Plant Omics Journal POJ

POJ 6(6): 371-376 (2013) ISSN:1836-3644

Supplementary data

# Metabolite profiling reveals the effect of drought on sorghum (*Sorghum bicolor* L. Moench) metabolism

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**Table 1.** Identified metabolites of sweet sorghum leaves and roots harvested from plants grown under normal or drought stress conditions at two stress levels. Drought stress was induced by polyethylene glycol (PEG) at two levels of stress 2.5 % and 5 % PEG.

**Suppl. Table 1a. Amino acids**

| | m/z | RT | Loadings | | Control | 2,5% PEG | 5% PEG | *P* |
|---|---|---|---|---|---|---|---|---|
| | | | PC-1 (68%) | PC-2 (14%) | Average | Average | Average | |
| LEAVES | | | | | | | | |
| Aspartic acid | 232 | 17.6199 | 0.003212 | -0.008828 | 2.75E-05 | 0.000159 | 0.00014 | 0.01 |
| b-alanine | 248 | 15.2100 | 0.008034 | -0.003557 | 4.89E-06 | 0.000142 | 0.00029 | 0.00 |
| DL-isoleucine | 158 | 11.8931 | 0.005819 | -0.006800 | 5.07E-05 | 0.000187 | 0.00026 | 0.05 |
| glycine | 174 | 12.1789 | 0.010352 | -0.005670 | 2.4E-05 | 0.000252 | 0.00034 | 0.00 |
| L-alanine | 116 | 7.2591 | 0.038672 | -0.030306 | 0.000199 | 0.001129 | 0.00138 | 0.00 |
| L-asparagine | 231 | 21.0587 | 0.180705 | -0.259678 | 0.00026 | 0.005044 | 0.0072 | 0.00 |
| L-cysteine | 220 | 18.3804 | n/d | n/d | n/d | n/d | n/d | - |
| L-glutamic acid | 201 | 18.6980 | 0.022087 | -0.019053 | 9.19E-05 | 0.000682 | 0.00087 | 0.00 |
| L-homoserine | 218 | 15.9019 | 0.000254 | -0.000432 | 5.11E-07 | 7.04E-06 | 1.1E-05 | 0.03 |
| L-lysine | 317 | 26.2457 | 0.005667 | 0.006311 | 0 | 0 | 0.00013 | 0.14 |
| L-methionine | 176 | 17.4389 | 0.000496 | -0.001212 | 1.21E-05 | 2.2E-05 | 4.7E-05 | 0.07 |
| L-ornithine | 174 | 24.1784 | 0.002399 | -0.000744 | 0 | 3.93E-05 | 7.7E-05 | 0.02 |
| L-serine | 204 | 13.6984 | 0.057229 | -0.066447 | 0.00025 | 0.001609 | 0.00229 | 0.00 |
| L-threonine | 218 | 14.3861 | 0.023377 | -0.016571 | 0.000103 | 0.000629 | 0.00087 | 0.00 |
| L-tryptophan | 202 | 31.6634 | 0.028823 | -0.033023 | 8.08E-05 | 0.000707 | 0.00114 | 0.00 |
| Tyrosine | 218 | 26.5646 | 0.050153 | -0.044486 | 9.94E-06 | 0.001044 | 0.0017 | 0.00 |
| L-valine | 144 | 9.9049 | 0.037676 | -0.005024 | 5.96E-05 | 0.000489 | 0.00141 | 0.00 |
| ROOTS | | | | | | | | |
| Aspartic acid | 232 | 17.6199 | 0.004640 | 0.003836 | 8.11E-05 | 0.000399 | 0.00024 | 0.02 |
| b-alanine | 248 | 15.2100 | 0.000158 | 0.002001 | 5.16E-06 | 3.57E-05 | 5.3E-06 | 0.01 |
| DL-isoleucine | 158 | 11.8931 | 0.000018 | -0.002300 | 0.000191 | 0.000138 | 0.0001 | 0.35 |
| glycine | 174 | 12.1789 | 0.006208 | 0.003953 | 3.98E-05 | 0.00027 | 0.00033 | 0.04 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| L-alanine | 116 | 7.2591 | 0.013118 | 0.014621 | 4.69E-05 | 0.000667 | 0.00053 | 0.05 |
| L-asparagine | 231 | 21.0587 | 0.000071 | 0.010315 | 1.14E-05 | 0.000136 | 1E-05 | 0.08 |
| L-cysteine | 220 | 18.3804 | -0.000086 | -0.000033 | 6.41E-06 | 0 | 0 | 0.00 |
| L-glutamic acid | 201 | 18.6980 | 0.020389 | 0.002293 | 0.000195 | 0.000884 | 0.00109 | 0.05 |
| L-homoserine | 218 | 15.9019 | 0.000213 | 0.000226 | 8.35E-08 | 5.86E-06 | 1.6E-05 | 0.46 |
| L-lysine | 317 | 26.2457 | 0.002038 | 0.008083 | 9.12E-05 | 0.000289 | 0.00011 | 0.01 |
| L-methionine | 176 | 17.4389 | -0.000107 | -0.000077 | 9.2E-06 | 2.78E-06 | 0 | 0.01 |
| L-ornithine | 174 | 24.1784 | 0.001466 | 0.002243 | 1.47E-05 | 0.000113 | 6.4E-05 | 0.05 |
| L-serine | 204 | 13.6984 | 0.012675 | 0.021249 | 0.000283 | 0.001001 | 0.00069 | 0.04 |
| L-threonine | 218 | 14.3861 | 0.001968 | 0.007839 | 9.76E-05 | 0.000283 | 0.00013 | 0.01 |
| L-tryptophan | 202 | 31.6634 | -0.001360 | 0.005405 | 0.00011 | 6.91E-05 | 1E-05 | 0.08 |
| Tyrosine | 218 | 26.5646 | 0.000529 | 0.003624 | 7.95E-05 | 0.000108 | 6.5E-05 | 0.42 |
| L-valine | 144 | 9.9049 | 0.000516 | 0.007929 | 0.000172 | 0.000238 | 0.00014 | 0.22 |

