranoside   |   |  |
| 6367 | -1.714 | -1.879 | Ph  | 519.187226 | 520.194503 | 0.078545  | C26H32O11    | 2  | Brusatol   | (-)-Pinoresinol glucoside   |  |
| 3918 | -1.713 | -2.081 | Cb  | 387.129645 | 388.136921 | -0.066108 | C17H24O10    | 5  | Secologanin; (-)-Secologanin   | Geniposide  | Verbenalin; Cornin (glycoside)   |
| 3969 | -1.713 | -1.783 | NM  | 389.145306 | 390.152582 | 0.415595  | C21H25ClN2O3 | 4  | Cl37 isotope of Cetirizine   | Cl37 isotope of Cetirizine (see KEGG C07778); 2-[2-[4-[(4-chlorophenyl)-phenyl-methyl]piperazin-1-yl]ethoxy]acetic acid [dialkyl ether] | Loganin  |
| 11   | -1.706 | -2.180 | Cb  | 161.045532 | 162.052809 | -0.091525 | C6H10O5      | 30 | Lichenin; Lichenan   | (R)-3,3-Dimethylmalate  | 3-Ethylmalate  |
| 1843 | -1.705 | -1.839 | Ph  | 310.093192 | 311.100468 | -0.108516 | C14H17NO7    | 4  | Taxiphyllin; (R)-4-Hydroxymandelonitrile β-D-glucoside   | Dhurrin; (S)-4-Hydroxymandelonitrile β-D-glucoside  | p-Glucosyloxymandelonitrile  |
| 2811 | -1.696 | -1.429 | Cb  | 347.171101 | 348.178377 | -0.116791 | C16H28O8     | 1  | Schizonepetoside E   |   |  |
| 4393 | -1.694 | -1.526 | Ph  | 407.171139 | 408.178415 | -0.005805 | C21H28O8     | 2  | Vernoflexuoside  |   |  |
| 4594 | -1.690 | -1.690 | Ph  | 419.134784 | 420.142061 | 0.067492  | C21H24O9     | 10 | Melampodin A   | Glycyphyllin; Phloretin 2'-O-rhamnoside   | Isorhapontin   |
| 2276 | -1.688 | -1.688 | Ph  | 327.144911 | 328.152188 | -0.047159 | C16H24O7     | 3  | Rhododendrin   | Tetranor-PGEM; 11R-hydroxy-9,15-dioxo-2,3,4,5-tetranor-prostan-1,20-dioic acid [Prostaglandins [FA0301]]                                | Prostaglandin M; 7R-hydroxy-5,11-dioxotetranorprostane-1,16-dioic acid [Prostaglandins [FA0301]] |
| 4985 | -1.682 | -1.799 | Ph  | 441.082837 | 442.090114 | 0.264769  | C22H18O10    | 10 | Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | ent-Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Catechin 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                       |
| 4292 | -1.672 | -1.672 | Ph  | 403.139861 | 404.147137 | 0.048967  | C21H24O8     | 4  | Mallotophenone   | Koaburanin [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Orientanol A [Pterocarpan [PK1207]]  |
| 4338 | -1.666 | -1.699 | Ph  | 405.140233 | 406.147509 | -0.005430 | C17H26O11    | 4  | Ipolamiide   | 10-Hydroxyloganin   | Morroniside  |
| 6989 | -1.658 | -1.658 | Ph  | 563.140743 | 564.148019 | 0.201658  | C26H28O14    | 52 | Apigenin 7-O-[β-D-apiosyl-(1->2)-β-D-glucoside]; 7-O-(β-D-Apiofuranosyl-1,2-β-D-glucosyl)-5,7,4'-trihydroxyflavone; Apiin; 7-[(2-O-D-Apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxy-phenyl)-4H-1-benzopyran-4-one; Apioside | Neoschaftoside  | Schaftoside  |
| 3591 | -1.657 | -1.724 | Ph  | 375.129648 | 376.136925 | -0.059642 | C16H24O10    | 3  | Loganate; Loganic acid   | 7-Epiloganic acid   |  |
| 3500 | -1.657 | -1.646 | Ph  | 371.134722 | 372.141998 | -0.092343 | C17H24O9     | 1  | Syringin; Eleutheroside B  |   |  |
| 3072 | -1.653 | -1.633 | AmS | 356.098668 | 357.105944 | -0.103781 | C15H19NO9    | 1  | cyclo-Dopa 5-O-glucoside   |   |  |
| 2539 | -1.650 | -1.757 | Ph  | 337.113983 | 338.121259 | 0.392818  | C12H20N2O9   | 1  | O18 isotope of 3-Epihydroxymugineic acid   |   |  |
| 4597 | -1.648 | -1.696 | Ph  | 419.155889 | 420.163166 | 0.009385  | C18H28O11    | 2  | Lamioside  | Lamioside (see KEGG C11645) [C10 isoprenoids (monoterpenes) [PR0102]]   |  |
| 3972 | -1.622 | -1.830 | Lp  | 389.181684 | 390.188961 | -0.055764 | C18H30O9     | 1  | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11-β-D-   |   |  |

|      |        |        |    |            |            |           |            |    |  |   |   |
|------|--------|--------|----|------------|------------|-----------|------------|----|--|---|---|
|      |        |        |    |            |            |           |            |    | glucoside; {(1R,2R)-2-[4-(β-D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]]   |   |   |
| 7153 | -1.619 | -1.227 | Ph | 577.135234 | 578.142510 | 0.145859  | C30H26O12  | 22 | Epicatechin-(4β->8)-ent-epicatechin  | Procyanidin B4; Catechin-(4α->8)-epicatechin  | Procyanidin B2; Procyanidol B2  |
| 1733 | -1.603 | -1.800 | Ph | 305.124160 | 306.131437 | 0.457167  | C12H20N2O7 | 1  | O18 isotope of 2'-Deoxymugineic acid   |   |   |
| 3967 | -1.597 | -1.371 | Ph | 389.124168 | 390.131444 | -0.060382 | C20H22O8   | 5  | Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside  | Populin   | Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                  |
| 3651 | -1.590 | -1.643 | Ph | 377.160554 | 378.167830 | -0.061522 | C20H26O7   | 5  | Chaparrinone   | Cnicin  | Eupahyssopin  |
| 4289 | -1.586 | -1.765 | Ph | 403.124570 | 404.131847 | -0.036646 | C17H24O11  | 2  | Gardenoside  | Scandoside methyl ester   |   |
| 4511 | -1.585 | -1.967 | Lp | 413.218120 | 414.225397 | 0.069673  | C21H34O8   | 3  | methyl 5-hydroperoxy-6,8,9,11-bisepidioxy-12,14-eicosadienoate [Hydroperoxy fatty acids [FA0104]]  | methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]]  | methyl 6,8-epidioxy-5,15-dihydroperoxy-9,11,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrienoic acids [FA0305]] |
| 2807 | -1.560 | -1.481 | Cb | 347.134705 | 348.141981 | -0.146980 | C15H24O9   | 1  | Leonuridine  |   |   |
| 1303 | -1.544 | -1.835 | Ph | 281.139425 | 282.146702 | -0.078970 | C15H22O5   | 6  | Hymenoxon  | Qing Hau Sau; Artemisinin   | Dihydrophaseic acid; (-)-Dihydrophaseic acid  |
| 4441 | -1.541 | -1.531 | Ph | 409.150412 | 410.157688 | 0.014166  | C20H26O9   | 2  | Bruceine D   | C20H26O9  |   |
| 80   | -1.538 | -1.984 | Cb | 179.056091 | 180.063368 | -0.114407 | C6H12O6    | 69 | D-Glucose; Grape sugar; Dextrose   | D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose   | D-Galactose   |
| 1351 | -1.532 | -1.627 | Cb | 285.097947 | 286.105223 | -0.104355 | C13H18O7   | 4  | Salicin; Salicoside  | Gastrodin; 4-(Hydroxymethyl)phenyl-β-D-glucopyranoside  | Methylarbutin   |
| 3540 | -1.529 | -1.619 | Ph | 373.113993 | 374.121269 | -0.074217 | C16H22O10  | 4  | Secologanate   | Swertiamarin  | Geniposidic acid  |
| 5778 | -1.528 | -1.528 | Cb | 485.082492 | 486.089768 | 0.446498  | C20H20O14  | 1  | O18 isotope of 1-O,6-O-Digalloyl-β-D-glucose   |   |   |
| 2684 | -1.519 | -1.787 | Cb | 343.124543 | 344.131820 | -0.121434 | C12H24O11  | 4  | Melibiiitol; 6-O-α-D-Galactosyl-D-glucitol   | Clusianose  | Maltitol; 4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol [acetal]                      |
| 2222 | -1.506 | -1.601 | Cb | 325.113981 | 326.121258 | -0.120525 | C12H22O10  | 6  | α-L-Fucosyl-1,2-β-D-galactoside; Glycoprotein α-L-fucosyl-(1,2)-D-galactose; Glycolipid α-L-fucosyl-1,2-β-D-galactose; α-L-Fucosyl-(1->2)-D-galactosyl-R | 2-O-α-L-Rhamnopyranosyl-D-glucopyranose; Neohesperidose   | Robinobiose   |
| 6404 | -1.504 | -1.603 | Ph | 521.202869 | 522.210145 | 0.064409  | C26H34O11  | 2  | Isobrucein A   | Quassamarin   |   |
| 3922 | -1.497 | -2.042 | Lp | 387.166034 | 388.173310 | -0.057526 | C18H28O9   | 2  | Tuberonic acid glucoside   | Tuberonic acid glucoside (see KEGG C08558); (1R,2S)-3-oxo-2-(5'-O-β-D-glucopyranosyloxy-2'Z-pentenyl)-cyclopentaneacetic acid [Fatty acyl glycosides of mono- and disaccharides [FA1301]] |   |