**Table 1b. Organic acids**

| | **m/z** | **RT** | **Loadings** | | **Control** | **2,5% PEG** | **5% PEG** | ***P*** |
|---|---|---|---|---|---|---|---|---|
| | | | **PC-1 (68%)** | **PC-2 (14%)** | **Average** | **Average** | **Average** | |
| LEAVES | | | | | | | | |
| a ketoglutaric acid | 147 | 18.9074 | -0.000110 | 0.000185 | 4.71E-06 | 0 | 0 | 0.00 |
| Caffeic acid | 396 | 30.1434 | 0.003445 | 0.001521 | 3.21E-05 | 5.46E-05 | 0.00014 | 0.00 |
| Citric acid | 347 | 24.3955 | 0.006900 | -0.020258 | 6.63E-05 | 0.000414 | 0.00025 | 0.01 |
| Dehydroascorbic acid | 173 | 24.9093 | -0.000033 | 0.000053 | 1.41E-06 | 0 | 0 | 0.01 |
| 4-hydroxycinnamic acid | 293 | 26.3507 | 0.002564 | -0.000184 | 6.4E-06 | 3.02E-05 | 8.1E-05 | 0.01 |
| DL-4-hydroxymandelic acid | 267 | 23.4074 | 0.026514 | -0.014107 | 1.6E-05 | 0.00063 | 0.00076 | 0.02 |
| D-malic acid | 147 | 16.8912 | 0.022863 | -0.045825 | 0.000168 | 0.001097 | 0.00072 | 0.04 |
| Fumaric acid | 245 | 13.1481 | 0.000215 | -0.000318 | 9.18E-07 | 6.24E-06 | 7.4E-06 | 0.03 |
| Gluconic acid | 333 | 28.1861 | 0.013507 | -0.021143 | 2.69E-05 | 0.000578 | 0.0004 | 0.02 |
| Glycolic acid | 147 | 6.7007 | 0.022164 | 0.031249 | 1.18E-05 | 6.67E-05 | 0.00062 | 0.06 |
| 3,4-dihydroxymandelic acid | 355 | 28.5997 | 0.000452 | -0.000264 | 0 | 1.07E-05 | 1.4E-05 | 0.02 |
| Mucic acid | 333 | 28.9875 | 0.001692 | -0.004968 | 1.22E-05 | 0.000105 | 5.3E-05 | 0.03 |
| Pipecolic acid | 156 | 13.5854 | 0.000401 | -0.000711 | 5.87E-06 | 2.2E-05 | 1.7E-05 | 0.02 |
| Pyruvic acid | 174 | 6.2359 | -0.000770 | 0.000946 | 3.8E-05 | 1.09E-05 | 3.4E-06 | 0.00 |
| Saccharic acid | 333 | 28.7452 | 0.001044 | -0.002392 | 2.54E-06 | 5E-05 | 3.4E-05 | 0.01 |
| Succinic acid | 148 | 12.3228 | 0.001887 | -0.002617 | 1.21E-05 | 6.9E-05 | 7.6E-05 | 0.00 |
| Trans-aconitic acid | 229 | 22.7348 | 0.037849 | -0.088046 | 2.15E-05 | 0.001431 | 0.00127 | 0.01 |
| Uric acid | 441 | 29.8723 | 0.000130 | -0.000055 | 7.7E-07 | 3.52E-06 | 4.5E-06 | 0.01 |
| ROOTS | | | | | | | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| a ketoglutaric acid | 147 | 18.9074 | n/d | n/d | n/d | n/d | n/d | - |
| Caffeic acid | 396 | 30.1434 | 0.000063 | 0.000090 | 1.2E-06 | 4.12E-06 | 3.7E-06 | 0.21 |
| Citric acid | 347 | 24.3955 | 0.000402 | 0.005524 | 0.000185 | 0.000364 | 3.9E-05 | 0.00 |
| Dehydroascorbic acid | 173 | 24.9093 | n/d | n/d | n/d | n/d | n/d | - |
| 4-hydroxycinnamic acid | 293 | 26.3507 | 0.001561 | 0.002647 | 2.25E-05 | 0.000122 | 0.00012 | 0.03 |
| DL-4-hydroxymandelic acid | 267 | 23.4074 | 0.004116 | 0.003047 | 4.63E-05 | 0.00029 | 0.0001 | 0.33 |
| D-malic acid | 147 | 16.8912 | -0.006469 | 0.008983 | 0.000779 | 0.000362 | 0.00019 | 0.01 |
| Fumaric acid | 245 | 13.1481 | 0.000557 | 0.000598 | 1.27E-05 | 3.22E-05 | 3.5E-05 | 0.14 |
| Gluconic acid | 333 | 28.1861 | 0.001480 | 0.002879 | 5.89E-05 | 0.000194 | 0.0001 | 0.00 |
| Glycolic acid | 147 | 6.7007 | 0.021758 | -0.015682 | 5.86E-05 | 0.000237 | 0.0016 | 0.00 |
| 3,4-dihydroxymandelic acid | 355 | 28.5997 | -0.000002 | -0.000001 | 1.63E-07 | 0 | 0 | 0.12 |
| Mucic acid | 333 | 28.9875 | -0.000036 | 0.001079 | 7.15E-06 | 1.72E-05 | 0 | 0.11 |
| Pipecolic acid | 156 | 13.5854 | -0.000166 | 0.000339 | 1.91E-05 | 8.01E-06 | 2.5E-06 | 0.11 |
| Pyruvic acid | 174 | 6.2359 | 0.000033 | -0.000133 | 5.87E-06 | 6.77E-06 | 8.4E-06 | 0.72 |
| Saccharic acid | 333 | 28.7452 | -0.000010 | 0.000251 | 2.04E-06 | 5.93E-06 | 0 | 0.00 |
| Succinic acid | 148 | 12.3228 | 0.002841 | 0.000598 | 4.02E-05 | 0.000139 | 0.00019 | 0.01 |
| Trans-aconitic acid | 229 | 22.7348 | 0.000074 | 0.001552 | 3.76E-06 | 1.1E-05 | 6.7E-06 | 0.80 |
| Uric acid | 441 | 29.8723 | n/d | n/d | n/d | n/d | n/d | - |

**Table 1c. Fatty acids**

| | **m/z** | **RT** | **Loadings** | | **Control** | **2,5% PEG** | **5% PEG** | ***P*** |
|---|---|---|---|---|---|---|---|---|
| | | | **PC-1 (68%)** | **PC-2 (14%)** | **Average** | **Average** | **Average** | |
| LEAVES | | | | | | | | |
| Capric acid | 229 | 15.7761 | n/d | n/d | n/d | n/d | n/d | - |
| 4-guanidinobutyric acid | 174 | 17.6937 | 0.013202 | -0.004076 | 1.65E-05 | 0.000277 | 0.00044 | 0.00 |
| 2-hydroxybutyric acid | 147 | 7.7499 | 0.000037 | 0.000018 | 0 | 6.38E-08 | 1.2E-06 | 0.03 |
| ROOTS | | | | | | | | |
| Capric acid | 229 | 15.7761 | 0.000092 | 0.000019 | 8.25E-07 | 1E-05 | 5.3E-06 | 0.04 |
| 4-guanidinobutyric acid | 174 | 17.6937 | 0.003566 | 0.005331 | 6.19E-05 | 0.000318 | 0.0002 | 0.01 |
| 2-hydroxybutyric acid | 147 | 7.7499 | n/d | n/d | n/d | n/d | n/d | - |

**Table 1d. Sugars**

| | **m/z** | **RT** | **Loadings** | | **Control** | **2,5% PEG** | **5% PEG** | ***P*** |
|---|---|---|---|---|---|---|---|---|
| | | | **PC-1 (68%)** | **PC-2 (14%)** | **Average** | **Average** | **Average** | |
| LEAVES | | | | | | | | |
| D-glucose | 319 | 26.2202 | 0.731198 | -0.104959 | 0.001403 | 0.007798 | 0.02154 | 0.01 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| D-lyxose | 307 | 21.2187 | 0.001893 | 0.000188 | 3.36E-05 | 6.68E-05 | 8.5E-05 | 0.05 |
| D-(+) trehalose | 361 | 40.8432 | 0.035573 | -0.015576 | 0.000242 | 0.001002 | 0.00125 | 0.02 |
| Fructose | 307 | 25.7157 | 0.296617 | -0.368847 | 0.004408 | 0.01308 | 0.01293 | 0.01 |
| Raffinose | 87 | 49.0069 | 0.024816 | 0.018845 | 6.15E-05 | 0.000236 | 0.00078 | 0.02 |
| Sedoheptulose anhydride monohydrate | 204 | 27.8032 | -0.004646 | -0.181400 | 0.000586 | 0.002895 | 0.00121 | 0.02 |
| Sophorose | 319 | 41.6028 | 0.000078 | 0.000116 | 3.35E-06 | 4.68E-06 | 4.6E-06 | 0.85 |
| Sucrose | 361 | 39.0483 | 0.174925 | -0.074017 | 0.001662 | 0.005294 | 0.00631 | 0.02 |
| Talose | 319 | 26.5018 | -0.112775 | 0.202728 | 0.005084 | 0.000143 | 0.00025 | 0.00 |
| ROOTS | | | | | | | | |
| D-glucose | 319 | 26.2202 | -0.040919 | 0.782006 | 0.005498 | 0.0101 | 0.00194 | 0.24 |
| D-lyxose | 307 | 21.2187 | 0.000862 | 0.004194 | 3.5E-05 | 0.000128 | 6.5E-05 | 0.01 |
| D-(+) trehalose | 361 | 40.8432 | 0.112013 | 0.160751 | 1.56E-05 | 0.004449 | 0.00621 | 0.02 |
| Fructose | 307 | 25.7157 | -0.092943 | 0.551804 | 0.006759 | 0.005579 | 0.00094 | 0.29 |
| Raffinose | 87 | 49.0069 | 0.000005 | -0.000002 | 1.71E-07 | 5.14E-07 | 0 | 0.50 |
| Sedoheptulose anhydride monohydrate | 204 | 27.8032 | -0.002582 | 0.030655 | 0.000125 | 0.000365 | 5.7E-05 | 0.33 |
| Sophorose | 319 | 41.6028 | -0.000093 | -0.000026 | 7.05E-06 | 0 | 0 | 0.01 |
| Sucrose | 361 | 39.0483 | -0.138201 | 0.184455 | 0.009577 | 0.004935 | 0.00036 | 0.11 |
| Talose | 319 | 26.5018 | -0.000183 | -0.000256 | 2.59E-05 | 5.96E-06 | 4.8E-06 | 0.12 |