|      |        |        |    |            |            |           |            |    |  |   |   |
|------|--------|--------|----|------------|------------|-----------|------------|----|--|---|---|
| 199  | -1.489 | -1.629 | Ph | 205.035328 | 206.042604 | -0.236504 | C7H10O7    | 7  | (R)-2-Hydroxybutane-1,2,4-tricarboxylate; Homocitrate; Homocitric acid; 3-Hydroxy-3-carboxyadipic acid; (R)-2-Hydroxy-1,2,4-butanetricarboxylic acid | 2-Methylcitrate; 2-Hydroxybutane-1,2,3-tricarboxylate; (2R,3S)-2-Hydroxybutane-1,2,3-tricarboxylate   | (2S,3R)-3-Hydroxybutane-1,2,3-tricarboxylate; Methylisocitrate; Methylisocitric acid                    |
| 2088 | -1.470 | -1.476 | Pp | 320.062277 | 321.069553 | -0.132751 | C11H15NO10 | 1  | $\beta$ -Citryl-L-glutamic acid; 3-[[[(2S)-1,5-dihydroxy-1, 5-dioxopentan-2-yl]carbamoyl]-3-hydroxypentanedioic acid [tertiary alcohol]              |   |   |
| 3977 | -1.467 | -1.400 | Cb | 389.218068 | 390.225344 | -0.061128 | C19H34O8   | 2  | Rehmaionoside A  | Rehmaionoside B   |   |
| 3598 | -1.437 | -1.789 | Cb | 375.202440 | 376.209716 | -0.005151 | C18H32O8   | 1  | 2,3-di-O-hexanoyl- $\alpha$ -glucopyranose [Other acyl sugars [SL05]]  |   |   |
| 3508 | -1.433 | -1.751 | Lp | 371.243903 | 372.251179 | -0.025932 | C20H36O6   | 5  | 8,8a-Deoxyoleandolide  | 19(R)-hydroxy-PGF1 $\alpha$ ; 9S,11R,15S,19R-tetrahydroxy-13E-prostaenoic acid [Prostaglandins [FA0301]]  | 13,14-dihydro-19(R)-hydroxyPGE1; 9-oxo-11R,15S,19R-trihydroxy-prostanoic acid [Prostaglandins [FA0301]] |
| 2074 | -1.420 | -1.372 | Cb | 319.139804 | 320.147080 | -0.116812 | C14H24O8   | 2  | Valproic acid glucuronide (see KEGG C03033); 3,4,5-trihydroxy-6-(2-propylpentanoyloxy)oxane-2-carboxylic acid [secondary alcohol]                    | Octanoylglucuronide (see KEGG C03033) [secondary alcohol]   |   |
| 6097 | -1.407 | -1.308 | Cb | 503.161797 | 504.169074 | 0.077257  | C18H32O16  | 21 | Raffinose; Melitose; Melitriose; Gossypose; 6G- $\alpha$ -D-galactosylsucrose  | Panose  | Galactomannan; Galactomannoglycan   |
| 7699 | -1.389 | -1.146 | Ph | 633.073451 | 634.080728 | 0.180016  | C27H22O18  | 1  | Corilagin  |   |   |
| 574  | -1.380 | -1.420 | Lp | 255.232918 | 256.240194 | -0.141782 | C16H32O2   | 23 | Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid   | Palmitic acid (see KEGG C00249); Hexadecanoic acid [carboxylic acid]  | Trimethyltridecanoic acid; 4,8,12-trimethyltridecanoic acid [carboxylic acid]                           |
| 1730 | -1.378 | -1.467 | Pp | 305.087764 | 306.095041 | 0.422086  | C11H16N2O8 | 2  | <i>O18 isotope of N-Acetyl-aspartyl-glutamate; NAAG</i>  | <i>O18 isotope of N-Acetylaspartylglutamic acid (see KEGG C12270); 2-[(2-acetamido-3-carboxypropanoyl)amino]pentanedioic acid [carboxylic acid]</i> |   |
| 1586 | -1.363 | -1.218 | Ph | 299.077209 | 300.084485 | -0.108396 | C13H16O8   | 1  | 4-( $\beta$ -D-Glucosyloxy)benzoate  |   |   |
| 4335 | -1.358 | -1.064 | Ph | 405.119098 | 406.126375 | -0.018591 | C20H22O9   | 7  | Astringin  | Trichocarpin  | Anadanthoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                     |
| 7306 | -1.352 | -1.032 | Cb | 593.130164 | 594.137440 | 0.167509  | C30H26O13  | 16 | Tribuloside  | Apigenin 7-glucoside-4'- <i>trans</i> -caffeate [Flavones and Flavonols [PK1211]]   | Apigenin 7-(6"-E-Caffeoylglucoside) [Flavones and Flavonols [PK1211]]                                   |
| 3145 | -1.292 | -1.382 | Cb | 359.098337 | 360.105614 | -0.091802 | C15H20O10  | 1  | 3-Methoxy-4-hydroxyphenylglycol glucuronide (see KEGG C03033);   |   |   |

|      |        |        |     |            |            |           |            |    |   |   |  |
|------|--------|--------|-----|------------|------------|-----------|------------|----|---|---|--|
| 2575 | -1.287 | -1.307 | Cb  | 339.093245 | 340.100522 | -0.117669 | C12H20O11  | 4  | (2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-hydroxy-2-(4-hydroxy-3-methoxy-phenyl)ethoxy]oxane-2-carboxylic acid [acetal]                                  | 3-Ketolactose   | 3-Ketosucrose; 3-Dehydro- $\alpha$ -D-glucosyl- $\beta$ -D-fructofuranoside  |
| 291  | -1.279 | -1.736 | Cb  | 221.066628 | 222.073904 | -0.220142 | C8H14O7    | 4  | Cellobiono-1,5-lactone; Cellobiose-1,5-lactone  | 6-Acetyl- $\beta$ -D-galactoside  | Ethyl glucuronide; (2S,3S,4S,5R)-6-ethoxy-3,4,5-trihydroxyoxane-2-carboxylic acid [acetal]   |
| 5262 | -1.261 | -1.114 | Ph  | 455.353108 | 456.360385 | 0.086530  | C30H48O3   | 20 | Betulinic acid  | $\alpha$ -Elemolic acid   | Ursolic acid   |
| 4329 | -1.226 | -1.712 | Ph  | 405.082709 | 406.089985 | -0.028041 | C19H18O10  | 7  | Lancerin; 4-C-Glucosyl-1,3,7-trihydroxyxanthone   | 5,7,3',5'-Tetrahydroxy-3,6,8,4'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]   | 5,7,3',4'-Tetrahydroxy-3,6,8,5'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]  |
| 5658 | -1.183 | -1.001 | Cb  | 479.083140 | 480.090416 | 0.053553  | C21H20O13  | 18 | Gossypin; Gossypetin 8-O-glucoside  | 4-o-Galloylbergenin   | 11-o-Galloylbergenin   |
| 224  | -1.134 | -1.746 | Cb  | 209.066629 | 210.073905 | -0.227478 | C7H14O7    | 5  | Sedoheptulose; D-altro-Heptulose; D-Sedoheptulose; Volemulose   | $\alpha$ -D-Mannoheptulopyranose; Mannoheptulose  | $\beta$ -D-Sedoheptulopyranose; $\beta$ -D-Sedoheptulose   |
| 2506 | -1.060 | -2.069 | AmS | 336.129968 | 337.137244 | -0.110462 | C13H23NO9  | 3  | Streptobiosamine  |   |  |
| 8856 | -1.010 | -0.816 | Lp  | 831.502796 | 832.510072 | -0.128394 | C43H77O13P | 12 | PI(14:0/20:3(8Z,11Z,14Z)); 1-tetradecanoyl-2-(8Z,11Z,14Z-eicosatrienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]] | PI(14:1(9Z)/20:2(11Z,14Z)); 1-(9Z-tetradecenoyl)-2-(11Z,14Z-eicosadienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]] | PI(17:1(9Z)/17:2(9Z,12Z)); 1-(9Z-heptadecenoyl)-2-(9Z,12Z-heptadecadienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]] |
| 6992 | -0.942 | -0.942 | Ph  | 563.177052 | 564.184328 | 0.065793  | C27H32O13  | 6  | Pinocembrin 7-rhamnosylglucoside  | Cascaroside D   | Cascaroside C  |
| 6072 | -0.779 | -0.905 | Cb  | 501.146171 | 502.153448 | 0.125686  | C18H30O16  | 1  | $\alpha$ -L-Rhamnopyranosyl-(1->2)- $\beta$ -D-galactopyranosyl-(1->2)- $\beta$ -D-glucuronopyranoside; $\beta$ -Fabatriose                           |   |  |

**j) List of the 165 identified compounds from the 761 common significant *m/z* of combined WSHS stresses samples at time A.** Functional category counts: Ph:87; Lp:23; Cb:35; Pp:6; AmS:4; Nu:0; NM:10.