**Table 1e. Polyols**

| | **m/z** | **RT** | **Loadings** | | **Control** | **2,5% PEG** | **5% PEG** | ***P*** |
|---|---|---|---|---|---|---|---|---|
| | | | **PC-1 (68%)** | **PC-2 (14%)** | **Average** | **Average** | **Average** | |
| LEAVES | | | | | | | | |
| D-mannitol | 319 | 26.8178 | -0.000811 | -0.005078 | 3.63E-06 | 7.44E-05 | 1.4E-05 | 0.08 |
| D-sorbitol | 319 | 27.0474 | 0.003639 | -0.001708 | 1.55E-06 | 8.71E-05 | 0.00015 | 0.00 |
| myo-inositol | 432 | 29.7437 | 0.190297 | -0.147333 | 0.002398 | 0.006161 | 0.00817 | 0.00 |
| D-threitol | 217 | 17.3574 | 0.001082 | 0.000871 | 2.66E-06 | 8.93E-06 | 3.8E-05 | 0.01 |
| ROOTS | | | | | | | | |
| D-mannitol | 319 | 26.8178 | 0.976739 | 0.087747 | 0.003333 | 0.039295 | 0.04937 | 0.02 |
| D-sorbitol | 319 | 27.0474 | 0.000727 | -0.002098 | 6.14E-06 | 3.37E-05 | 8.6E-05 | 0.00 |
| myo-inositol | 432 | 29.7437 | 0.002516 | 0.037217 | 0.000634 | 0.000622 | 0.00087 | 0.78 |
| D-threitol | 217 | 17.3574 | 0.007972 | -0.002757 | 8.18E-06 | 7.62E-05 | 0.00046 | 0.06 |

**Table 1f. Phosphates**

| | m/z | RT | Loadings | | Control | 2,5% PEG | 5% PEG | *P* |
|---|---|---|---|---|---|---|---|---|
| | | | PC-1 (68%) | PC-2 (14%) | Average | Average | Average | |
| LEAVES | | | | | | | | |
| D-glucose-6-phosphate | 387 | 33.9694 | 0.000143 | -0.006922 | 9.18E-05 | 0.000206 | 8.6E-05 | 0.01 |
| Glycerol 1-phosphate | 357 | 23.2557 | 0.001401 | -0.005874 | 2.65E-05 | 0.000126 | 0.00014 | 0.14 |
| Phosphoric acid | 299 | 11.4449 | 0.105162 | -0.168933 | 0.001059 | 0.003924 | 0.00414 | 0.03 |
| O-phosphocolamine | 299 | 23.5399 | 0.001582 | -0.001420 | 1.49E-05 | 4.82E-05 | 6.8E-05 | 0.00 |
| Ribulose-5-phosphate | 357 | 30.4788 | -0.000040 | 0.000041 | 2.4E-06 | 1.05E-06 | 5.2E-07 | 0.04 |
| ROOTS | | | | | | | | |
| D-glucose-6-phosphate | 387 | 33.9694 | -0.000618 | 0.000475 | 7E-05 | 2.74E-05 | 8.6E-06 | 0.01 |
| Glycerol 1-phosphate | 357 | 23.2557 | 0.015894 | 0.003408 | 5.65E-05 | 0.000699 | 0.00066 | 0.08 |
| Phosphoric acid | 299 | 11.4449 | 0.046304 | 0.103660 | 0.000852 | 0.003849 | 0.00255 | 0.02 |
| O-phosphocolamine | 299 | 23.5399 | n/d | n/d | n/d | n/d | n/d | - |
| Ribulose-5-phosphate | 357 | 30.4788 | n/d | n/d | n/d | n/d | n/d | - |

**Table 1g. Polyamines**

| | m/z | RT | Loadings | | Control | 2,5% PEG | 5% PEG | *P* |
|---|---|---|---|---|---|---|---|---|
| | | | PC-1 (68%) | PC-2 (14%) | Average | Average | Average | |
| LEAVES | | | | | | | | |
| 1,3-diaminopropane | 174 | 20.3561 | 0.002079 | -0.001720 | 2.73E-05 | 4.68E-05 | 9.3E-05 | 0.01 |
| Putrescine | 174 | 22.3494 | -0.004973 | -0.000420 | 0.000378 | 0.000281 | 0.0002 | 0.05 |
| ROOTS | | | | | | | | |
| 1,3-diaminopropane | 174 | 20.3561 | -0.000106 | -0.000029 | 7.87E-06 | 0 | 0 | 0.00 |
| Putrescine | 174 | 22.3494 | -0.010487 | -0.000437 | 0.000813 | 8.66E-05 | 2.4E-05 | 0.00 |