| ID   | WSHS<br><i>Ds</i> -NI | WSHS<br><i>Np</i> -NI | Cat. | <i>m/z</i> | Mass       | error<br>(ppm) | Formula    | n | Identification  |   |                |
|------|-----------------------|-----------------------|------|------------|------------|----------------|------------|---|---|---|----------------|
| 5781 | -2.818                | -2.818                | Ph   | 485.108961 | 486.116238 | 0.054370       | C24H22O11  | 2 | Flavonol 3-O-(6-O-malonyl- $\beta$ -D-glucoside)      | Epigallocatechin 3-O-(3,5-di-O-methylgallate) [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] |                |
| 1087 | -2.766                | -2.766                | Pp   | 265.144542 | 266.151818 | 0.677275       | C14H20N2O3 | 6 | <i>O18</i> isotope of Subaphyllin; Feruloylputrescine | <i>Mukaadial</i>  | <i>Rugosal</i> |



|      |        |        |    |            |            |           |           |    |   |   |   |
|------|--------|--------|----|------------|------------|-----------|-----------|----|---|---|---|
| 5566 | -2.662 | -2.298 | Ph | 473.363676 | 474.370953 | 0.090535  | C30H50O4  | 15 | Sapelin A   | Bryodulcosigenin  | Soyasapogenol A   |
| 4717 | -2.655 | -2.791 | Ph | 425.087827 | 426.095103 | 0.049636  | C22H18O9  | 2  | Epiafzelechin 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                   | Epigallocatechin 3-O-(4-hydroxybenzoate) [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                      |   |
| 1130 | -2.584 | -2.584 | Ph | 269.045564 | 270.052841 | 0.064429  | C15H10O5  | 42 | Apigenin; 4',5,7-Trihydroxyflavone; 5,7,4'-Trihydroxyflavone                                      | 2'-Hydroxydaidzein  | Genistein; 5,7,4'-Trihydroxyisoflavone  |
| 7699 | -2.575 | -2.997 | Ph | 633.073451 | 634.080728 | 0.180016  | C27H22O18 | 1  | Corilagin   |   |   |
| 5278 | -2.563 | -2.563 | Ph | 457.077691 | 458.084967 | 0.122575  | C22H18O11 | 7  | Epigallocatechin 3-gallate  | 8-Demethyltetracenomycin C  | Epigallocatechin gallate (see KEGG C09731); [(2R,3R)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)chroman-3-yl] 3,4,5-trihydroxybenzoate [phenol or hydroxyhetarene] Traumatins; (10E)-12-Oxododecenoic acid |
| 233  | -2.480 | -2.480 | Lp | 211.133944 | 212.141220 | -0.115861 | C12H20O3  | 15 | Cucurbitic acid   | Putaminoxin   |   |
| 5457 | -2.465 | -2.645 | Ph | 467.098394 | 468.105671 | 0.051411  | C24H20O10 | 2  | Epigallocatechin 3-O-cafeate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                | Apocynin A [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |   |
| 3970 | -2.462 | -2.462 | Ph | 389.160552 | 390.167829 | -0.062778 | C21H26O7  | 2  | Erioflorin acetate  |   |   |
| 5778 | -2.458 | -2.458 | Cb | 485.082492 | 486.089768 | 0.446498  | C20H20O14 | 1  | <i>O18 isotope of 1-O,6-O-Digalloyl-β-D-glucose</i>   |   |   |
| 132  | -2.410 | -2.410 | Ph | 191.034952 | 192.042228 | -0.159394 | C10H8O4   | 10 | Scopoletin  | Naphthazarin; 5,8-Dihydroxy-1,4-naphthoquinone  | 3,4-Dehydro-6-hydroxymellein  |
| 5733 | -2.375 | -2.375 | Ph | 483.093470 | 484.100746 | 0.382970  | C24H20O11 | 2  | Tetracenomycin X  |   |   |
| 3099 | -2.369 | -2.369 | Ph | 357.107697 | 358.114974 | -0.013607 | C16H20O9  | 4  | <i>O18 isotope of Gentiopicroin; Gentiopicroside</i>  | <i>O18 isotope of 1-O-Feruloyl-β-D-glucose; 1-Feruloyl-D-glucose</i>  | <i>O18 isotope of Gentiopicroin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]</i>   |
| 3831 | -2.353 | -2.353 | Ph | 384.145333 | 385.152609 | 0.187448  | C21H23NO6 | 1  | Polycarpine   |   |   |
| 6042 | -2.337 | -2.337 | NM | 499.291301 | 500.298577 | 0.088261  | C26H44O9  | 1  | Mupirocin   |   |   |
| 1843 | -2.335 | -2.474 | Ph | 310.093192 | 311.100468 | -0.108516 | C14H17NO7 | 4  | Taxiphyllin; (R)-4-Hydroxymandelonitrile β-D-glucoside  | Dhurrin; (S)-4-Hydroxymandelonitrile β-D-glucoside  | p-Glucosyloxymandelonitrile   |
| 4635 | -2.320 | -2.320 | Ph | 421.186827 | 422.194104 | 0.084740  | C22H30O8  | 4  | Valtratum; Valtrate   | Isovaltrate   | Picrasin F  |
| 3088 | -2.319 | -2.319 | Ph | 357.061579 | 358.068856 | -0.032332 | C18H14O8  | 10 | 5,3'-Dihydroxy-4',5'-dimethoxy-6,7-methylenedioxyisoflavone [Isoflavonoids [PK1205]]              | Dalpalatin [Isoflavonoids [PK1205]]   | Luteolin 7-lactate [Flavones and Flavonols [PK1211]]  |
| 5262 | -2.317 | -2.187 | Ph | 455.353108 | 456.360385 | 0.086530  | C30H48O3  | 20 | Betulonic acid  | α-Elementic acid  | Ursolic acid  |
| 4511 | -2.304 | -1.932 | Lp | 413.218120 | 414.225397 | 0.069673  | C21H34O8  | 3  | methyl 5-hydroperoxy-6,8,9,11-bisepidioxy-12,14-eicosadienoate [Hydroperoxy fatty acids [FA0104]] | methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrien oic acids [FA0305]] | methyl 6,8-epidioxy-5,15-dihydroperoxy-9,11,13-eicosatrienoate [Hydroxy/hydroperoxyeicosatrien oic acids [FA0305]]  |
| 4985 | -2.295 | -2.728 | Ph | 441.082837 | 442.090114 | 0.264769  | C22H18O10 | 10 | Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                   | ent-Robinetinidol 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                                 | Catechin 3-O-gallate [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 4377 | -2.291 | -2.291 | Ph | 407.077314 | 408.084590 | 0.179320  | C22H16O8  | 4  | Tetracenomycin E  | Tetracenomycin B2   | Torosaflavone C [Flavones and Flavonols [PK1211]]   |

|      |        |        |    |            |            |           |           |    |  |   |  |
|------|--------|--------|----|------------|------------|-----------|-----------|----|--|---|--|
| 2893 | -2.258 | -2.258 | Lp | 350.306446 | 351.313723 | -0.019531 | C22H41NO2 | 11 | Anandamide (20:2, n-6); N-(11Z,14Z-eicosadienoyl)-ethanolamine [N-acyl ethanolamines (endocannabinoids) [FA0804]]  |   |  |
| 3591 | -2.248 | -2.415 | Ph | 375.129648 | 376.136925 | -0.059642 | C16H24O10 | 3  | Loganate; Loganic acid   | 7-Epiloganic acid   | $\alpha$ -Tocotrienol (see KEGG C14153); (2R)-2,5,7,8-tetramethyl-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trienyl]chroman-6-ol [phenol or hydroxyhetarene] |
| 4688 | -2.246 | -2.246 | Lp | 423.326893 | 424.334170 | 0.092124  | C29H44O2  | 4  | $\alpha$ -Tocotrienol  | 4,4'-Methylenebis(2,6-di-tert-butylphenol)  |  |
| 4730 | -2.237 | -2.237 | Ph | 425.181737 | 426.189014 | 0.073384  | C21H30O9  | 2  | Absciscic acid glucose ester; absciscic acid- $\beta$ -D-glucopyranosyl ester  | $\gamma$ -CEHC Glc; $\gamma$ -carboxyethyl-hydroxychroman $\beta$ -D-glucoside [Vitamin E [PR0202]]                     |  |
| 2684 | -2.216 | -2.383 | Cb | 343.124543 | 344.131820 | -0.121434 | C12H24O11 | 4  | Melibiotol; 6-O- $\alpha$ -D-Galactosyl-D-glucitol   | Clusianose  | Maltitol; 4-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol [acetal]   |
| 5171 | -2.211 | -2.372 | Ph | 451.103475 | 452.110751 | 0.041592  | C24H20O9  | 6  | Cinchonain 1a  | 9,10-Dihydro-10-(3,4-dihydroxyphenyl)-pyrano[2,3-h]catechin-8-one [Flavans, Flavanols and Leucoanthocyanidins [PK1202]] | Cinchonain Ib [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 4599 | -2.210 | -2.210 | Ph | 419.171164 | 420.178440 | 0.053946  | C22H28O8  | 6  | Eupacunolin  | Eupacunoxin   | Eupaformosanin   |
| 4636 | -2.209 | -2.114 | Cb | 421.207924 | 422.215201 | 0.008100  | C19H34O10 | 1  | 1-Octen-3-ol-3-o- $\beta$ -D-xylopyranosyl(1->6)- $\beta$ -D-glucopyranoside   |   |  |
| 306  | -2.204 | -2.204 | Ph | 223.133928 | 224.141204 | -0.180408 | C13H20O3  | 8  | Vomifoliol; (6S,9R)-6-hydroxy-3-oxo- $\alpha$ -ionol   | (+/-)-6-Hydroxy-3-oxo- $\alpha$ -ionol  | Methyl jasmonate; (-)-Methyl jasmonate   |
| 1722 | -2.181 | -1.809 | Ph | 305.066640 | 306.073916 | -0.120233 | C15H14O7  | 11 | Leucocyanidin; 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol; 3,3',4,4',5,7-Flavanhexol; 3,4-Cyanidiol; Leucoanthocyanidol; Leucocianidol; Leucocyanidol; Leukocyanidine; Procyanidol; Resivit; 2,3-trans-3,4-cis-Leucocyanidin | (+)-Gallocatechin; Gallocatechol  | (-)-Epigallocatechin   |
| 1583 | -2.176 | -2.176 | Ph | 299.056112 | 300.063389 | 0.002400  | C16H12O6  | 77 | 5,7,4'-Trihydroxy-3'-methoxyflavone; 3'-O-Methylfluteolin; Chrysoeriol   | 3-Methoxyapigenin; 3-O-Methylkaempferol   | Leptosidin   |
| 3926 | -2.176 | -2.584 | Cb | 387.202414 | 388.209691 | -0.070880 | C19H32O8  | 5  | Rehmaionoside C  | methyl 9-hydroperoxy-10,12,13,15-bisepidioxy-16E-octadecenoate [Hydroperoxy fatty acids [FA0104]]                       | methyl 10,12,13,15-bisepidioxy-16-hydroperoxy-8E-octadecenoate [Hydroperoxy fatty acids [FA0104]]  |
| 6299 | -2.172 | -2.172 | Lp | 515.286219 | 516.293495 | 0.092665  | C26H44O10 | 2  | L-Olivosyl-oleandolide   | L-Olivosyl-oleandolide (see KEGG C11991) [Macrolides and lactone polyketides [PK04]]                                    |  |