**Table 1h. N-compounds**

| | m/z | RT | Loadings | | Control | 2,5% PEG | 5% PEG | *P* |
|---|---|---|---|---|---|---|---|---|
| | | | PC-1 (68%) | PC-2 (14%) | Average | Average | Average | |
| LEAVES | | | | | | | | |
| Acetyl-L-serine | 174 | 14.4827 | 0.000224 | 0.000561 | 1.84E-06 | 3.93E-06 | 8E-06 | 0.44 |
| Adenine | 264 | 24.9660 | 0.002173 | -0.001493 | 1.45E-05 | 4.58E-05 | 9.6E-05 | 0.00 |
| Adenosine | 236 | 38.4360 | 0.004016 | -0.006006 | 4.11E-05 | 0.00018 | 0.00016 | 0.01 |
| b-cyano-L-alanine | 141 | 13.8776 | 0.009878 | -0.014927 | 2.86E-05 | 0.000283 | 0.00037 | 0.01 |
| 1-aminocyclopropane-1-carboxylic acid | 147 | 10.8258 | 0.000573 | -0.000186 | 4.74E-06 | 9.97E-06 | 2.3E-05 | 0.01 |
| 5-aminovaleric acid | 174 | 19.7646 | -0.000133 | 0.000270 | 2E-05 | 6.64E-06 | 5.3E-06 | 0.15 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Carbamic acid ethyl ester (urethane) | 146 | 4.7187 | 0.005169 | -0.001134 | 2.05E-05 | 0.000109 | 0.00019 | 0.00 |
| D-panthenol | 277 | 26.7673 | -0.000016 | -0.000497 | 1.54E-06 | 1.03E-05 | 1.6E-06 | 0.00 |
| Gly-pro | 174 | 27.4069 | 0.000064 | -0.000014 | 3.14E-08 | 8.69E-07 | 2.7E-06 | 0.00 |
| 4-hydroxybenzyl cyanide | 190 | 17.1553 | 0.000233 | -0.000282 | 1.94E-06 | 6.9E-06 | 9.7E-06 | 0.01 |
| Hypoxanthine | 265 | 23.7548 | -0.000017 | 0.000028 | 7.56E-07 | 0 | 0 | 0.01 |
| N-acetyl-D-glucosamine | 319 | 30.7496 | 0.000879 | -0.002054 | 2.4E-05 | 6.75E-05 | 5.3E-05 | 0.07 |
| N-acetyl-D-mannosamine | 205 | 29.6268 | n/d | n/d | n/d | n/d | n/d | - |
| N-methylglutamic acid | 260 | 22.0275 | 0.003073 | -0.001360 | 9.81E-07 | 5.69E-05 | 0.00012 | 0.00 |
| 1-methyl nicotinamide | 179 | 16.2677 | 0.000151 | -0.000134 | 1.09E-06 | 4.72E-06 | 6.1E-06 | 0.00 |
| L-mimosine | 188 | 9.3364 | 0.000679 | -0.000748 | 1.33E-05 | 2.7E-05 | 2.7E-05 | 0.38 |
| L-norleucine | 158 | 11.3417 | 0.004475 | -0.001549 | 1.4E-05 | 6.89E-05 | 0.00017 | 0.00 |
| N,N-dimethylglycine | 160 | 5.2735 | 0.000290 | -0.000106 | 3.3E-06 | 8.04E-06 | 1.2E-05 | 0.04 |