|      |        |        |     |            |            |           |            |    |  |   |   |
|------|--------|--------|-----|------------|------------|-----------|------------|----|--|---|---|
| 1247 | -2.143 | -2.143 | Ph  | 277.092868 | 278.100145 | -0.082506 | C11H18O8   | 5  | Tuliposide A   | Isovalerylglucuronide (see KEGG C03033); (2S,3S,4S,5R,6S)-3,4,5-trihydroxy-6-(3-methylbutanoyloxy)oxane-2-carboxylic acid [secondary alcohol] |   |
| 2506 | -2.134 | -2.071 | AmS | 336.129968 | 337.137244 | -0.110462 | C13H23NO9  | 3  | Streptobiosamine   |   |   |
| 5460 | -2.126 | -2.126 | Ph  | 467.119547 | 468.126824 | 0.101485  | C21H24O12  | 3  | Catechin-4-ol 3-O-β-D-galactopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Catechin-4-ol 3-O-β-D-glycopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   | Leucodelphinidin 3-O-α-L-rhamnopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 6097 | -2.126 | -2.102 | Cb  | 503.161797 | 504.169074 | 0.077257  | C18H32O16  | 21 | Raffinose; Melitose; Melitriose; Gossypose; 6G-α-D-galactosylsucrose   | Panose  | Galactomannan; Galactomannoglycan   |
| 1303 | -2.121 | -2.121 | Ph  | 281.139425 | 282.146702 | -0.078970 | C15H22O5   | 6  | Hymenoxon  | Qing Hau Sau; Artemisinin   | Dihydrophaseic acid; (-)-Dihydrophaseic acid  |
| 4338 | -2.116 | -2.362 | Ph  | 405.140233 | 406.147509 | -0.005430 | C17H26O11  | 4  | Ipolamiide   | 10-Hydroxyloganin   | Morroniside   |
| 2347 | -2.105 | -2.304 | AmS | 330.119400 | 331.126676 | -0.122722 | C14H21NO8  | 1  | 5'-O-β-D-Glucosylpyridoxine  |   |   |
| 4393 | -2.102 | -2.795 | Ph  | 407.171139 | 408.178415 | -0.005805 | C21H28O8   | 2  | Vernoflexuoside  |   |   |
| 3153 | -2.095 | -2.156 | Ph  | 359.134719 | 360.141996 | -0.102120 | C16H24O9   | 2  | 7-Deoxyloganate  | 8-Epideoxyloganic acid  |   |
| 3540 | -2.086 | -2.238 | Ph  | 373.113993 | 374.121269 | -0.074217 | C16H22O10  | 4  | Secologanate   | Swertiamarin  | Geniposidic acid  |
| 4590 | -2.077 | -1.202 | Ph  | 419.098382 | 420.105659 | 0.027948  | C20H20O10  | 7  | 5,3',5'-Trihydroxy-3,6,7,8,4'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]  | 5,7,4'-Trihydroxy-3,6,8,3',5'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]   | 5,7,3'-Trihydroxy-3,6,8,4',5'-pentamethoxyflavone [Flavones and Flavonols [PK1211]]   |
| 3355 | -2.075 | -1.508 | AmS | 366.140542 | 367.147819 | -0.074144 | C14H25NO10 | 3  | N-Acetyl-6-O-L-fucosyl-D-glucosamine [aldehyde]  | 2-Acetamido-2-deoxy-6-O-α-L-fucopyranosyl-D-glucose [aldehyde]  | 3-O-fucopyranosyl-2-acetamido-2-deoxyglucopyranose; N-[(2R,3R,4R,5R)-4,5,6-trihydroxy-1-oxo-3-[(2R,3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyl-oxan-2-yl]oxy-hexan-2-yl]acetamide [aldehyde] |
| 1158 | -2.056 | -2.056 | Ph  | 271.061181 | 272.068458 | -0.058348 | C15H12O5   | 37 | Naringenin; 4',5,7-Trihydroxyflavanone   | (6aS,11aS)-3,6a,9-Trihydroxypterocarpan; 3,6,9-Trihydroxypterocarpan; (-)-Glycinol  | Licodione   |
| 5493 | -2.050 | -1.744 | Ph  | 469.135176 | 470.142452 | 0.055729  | C21H26O12  | (1 | Plumieride   |   |   |
| 1376 | -2.043 | -2.159 | Ph  | 287.056089 | 288.063365 | -0.079954 | C15H12O6   | 33 | Dihydrokaempferol; Aromadendrin; (+)-Dihydrokaempferol; (+)-Aromadendrin   | Fustin; 2,3-Dihydrofisetin  | Eriodictyol   |
| 80   | -2.026 | -2.246 | Cb  | 179.056091 | 180.063368 | -0.114407 | C6H12O6    | 69 | D-Glucose; Grape sugar; Dextrose   | D-Fructose; Levulose; Fruit sugar; D-arabino-Hexulose   | D-Galactose   |
| 2222 | -2.026 | -2.601 | Cb  | 325.113981 | 326.121258 | -0.120525 | C12H22O10  | 6  | α-L-Fucosyl-1,2-β-D-galactoside; Glycoprotein α-L-fucosyl-(1,2)-D-galactose; Glycolipid α-L-fucosyl-1,2-β-D-galactose; α-L-Fucosyl-(1->2)-D-galactosyl-R | 2-O-α-L-Rhamnopyranosyl-D-glucopyranose; Neohesperidose   | Robinobiose   |
| 3977 | -2.025 | -2.552 | Cb  | 389.218068 | 390.225344 | -0.061128 | C19H34O8   | 2  | Rehmaionoside A  | Rehmaionoside B   |   |

|      |        |        |    |            |            |           |              |    |  |  |  |
|------|--------|--------|----|------------|------------|-----------|--------------|----|--|--|--|
| 4022 | -2.017 | -2.017 | Ph | 391.128449 | 392.135726 | 0.030165  | C20H22O8     | 5  | O18 isotope of Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3- $\beta$ -monoglucoside   | O18 isotope of Populin   | O18 isotope of Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 328  | -2.015 | -1.457 | Ph | 227.071321 | 228.078597 | -0.205916 | C14H12O3     | 10 | 3,4',5-Trihydroxystilbene; Resveratrol   | Seselin  | Trioxsalen; Trioxysalen; 4,8,5'-Trimethylpsoralen  |
| 3544 | -2.003 | -2.128 | Ph | 373.150383 | 374.157659 | -0.062393 | C17H26O9     | 4  | Deoxyloganin; 7-Deoxyloganin   | 8-Epideoxyloganin  | Deoxyloganin (see KEGG C06071) [C10 isoprenoids (monoterpenes) [PR0102]]   |
| 1409 | -1.978 | -1.666 | Ph | 289.071731 | 290.079007 | -0.106598 | C15H14O6     | 35 | cis-3,4-Leucopelargonidin  | Luteoforol; 3-Deoxyleuocyanidin  | (+)-Catechin; D-Catechin; Cyanidanol; (2R-trans)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-Benzopyran-3,5,7-triol; (2R,3S)-Catechin; (2R,3S)-(+)-Catechin; Cianidanol |
| 3927 | -1.972 | -1.972 | Lp | 387.238811 | 388.246087 | -0.041617 | C20H36O7     | 1  | 5,6-Dihydroxyprostaglandin F1a (see KEGG C06475) [secondary alcohol]   |  |  |
| 4441 | -1.971 | -2.412 | Ph | 409.150412 | 410.157688 | 0.014166  | C20H26O9     | 2  | Bruceine D   |  |  |
| 3594 | -1.966 | -2.088 | NM | 375.166033 | 376.173310 | 0.410054  | C21H27ClN2O2 | 1  | Cl37 isotope of Hydroxyzine  |  |  |
| 1677 | -1.963 | -2.020 | Ph | 303.050993 | 304.058270 | -0.108829 | C15H12O7     | 7) | Taxifolin; Dihydroquercetin; (+)-Dihydroquercetin; (+)-Taxifolin; trans-Dihydroquercetin   | Pentahydroxyflavanone; Dihydrotricetin   | cis-Dihydroquercetin   |
| 7306 | -1.938 | -1.894 | Cb | 593.130164 | 594.137440 | 0.167509  | C30H26O13    | 16 | Tribuloside  | Apigenin 7-glucoside-4'-trans-caffeate [Flavones and Flavonols [PK1211]]               | Apigenin 7-(6"-E-Caffeoylglucoside) [Flavones and Flavonols [PK1211]]  |
| 4779 | -1.915 | -1.915 | Ph | 429.082814 | 430.090090 | 0.218359  | C21H18O10    | 4  | Coumestrol 3-O-glucoside [Coumestan flavonoids [PK1209]]   | Chrysin 7-glucuronide [Flavones and Flavonols [PK1211]]                                | Derhamnosylmaysin [Flavones and Flavonols [PK1211]]  |
| 2179 | -1.911 | -1.962 | Cb | 323.098329 | 324.105606 | -0.127735 | C12H20O10    | 2  | Bis-D-fructose 2',1:2,1'-dianhydride; Difructose anhydride I; Di-D-fructose 1,2'; 2,1' dianhydride   | D-Fructofuranose 1,2':2,3'-dianhydride   |  |
| 4289 | -1.902 | -2.539 | Ph | 403.124570 | 404.131847 | -0.036646 | C17H24O11    | 2  | Gardenoside  | Scandoside methyl ester  |  |
| 1864 | -1.896 | -2.139 | Cb | 311.098334 | 312.105610 | -0.117249 | C11H20O10    | 6  | Vicianose; O- $\alpha$ -L-Arabinopyranosyl-(1-6)-D-glucopyranose   | Arabino-galactose  | 6-O- $\beta$ -D-Xylopyranosyl-D-glucose; Primeverose   |
| 3972 | -1.878 | -2.124 | Lp | 389.181684 | 390.188961 | -0.055764 | C18H30O9     | 1  | (-)-11-hydroxy-9,10-dihydrojasmonic acid 11- $\beta$ -D-glucoside; {(1R,2R)-2-[4-( $\beta$ -D-glucopyranosyloxy)pentyl]-3-oxocyclopentyl}acetic acid [Jasmonic acids [FA0202]] |  |  |
| 191  | -1.857 | -2.203 | Pp | 203.082553 | 204.089830 | -0.236798 | C11H12N2O2   | 10 | L-Tryptophan; Tryptophan; (S)- $\alpha$ -Amino- $\beta$ -(3-indolyl)-propionic acid  | D-Tryptophan   | Tryptophan; $\alpha$ -Amino- $\beta$ -(3-indolyl)-propionic acid   |
| 8565 | -1.851 | -1.473 | Lp | 741.471328 | 742.478604 | 0.160654  | C40H71O10P   | 18 | PG(16:1(9Z)/18:3(6Z,9Z,12Z)); 1-(9Z-hexadecenoyl)-2-(6Z,9Z,12Z-octadecatrienoyl)-sn-   | PG(16:1(9Z)/18:3(9Z,12Z,15Z)); 1-(9Z-hexadecenoyl)-2-(9Z,12Z,15Z-octadecatrienoyl)-sn- | PG(18:3(6Z,9Z,12Z)/16:1(9Z)); 1-(6Z,9Z,12Z-octadecatrienoyl)-2-(9Z-hexadecenoyl)-sn-glycero-   |

|      |        |        |    |            |            |           |              |    |   |  |   |
|------|--------|--------|----|------------|------------|-----------|--------------|----|---|--|---|
| 7153 | -1.835 | -1.624 | Ph | 577.135234 | 578.142510 | 0.145859  | C30H26O12    | 22 | glycero-3-phospho-(1'-sn-glycerol) [primary alcohol]<br>Epicatechin-(4β->8)-ent-epicatechin   | glycero-3-phospho-(1'-sn-glycerol) [primary alcohol]<br>Procyanidin B4; Catechin-(4α->8)-epicatechin   | 3-phospho-(1'-sn-glycerol) [primary alcohol]<br>Procyanidin B2; Procyanidol B2  |
| 5489 | -1.833 | -2.011 | Ph | 469.114066 | 470.121342 | 0.096923  | C24H22O10    | 2  | Pongamoside B [Flavones and Flavonols [PK1211]]   | Pongamoside C [Flavones and Flavonols [PK1211]]  |   |
| 5001 | -1.830 | -2.096 | Cb | 441.176638 | 442.183914 | 0.038479  | C21H30O10    | 1  | Lusitanicoside  |  |   |
| 2057 | -1.817 | -1.992 | Ph | 319.045905 | 320.053181 | -0.113324 | C15H12O8     | 3  | Dihydromyricetin; Ampelopsin; (+)-Dihydromyricetin; (+)-Ampelopsin  | 2,3-Dihydrogossypetin  | Amaranol A; (+)- 2,4,6-Trihydroxy-2-[(3,4,5-trihydroxyphenyl)methyl]-3(2H)-benzofuranone [Aurone flavonoids [PK1213]]                         |
| 6216 | -1.816 | -2.313 | Ph | 511.218562 | 512.225838 | 0.149097  | C25H36O11    | 1  | gibberellin A2 O-β-D-glucoside [C20 isoprenoids (diterpenes) [PR0104]]  |  |   |
| 1135 | -1.814 | -2.546 | Lp | 269.081904 | 270.089181 | -0.104475 | C16H14O4     | 35 | (+)-Medicarpin; 3-Hydroxy-9-methoxypterocarpan  | Vignafuran   | Alloimperatorin   |
| 1730 | -1.813 | -1.593 | Pp | 305.087764 | 306.095041 | 0.422086  | C11H16N2O8   | 2  | O18 isotope of N-Acetyl-aspartyl-glutamate; NAAG  | O18 isotope of N-Acetyl-aspartylglutamic acid (see KEGG C12270); 2-[(2-acetamido-3-carboxy-propanoyl)amino]pentanedioic acid [carboxylic acid] |   |
| 3969 | -1.809 | -2.378 | NM | 389.145306 | 390.152582 | 0.415595  | C21H25ClN2O3 | 4  | Cl37 isotope of Cetirizine  | Cl37 isotope of Cetirizine (see KEGG C07778); 2-[2-[4-[(4-chlorophenyl)-phenyl-methyl]piperazin-1-yl]ethoxy]acetic acid [dialkyl ether]        | Loganin   |
| 4794 | -1.809 | -1.706 | Lp | 429.373813 | 430.381089 | 0.020016  | C29H50O2     | 11 | α-Tocopherol; Vitamin E   | 4β-Hydroxymethyl-4α-methyl-5α-cholest-7-en-3β-ol   | α-Tocopherol (see KEGG C02477); (2R)-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]chroman-6-ol [phenol or hydroxyhetarene]         |
| 8383 | -1.801 | -1.703 | Lp | 712.492329 | 713.499605 | 0.070622  | C39H72NO8P   | 30 | PE(14:0/20:3(5Z,8Z,11Z)) (see KEGG C00350); 1-tetradecanoyl-2-(5Z,8Z,11Z-eicosatrienoyl)-sn-glycero-3-phosphoethanolamine [primary amine] | PE(14:0/20:3(8Z,11Z,14Z)) (see KEGG C00350); 1-tetradecanoyl-2-(8Z,11Z,14Z-eicosatrienoyl)-sn-glycero-3-phosphoethanolamine [primary amine]    | PE(14:1(9Z)/20:2(11Z,14Z)) (see KEGG C00350); 1-(9Z-tetradecenoyl)-2-(11Z,14Z-eicosadienoyl)-sn-glycero-3-phosphoethanolamine [primary amine] |
| 291  | -1.778 | -2.619 | Cb | 221.066628 | 222.073904 | -0.220142 | C8H14O7      | 4  | 6-Acetyl-D-glucose  | 6-Acetyl-β-D-galactoside   | Ethyl glucuronide; (2S,3S,4S,5R)-6-ethoxy-3,4,5-trihydroxyoxane-2-carboxylic acid [acetal]  |
| 2331 | -1.778 | -1.733 | Ph | 329.139407 | 330.146683 | -0.123563 | C19H22O5     | 7  | Podolide  | Gibberellin A51-catabolite   | Gibberellin A7  |
| 449  | -1.767 | -2.125 | Ph | 243.066250 | 244.073527 | -0.131492 | C14H12O4     | 10 | 3,3',4'5-Tetrahydroxystilbene; Piceatannol  | Wyerone acid   | Eriobofuran   |
| 170  | -1.761 | -1.761 | Lp | 199.170322 | 200.177598 | -0.159280 | C12H24O2     | 13 | Dodecanoic acid; Dodecanoate; Dodecylcarboxylate; Lauric acid   | Dodecanoic acid (see KEGG C02679); Dodecanoic acid [carboxylic acid]   | Lauric acid (see KEGG C02679); dodecanoic acid [Straight chain fatty acids [FA0101]]  |