| Pantothenic acid | 291 | 27.6738 | 0.001003 | -0.001440 | 6.87E-06 | 4.78E-05 | 4E-05 | 0.01 |
| Uracil | 241 | 13.0040 | n/d | n/d | n/d | n/d | n/d | - |
| ROOTS | | | | | | | | |
| Acetyl-L-serine | 174 | 14.4827 | -0.000042 | -0.000008 | 3.12E-06 | 0 | 0 | 0.00 |
| Adenine | 264 | 24.9660 | 0.000232 | 0.000370 | 6.18E-06 | 2.08E-05 | 1.8E-05 | 0.01 |
| Adenosine | 236 | 38.4360 | -0.000118 | 0.001161 | 5.78E-05 | 4.75E-05 | 2.3E-05 | 0.10 |
| b-cyano-L-alanine | 141 | 13.8776 | 0.000089 | 0.002606 | 1.72E-06 | 3.87E-05 | 7E-06 | 0.06 |
| 1-aminocyclopropane-1-carboxylic acid | 147 | 10.8258 | n/d | n/d | n/d | n/d | n/d | - |
| 5-aminovaleric acid | 174 | 19.7646 | -0.000479 | 0.000061 | 4.66E-05 | 1.59E-05 | 0 | 0.00 |
| Carbamic acid ethyl ester (urethane) | 146 | 4.7187 | n/d | n/d | n/d | n/d | n/d | - |
| D-panthenol | 277 | 26.7673 | n/d | n/d | n/d | n/d | n/d | - |
| Gly-pro | 174 | 27.4069 | 0.000009 | 0.000018 | 0 | 1.16E-06 | 0 | 0.00 |
| 4-hydroxybenzyl cyanide | 190 | 17.1553 | 0.000028 | -0.000101 | 6.23E-07 | 1.54E-06 | 3E-06 | 0.48 |
| Hypoxanthine | 265 | 23.7548 | -0.000013 | 0.000006 | 9.91E-07 | 0 | 0 | 0.10 |
| N-acetyl-D-glucosamine | 319 | 30.7496 | 0.001173 | -0.000011 | 1.71E-05 | 3.47E-05 | 8.1E-05 | 0.02 |
| N-acetyl-D-mannosamine | 205 | 29.6268 | 0.000186 | -0.000164 | 0 | 3.19E-05 | 7.5E-06 | 0.04 |
| N-methylglutamic acid | 260 | 22.0275 | 0.000093 | 0.000102 | 4.03E-07 | 4.2E-06 | 3.9E-06 | 0.20 |
| 1-methyl nicotinamide | 179 | 16.2677 | 0.000124 | 0.000140 | 1.59E-06 | 7.36E-06 | 3.3E-06 | 0.42 |
| L-mimosine | 188 | 9.3364 | 0.000095 | 0.000150 | 1.88E-06 | 1.32E-05 | 4E-06 | 0.02 |
| L-norleucine | 158 | 11.3417 | 0.000218 | 0.001968 | 0.000139 | 0.000131 | 8.2E-05 | 0.71 |
| N,N-dimethylglycine | 160 | 5.2735 | n/d | n/d | n/d | n/d | n/d | - |
| Pantothenic acid | 291 | 27.6738 | -0.000140 | 0.000225 | 1.23E-05 | 4.71E-06 | 0 | 0.01 |
| Uracil | 241 | 13.0040 | 0.001171 | 0.000204 | 9.61E-06 | 6.69E-05 | 7.6E-05 | 0.00 |