|      |        |        |     |            |            |           |            |    |  |   |   |
|------|--------|--------|-----|------------|------------|-----------|------------|----|--|---|---|
| 6989 | -1.754 | -1.754 | Ph  | 563.140743 | 564.148019 | 0.201658  | C26H28O14  | 52 | Apigenin 7-O-[β-D-apiosyl-(1->2)-β-D-glucoside]; 7-O-(β-D-Apiofuranosyl-1,2-β-D-glucosyl)-5,7,4'-trihydroxyflavone; Apiin; 7-[(2-O-D-Apio-β-D-furanosyl-β-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxy-phenyl)-4H-1-benzopyran-4-one; Apioside | Neoschaftoside  | Schaftoside   |
| 4292 | -1.751 | -1.751 | Ph  | 403.139861 | 404.147137 | 0.048967  | C21H24O8   | 4  | Mallotophenone   | Koaburanin [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Orientanol A [Pterocarpanes [PK1207]]   |
| 6404 | -1.747 | -1.948 | Ph  | 521.202869 | 522.210145 | 0.064409  | C26H34O11  | 2  | Isobrucein A   | Quassamarin   |   |
| 11   | -1.738 | -2.234 | Cb  | 161.045532 | 162.052809 | -0.091525 | C6H10O5    | 30 | Lichenin; Lichenan   | (R)-3,3-Dimethylmalate  | 3-Ethylmalate   |
| 3598 | -1.736 | -2.111 | Cb  | 375.202440 | 376.209716 | -0.005151 | C18H32O8   | 1  | 2,3-di-O-hexanoyl-α-glucopyranose [Other acyl sugars [SL05]]   |   |   |
| 5732 | -1.716 | -1.835 | Cb  | 483.078040 | 484.085316 | 0.022519  | C20H20O14  | 1  | 1-O,6-O-Digalloyl-β-D-glucose  |   |   |
| 2539 | -1.714 | -1.762 | Ph  | 337.113983 | 338.121259 | 0.392818  | C12H20N2O9 | 1  | O18 isotope of 3-Epihydroxymugineic acid   |   |   |
| 2271 | -1.706 | -1.789 | Ph  | 327.108499 | 328.115775 | -0.129529 | C15H20O8   | 3  | Anisatin   | Paeonoside  |   |
| 3967 | -1.697 | -1.797 | Ph  | 389.124168 | 390.131444 | -0.060382 | C20H22O8   | 5  | Piceid; Polydatin; 3,4,5-Trihydroxystilbene-3-β-monoglucoside  | Populin   | Apigeniflavan 5-O-xyloside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]                        |
| 3918 | -1.691 | -2.229 | Cb  | 387.129645 | 388.136921 | -0.066108 | C17H24O10  | 5  | Secologanin; (-)-Secologanin   | Geniposide  | Verbenalin; Cornin (glycoside)  |
| 224  | -1.686 | -1.919 | Cb  | 209.066629 | 210.073905 | -0.227478 | C7H14O7    | 5  | Sedoheptulose; D-altro-Heptulose; D-Sedoheptulose; Volemulose  | α-D-Mannoheptulopyranose; Mannoheptulose  | β-D-Sedoheptulopyranose; β-D-Sedoheptulose  |
| 865  | -1.662 | -1.427 | Pp  | 263.077210 | 264.084487 | 0.530806  | C9H14N2O7  | 1  | O18 isotope of L-β-aspartyl-L-glutamic acid [primary amine]  |   |   |
| 4847 | -1.659 | -1.690 | Ph  | 433.114041 | 434.121318 | 0.048061  | C21H22O10  | 32 | Naringenin 7-O-β-D-glucoside; Prunin   | Phlorizin chalcone; Chalcone 2'-O-glucoside   | 2',4,4',6'-Tetrahydroxychalcone 4'-O-glucoside; THC 4'-glucoside  |
| 3922 | -1.659 | -1.817 | Lp  | 387.166034 | 388.173310 | -0.057526 | C18H28O9   | 2) | Tuberonic acid glucoside   | Tuberonic acid glucoside (see KEGG C08558); (1R,2S)-3-oxo-2-(5'-O-β-D-glucopyranosyloxy-2'Z-pentenyl)-cyclopentaneacetic acid [Fatty acyl glycosides of mono- and disaccharides [FA1301]] |   |
| 4814 | -1.654 | -1.784 | Cb  | 431.155905 | 432.163181 | 0.044900  | C19H28O11  | 1  | Zizybeoside I  |   |   |
| 4594 | -1.646 | -1.920 | Ph  | 419.134784 | 420.142061 | 0.067492  | C21H24O9   | 10 | Melampodin A   | Glycyphyllin; Phloretin 2'-O-rhamnoside   | Isorhapontin  |
| 3508 | -1.635 | -1.997 | Lp  | 371.243903 | 372.251179 | -0.025932 | C20H36O6   | 5  | 8,8a-Deoxyoleandolide  | 19(R)-hydroxy-PGF1α; 9S,11R,15S,19R-tetrahydroxy-13E-prostaenoic acid [Prostaglandins [FA0301]]   | 13,14-dihydro-19(R)-hydroxyPGE1; 9-oxo-11R,15S,19R-trihydroxy-prostanoic acid [Prostaglandins [FA0301]] |
| 6824 | -1.633 | -1.298 | Ph  | 549.182543 | 550.189820 | 0.089857  | C23H34O15  | 1  | Genipin 1-β-gentiobioside  |   |   |
| 3072 | -1.628 | -2.222 | AmS | 356.098668 | 357.105944 | -0.103781 | C15H19NO9  | 1  | cyclo-Dopa 5-O-glucoside   |   |   |



|      |        |        |    |            |            |           |              |    |  |   |  |
|------|--------|--------|----|------------|------------|-----------|--------------|----|--|---|--|
| 280  | -1.628 | -1.354 | Ph | 219.029852 | 220.037128 | -0.204938 | C11H8O5      | 4  | (3E)-4-(2-Carboxyphenyl)-2-oxobut-3-enoate; <i>trans</i> -2'-Carboxybenzalpyruvate   | Purpurogallin   | (3Z)-4-(2-Carboxyphenyl)-2-oxobut-3-enoate; <i>cis</i> -2'-Carboxybenzalpyruvate   |
| 2614 | -1.627 | -1.623 | Cb | 341.108884 | 342.116161 | -0.149462 | C12H22O11    | 45 | Sucrose; Cane sugar; Saccharose; 1- $\alpha$ -D-Glucopyranosyl-2- $\beta$ -D-fructofuranoside  | Cellobiose; 1- $\beta$ -D-Glucopyranosyl-4-D-glucopyranose  | Maltose; Malt sugar; $\alpha$ -D-Glucopyranosyl-(1->4)-D-glucopyranose   |
| 1733 | -1.595 | -2.225 | Ph | 305.124160 | 306.131437 | 0.457167  | C12H20N2O7   | 1  | <i>O18 isotope of 2'-Deoxymugineic acid</i>  |   |  |
| 1252 | -1.589 | -2.153 | NM | 277.144506 | 278.151783 | -0.095744 | C16H22O4     | 7  | 2-Ethylhexyl phthalate   | Dibutyl phthalate; Di-n-butyl phthalate; Dibutyl 1,2-benzenedicarboxylate   | Diisobutyl phthalate; DIBP   |
| 8856 | -1.589 | -1.463 | Lp | 831.502796 | 832.510072 | -0.128394 | C43H77O13P   | 12 | PI(14:0/20:3(8Z,11Z,14Z)); 1-tetradecanoyl-2-(8Z,11Z,14Z-eicosatrienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]]  | PI(14:1(9Z)/20:2(11Z,14Z)); 1-(9Z-tetradecenoyl)-2-(11Z,14Z-eicosadienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]] | PI(17:1(9Z)/17:2(9Z,12Z)); 1-(9Z-heptadecenoyl)-2-(9Z,12Z-heptadecadienoyl)-glycero-3-phospho-(1'-myo-inositol) [Diacylglycerophosphoinositols [GP0601]] |
| 5133 | -1.589 | -1.698 | Ph | 449.108952 | 450.116229 | 0.038519  | C21H22O11    | 25 | Neoastilbin; (2S,3S)-Taxifolin 3-rhamnoside  | 2',3,4,4',6'-Peptahydroxychalcone 4'-O-glucoside; PHC 4'-O-glucoside  | Astilbin   |
| 3500 | -1.572 | -1.811 | Ph | 371.134722 | 372.141998 | -0.092343 | C17H24O9     | 1  | Syringin; Eleutheroside B  |   |  |
| 1977 | -1.563 | -1.563 | NM | 315.144882 | 316.152158 | 0.418470  | C19H23ClN2   | 1  | <i>Cl37 isotope of Clomipramine</i>  |   |  |
| 2745 | -1.561 | -1.756 | Lp | 345.119057 | 346.126333 | -0.142585 | C15H22O9     | 4  | Aucubin  | Deutzioside   | Aucubin (see KEGG C09771) [C10 isoprenoids (monoterpenes) [PR0102]]  |
| 3101 | -1.559 | -2.041 | Cb | 357.119069 | 358.126345 | -0.103262 | C16H22O9     | 3  | Tarennoside  | 10-Deoxygeniposidic acid  | Sweroside  |
| 3145 | -1.552 | -1.851 | Cb | 359.098337 | 360.105614 | -0.091802 | C15H20O10    | 1  | 3-Methoxy-4-hydroxyphenylglycol glucuronide (see KEGG C03033); (2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)ethoxy]oxane-2-carboxylic acid [acetal]                 |   |  |
| 4329 | -1.550 | -1.135 | Ph | 405.082709 | 406.089985 | -0.028041 | C19H18O10    | 7  | Lancerin; 4-C-Glucosyl-1,3,7-trihydroxyxanthone  | 5,7,3',5'-Tetrahydroxy-3,6,8,4'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]   | 5,7,3',4'-Tetrahydroxy-3,6,8,5'-tetramethoxyflavone [Flavones and Flavonols [PK1211]]  |
| 2867 | -1.547 | -1.591 | NM | 349.114002 | 350.121279 | 0.454376  | C18H21ClN2O3 | 1  | <i>Cl37 isotope of Compound VII; 5-(5-(6-Chloro-4-(4,5-dihydro-2-oxazolyl)phenoxy)pentyl)-3-methylisoxazole</i>  |   |  |
| 5363 | -1.544 | -1.544 | Lp | 461.363655 | 462.370932 | 0.047187  | C29H50O4     | 1  | 2 $\alpha$ -(3-Hydroxypropyl)-1 $\alpha$ ,25-dihydroxy-19-norvitamin D3; (5Z,7E)-(1R,2R,3R)-3-(hydroxypropyl)-19-nor-9,10-seco-5,7-cholestadien-1,3,25-triol [Vitamin D3 and derivatives [ST0302]] |   |  |
| 93   | -1.534 | -1.586 | Ph | 181.050603 | 182.057880 | -0.160171 | C9H10O4      | 17 | 3-(4-Hydroxyphenyl)lactate; 4-Hydroxyphenyllactate; p-Hydroxyphenyllactate; 2-   | (R)-3-(4-Hydroxyphenyl)lactate  | 3-(2,3-Dihydroxyphenyl)propanoate; 2,3-Dihydroxyphenylpropanoate   |



|      |        |        |    |            |            |           |              |    |  |   |  |
|------|--------|--------|----|------------|------------|-----------|--------------|----|--|---|--|
| 2276 | -1.509 | -1.978 | Ph | 327.144911 | 328.152188 | -0.047159 | C16H24O7     | 3  | Hydroxy-3-(4-hydroxyphenyl)propanoate<br>Rhododendrin  | Tetranor-PGEM; 11R-hydroxy-9,15-dioxo-2,3,4,5-tetranor-prostan-1,20-dioic acid [Prostaglandins [FA0301]]<br>ZZZ   | Prostaglandin M; 7R-hydroxy-5,11-dioxotetranorpropane-1,16-dioic acid [Prostaglandins [FA0301]]<br>ZZZ |
| 5695 | -1.507 | -1.486 | Ph | 481.135145 | 482.142422 | -0.009034 | C22H26O12    | 1  | Catalposide  | 1-O-Feruloyl-β-D-glucose; 1-Feruloyl-D-glucose  | Gentiopicroin (see KEGG C09782) [C10 isoprenoids (monoterpenes) [PR0102]]                              |
| 3049 | -1.507 | -1.808 | Ph | 355.103413 | 356.110690 | -0.119119 | C16H20O9     | 3  | Gentiopicroin; Gentiopicroside   | 4-O-β-D-Glucosyl-sinapate   |  |
| 3857 | -1.506 | -1.773 | Ph | 385.113996 | 386.121273 | -0.063172 | C17H22O10    | 2  | 1-O-Sinapoyl-β-D-glucose; 1-O-Sinapoyl β-D-glucoside   | Plantagoside  | 3,4,5,2',4',6'-Hexahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]]              |
| 5431 | -1.499 | -1.784 | Ph | 465.103882 | 466.111159 | 0.069908  | C21H22O12    | 6  | Quercetin 7-O-glucoside  | (9Z,12Z,15Z)-Octadecatrienoic acid; α-Linolenic acid; 9,12,15-Octadecatrienoic acid; Linolenate; α-Linolenate   | Crepenynate; (9Z)-Octadec-9-en-12-ynoate; (Z)-9-Octadecen-12-ynoic acid; Crepenynic acid               |
| 1255 | -1.481 | -1.432 | Lp | 277.217271 | 278.224548 | -0.117541 | C18H30O2     | 47 | (6Z,9Z,12Z)-Octadecatrienoic acid; 6,9,12-Octadecatrienoic acid; γ-Linolenic acid; Gamolenic acid  |   |  |
| 1918 | -1.477 | -1.477 | NM | 313.147866 | 314.155142 | 0.528679  | C19H23ClN2   | 1  | Clomipramine   |   |  |
| 5036 | -1.454 | -1.557 | Cb | 443.192275 | 444.199552 | 0.009678  | C21H32O10    | 1  | dihydrophaseic acid 4-O-β-D-glucoside; (2Z,4E)-5-[(1R,3S,5R,8S)-3-(β-D-glucopyranosyloxy)-8-hydroxy-1,5-dimethyl-6-oxabicyclo[3,2,1]oct-8-yl]-3-methylpenta-2,4-dienoic acid [C15 isoprenoids (sesquiterpenes) [PR0103]] |   |  |
| 4853 | -1.449 | -1.966 | NM | 433.156296 | 434.163573 | -0.914956 | C23H25F3N2OS | 1  | cis-(Z)-Flupenthixol   |   |  |
| 3651 | -1.399 | -1.920 | Ph | 377.160554 | 378.167830 | -0.061522 | C20H26O7     | 5  | Chaparrinone   | Cnicin  | Eupahyssopin   |
| 3109 | -1.373 | -1.879 | Lp | 357.264681 | 358.271958 | 0.093990  | C20H38O5     | 6  | 13,14-Dihydro PGF-1a; 7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3S)-3-hydroxyoctyl]cyclopentyl]heptanoic acid [secondary alcohol]   | 9,13-dihydroxy-10-ethoxy-11-octadecenoic acid [Hydroxy fatty acids [FA0105]]  | 9,13-dihydroxy-12-ethoxy-10-octadecenoic acid [Hydroxy fatty acids [FA0105]]                           |
| 2575 | -1.360 | -1.552 | Cb | 339.093245 | 340.100522 | -0.117669 | C12H20O11    | 4  | Cellobiono-1,5-lactone; Cellobiose-1,5-lactone   | 3-Ketolactose   | 3-Ketosucrose; 3-Dehydro-α-D-glucosyl-β-D-fructofuranoside   |
| 1346 | -1.313 | -1.319 | Ph | 285.040436 | 286.047712 | -0.089823 | C15H10O6     | 34 | Luteolin; 3',4',5,7-Tetrahydroxyflavone; 5,7,3',4'-Tetrahydroxyflavone   | Kaempferol; 3,4',5,7-Tetrahydroxyflavone; 4H-1-Benzopyran-4-one,3,5,7-trihydroxy-2-(4-hydroxyphenyl)-5,7,4'-Trihydroxyflavonol; C,I,75640; Indigo yellow; Kaempferol; Kempferol; Nimbecetin; Pelargidenolon; Populnetin; Rhamnolutein; Rhamnolutin; Robigenin; Swartzol; Trifolitin | Aureusidin   |

|      |        |        |    |            |            |           |           |    |   |   |  |
|------|--------|--------|----|------------|------------|-----------|-----------|----|---|---|--|
| 2224 | -1.312 | -1.899 | NM | 325.129232 | 326.136508 | -0.138273 | C16H22O7  | 1  | Hinokitiol glucoside; β-Thujaplicin 2-O-β-D-glucoside   |   |  |
| 1138 | -1.291 | -2.284 | Lp | 269.175813 | 270.183090 | -0.072009 | C15H26O4  | 1  | (10S)-Juvenile hormone III acid diol  |   |  |
| 2111 | -1.281 | -1.568 | Ph | 321.061550 | 322.068827 | -0.126928 | C15H14O8  | 3  | Leucodelphinidin  | Elephantorrhizol [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  | Galocatechin-4β-ol [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]   |
| 1217 | -1.275 | -2.167 | Cb | 275.077209 | 276.084485 | -0.116446 | C11H16O8  | 1  | Ranunculin  |   |  |
| 2579 | -1.261 | -1.687 | Cb | 339.129643 | 340.136919 | -0.081507 | C13H24O10 | 1  | Methyl-2-α-L-fucopyranosyl-β-D-galactoside  |   |  |
| 5691 | -1.256 | -1.697 | Ph | 481.098785 | 482.106061 | 0.042399  | C21H22O13 | 1  | 3,4,2',3',4',6',α-Heptahydroxychalcone 2'-glucoside [Chalcones and dihydrochalcones [PK1212]]   |   |  |
| 2219 | -1.245 | -1.191 | Ph | 325.092849 | 326.100126 | -0.128228 | C15H18O8  | 8  | 4-O-β-D-Glucosyl-4-hydroxycinnamate   | <i>trans</i> -β-D-Glucosyl-2-hydroxycinnamate; β-D-Glucosyl-2-coumarate   | <i>cis</i> -β-D-Glucosyl-2-hydroxycinnamate; β-D-Glucosyl-2-coumarinate    |
| 6367 | -1.245 | -1.604 | Ph | 519.187226 | 520.194503 | 0.078545  | C26H32O11 | 2  | Brusatol  | (-)-Pinoresinol glucoside   | ZZZ  |
| 1304 | -1.212 | -1.257 | Lp | 281.248574 | 282.255850 | -0.106353 | C18H34O2  | 58 | (9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; Oleate; Oleic acid  | (9E)-Octadecenoic acid; 9-Octadecenoic acid, (E)-; (E)-Oleic acid; D9- <i>trans</i> -Octadecenoic acid; 9- <i>trans</i> -Octadecenoic acid; <i>trans</i> -D9-Octadecenoic acid; <i>trans</i> -9-Octadecenoic acid; <i>trans</i> -Elaidic acid; <i>trans</i> -Oleic acid; Elaidic acid; Acide elaidique; Elaidinsauire | (6Z)-Octadecenoic acid; Petroselinic acid; <i>cis</i> -6-Octadecenoic acid |
| 3121 | -1.210 | -2.451 | Pp | 358.114330 | 359.121606 | -0.070431 | C15H21NO9 | 1  | Epinephrine glucuronide (see KEGG C03033); (2S,3S,4S,6S)-3,4,5,5-tetrahydroxy-3-[(1R)-1-hydroxy-2-methylaminoethyl]-6-(phenoxy)oxane-2-carboxylic acid [acetal] |   |  |
| 1351 | -1.201 | -1.738 | Cb | 285.097947 | 286.105223 | -0.104355 | C13H18O7  | 4  | Salicin; Salicoside   | Gastrodin; 4-(Hydroxymethyl)phenyl-β-D-glucopyranoside  | Methylarbutin  |
| 1590 | -1.196 | -1.342 | Cb | 299.113594 | 300.120870 | -0.109047 | C14H20O7  | 1  | Salidroside; p-Hydroxyphenethyl alcohol 1-O-β-D-glucoside; Tyrosol glucoside  |   |  |
| 2074 | -1.195 | -1.764 | Cb | 319.139804 | 320.147080 | -0.116812 | C14H24O8  | 2  | Valproic acid glucuronide (see KEGG C03033); 3,4,5-trihydroxy-6-(2-propylpentanoyloxy)oxane-2-carboxylic acid [secondary alcohol]                               | Octanoylglucuronide (see KEGG C03033) [secondary alcohol]   |  |
| 6826 | -1.180 | -1.180 | Ph | 549.197747 | 550.205023 | -0.006175 | C27H34O12 | 1  | Eucommin A; Medioresinol 4'-O-β-D-glucopyranoside   |   |  |