**Table 1i. Other compounds**

| | m/z | RT | Loadings | | Control | 2,5% PEG | 5% PEG | *P* |
|---|---|---|---|---|---|---|---|---|
| | | | PC-1 (68%) | PC-2 (14%) | Average | Average | Average | |
| LEAVES | | | | | | | | |
| Acetol | 217 | 19.9778 | -0.000023 | 0.000037 | 9.93E-07 | 0 | 0 | 0.00 |
| Arbutin | 254 | 37.9619 | 0.000814 | 0.000501 | 1.87E-05 | 2.12E-05 | 4.1E-05 | 0.15 |
| Galacturonic acid | 333 | 24.5397 | 0.002229 | -0.001768 | 1.75E-05 | 7.37E-05 | 8.5E-05 | 0.01 |
| Isopropyl b-D-1-thiogalactopyranoside | 217 | 27.2213 | -0.001081 | -0.010687 | 0.000246 | 0.000411 | 0.00018 | 0.01 |
| 2-keto-L-gulonic acid | 204 | 24.4794 | -0.001595 | -0.015615 | 0 | 0.000219 | 3.8E-05 | 0.04 |
| Ribonic acid-g-lactone | 147 | 20.6655 | -0.000028 | 0.000032 | 8.78E-07 | 3.71E-07 | 0 | 0.07 |
| ROOTS | | | | | | | | |
| Acetol | 217 | 19.9778 | 0.000025 | -0.000057 | 0 | 0 | 2.1E-06 | 0.21 |
| Arbutin | 254 | 37.9619 | -0.000200 | 0.000158 | 1.54E-05 | 1.93E-06 | 4.7E-07 | 0.00 |
| Galacturonic acid | 333 | 24.5397 | -0.000580 | 0.001859 | 3.94E-05 | 1.89E-05 | 0 | 0.05 |
| Isopropyl b-D-1-thiogalactopyranoside | 217 | 27.2213 | -0.000354 | 0.001440 | 2.27E-05 | 1.22E-05 | 0 | 0.15 |
| 2-keto-L-gulonic acid | 204 | 24.4794 | n/d | n/d | n/d | n/d | n/d | - |
| Ribonic acid-g-lactone | 147 | 20.6655 | -0.000024 | 0.000004 | 1.76E-06 | 0 | 0 | 0.03 |

*For each identified metabolite GC-MS characteristics (fragment mass, RI: Retention Index), loadings in principal components and average response (resulting from 4 biological replications) are presented. P value represents the level of significance (ANOVA)*