|      |        |        |    |            |            |           |              |    |   |  |  |
|------|--------|--------|----|------------|------------|-----------|--------------|----|---|--|--|
| 60   | -1.134 | -1.163 | Ph | 175.024794 | 176.032070 | -0.100946 | C6H8O6       | 14 | Ascorbate; Ascorbic acid; L-Ascorbate; L-Ascorbic acid; Vitamin C   | D-Glucuronolactone; Glucurone; Glucofuranurono-6,3-lactone; D-Glucurono-3,6-lactone; D-Glucurone | 2-Hydroxy-3-oxoadipate   |
| 2088 | -1.128 | -1.784 | Pp | 320.062277 | 321.069553 | -0.132751 | C11H15NO10   | 1  | B-Citryl-L-glutamic acid; 3-[[[(2S)-1,5-dihydroxy-1, 5-dioxopentan-2-yl]carbamoyl]-3-hydroxypentanedioic acid [tertiary alcohol]            |  |  |
| 1966 | -1.101 | -1.967 | Ph | 315.087373 | 316.094649 | -0.123479 | C17H16O6     | 42 | Cajanol   | Homoferreirin  | 2,3-Dihydro-6-hydroxy-2-(4-hydroxyphenyl)-5,7-dimethoxy-4H-1-benzopyran-4-one; 4',6-Dihydroxy-5,7-dimethoxyflavanone<br>ZZZ      |
| 1159 | -1.096 | -1.875 | Cb | 271.082290 | 272.089566 | -0.135033 | C12H16O7     | 2  | Arbutin; Ursin; Uvasol; Hydroquinone-O-β-D-glucopyranoside  | α-Arbutin  |  |
| 5385 | -1.075 | -1.386 | Ph | 463.088225 | 464.095501 | 0.054352  | C21H20O12    | 52 | Quercetin 3-O-glucoside; Isoquercitrin; 2-(3,4-Dihydroxyphenyl)-3-(β-D-glucofuranosyloxy)-5,7-dihydroxy-4H-1-benzopyran-4-one; Isotrifoliin | Gossypetin 8-rhamnoside  | Hyperin; Quercetin 3-galactoside   |
| 4027 | -1.074 | -2.182 | NM | 391.160971 | 392.168248 | 0.453424  | C21H27ClN2O3 | 1  | Cl37 isotope of Compound II(R/S); 5-(7-(6-Chloro-4-(5-hydro-4-methyl-2-oxazolyl)phenoxy)heptyl)-3-methylisoxazole                           |  |  |
| 4887 | -1.073 | -1.375 | Ph | 435.129686 | 436.136963 | 0.036110  | C21H24O10    | 16 | Phlorizin; Phlorhizin; Phloridzin   | Epiafzelechin 3-O-β-D-allopyranoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]       | Arthromerin B [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 5658 | -1.052 | -1.601 | Cb | 479.083140 | 480.090416 | 0.053553  | C21H20O13    | 18 | Gossypin; Gossypetin 8-O-glucoside  | 4-o-Galloylbergenin  | 11-o-Galloylbergenin   |
| 557  | -0.994 | -1.259 | Cb | 253.092852 | 254.100128 | -0.155851 | C9H18O8      | 4  | 3-β-D-Galactosyl-sn-glycerol; Galactosylglycerol  | 2-(β-D-Glucosyl)-sn-glycerol   | Galactosylglycerol (see KEGG C05401); (2R,3R,4S,5R,6R)-2-[(2R)-2,3-dihydroxypropoxy]-6-(hydroxymethyl)oxane-3,4,5-triol [acetal] |
| 4335 | -0.982 | -1.113 | Ph | 405.119098 | 406.126375 | -0.018591 | C20H22O9     | 7  | Astringin   | Trichocarpin   | Ananthoside [Flavans, Flavanols and Leucoanthocyanidins [PK1202]]  |
| 574  | -0.956 | -0.981 | Lp | 255.232918 | 256.240194 | -0.141782 | C16H32O2     | 23 | Hexadecanoic acid; Hexadecanoate; Hexadecylic acid; Palmitic acid; Palmitate; Cetylic acid  | Palmitic acid (see KEGG C00249); Hexadecanoic acid [carboxylic acid]                             | Trimethyltridecanoic acid; 4,8,12-trimethyltridecanoic acid [carboxylic acid]  |
| 2811 | -0.946 | -1.998 | Cb | 347.171101 | 348.178377 | -0.116791 | C16H28O8     | 1  | Schizonepetoside E  |  |  |
| 51   | -0.937 | -1.303 | Ph | 173.009145 | 174.016422 | -0.092226 | C6H6O6       | 6  | cis-Aconitate; cis-Aconitic acid  | trans-Aconitate; trans-Aconitic acid   | Dehydroascorbate; Dehydroascorbic acid; L-   |

|      |        |        |    |            |            |           |             |    |   |   |   |
|------|--------|--------|----|------------|------------|-----------|-------------|----|---|---|---|
| 3141 | -0.931 | -1.474 | Ph | 359.077202 | 360.084478 | -0.109923 | C18H16O8    | 63 | Rosmarinate; Rosmarinic acid  | 3',4',5-Trihydroxy-3,6,7-trimethoxyflavone  | Dehydroascorbate; L-Dehydroascorbic acid  |
| 1329 | -0.900 | -0.949 | Lp | 283.264219 | 284.271495 | -0.124815 | C18H36O2    | 16 | Octadecanoic acid; Stearate; Stearic acid   | Stearic acid (see KEGG C01530); Octadecanoic acid [carboxylic acid]   | 6-Methoxyaromadendrin 3-O-acetate   |
| 4597 | -0.870 | -2.126 | Ph | 419.155889 | 420.163166 | 0.009385  | C18H28O11   | 2  | Lamioside   | Lamioside (see KEGG C11645) [C10 isoprenoids (monoterpenes) [PR0102]]   | Stearic acid (see KEGG C01530); octadecanoic acid [Straight chain fatty acids [FA0101]] |
| 3093 | -0.754 | -1.035 | Ph | 357.086062 | 358.093339 | 0.982887  | C14H19N2O7P | 2  | N1-(5-Phospho- $\alpha$ -D-ribose)-5,6-dimethylbenzimidazole; $\alpha$ -Ribazole 5'-phosphate                               | N1-(5-Phospho- $\alpha$ -D-ribose)-5,6-dimethylbenzimidazole (see KEGG C04778); [(2R,3R,4R,5S)-5-(5,6-dimethylbenzimidazol-1-yl)-3,4-dihydroxy-oxolan-2-yl]methoxyphosphonic acid [secondary alcohol] |   |
| 6072 | -0.725 | -0.969 | Cb | 501.146171 | 502.153448 | 0.125686  | C18H30O16   | 1  | $\alpha$ -L-Rhamnopyranosyl-(1->2)- $\beta$ -D-galactopyranosyl-(1->2)- $\beta$ -D-glucuronopyranoside; $\beta$ -Fabatriose |   |   |
| 2807 | -0.702 | -1.973 | Cb | 347.134705 | 348.141981 | -0.146980 | C15H24O9    | 1  | Leonuridine   |   |   |
| 1186 | -0.699 | -1.496 | Ph | 273.076829 | 274.084105 | -0.067655 | C15H14O5    | 26 | Phloretin   | $\alpha$ -Pyrufuran   | $\beta$ -Pyrufuran  |