# **Supplementary materials**

# Table S1. Loading values of partial least square discriminant analysis (PLS-DA) performed with a public web tool (MetaboAnalyst 4.0, http://www.metaboanalyst.ca/).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Drought | | | Recovery | | |
| Parameters | Component 1 | Component 2 | Component 3 | Component 1 | Component 2 | Component 3 |
| β-D-Galactopyranosyl-1,3-arabinose | -0.10877 | 0.12849 | 0.06358 | -0.08923 | 0.10845 | -0.05145 |
| 3-hydroxy-3-methyl-Glutaric acid | -0.019398 | -0.071867 | -0.094975 | -0.02988 | -0.01988 | 0.15492 |
| 4-hydroxy-Benzoic acid | -0.10905 | -0.053358 | -0.072587 | -0.04895 | -0.03925 | -0.11541 |
| 5,8,11,14-Eicosatetraenoic acid (20:4) | 0.10499 | -0.13082 | -0.066188 | 0.063142 | -0.01637 | 0.19724 |
| 5-Hydroxypentanoic acid | -0.13105 | -0.028932 | -0.13323 | -0.14607 | -0.05839 | -0.02523 |
| 6-Kestose | 0.018119 | 0.033034 | 0.049699 | -0.02607 | 0.13252 | 0.20792 |
| Acetylornithine | -0.15936 | -0.10107 | 0.019776 | -0.16257 | 0.003654 | -0.01974 |
| Alanine | 0.15119 | -0.028434 | -0.14762 | 0.15349 | 0.061347 | -0.06028 |
| α-Tocopherol | 0.039023 | 0.074672 | 0.07056 | 0.028577 | 0.14463 | 0.079898 |
| Arbutin | -0.0081935 | 0.020581 | -0.032483 | 0.044068 | 0.077152 | 0.008336 |
| Arginine | 0.14879 | -0.073915 | -0.16202 | 0.077649 | -0.06705 | -0.04314 |
| Aspartic acid | 0.036047 | -0.057416 | -0.19519 | -0.04846 | -0.02042 | -0.09706 |
| β-Alanine | 0.11452 | -0.19364 | -0.047621 | -0.06997 | -0.02862 | -0.0135 |
| β-Sitosterol | -0.027117 | 0.023274 | -0.063839 | -0.02906 | 0.001903 | 0.037506 |
| C/N (carbon/nitrogen) | -0.060627 | 0.063154 | 0.041778 | 0.010501 | 0.20486 | 0.084442 |
| Caproic acid 60 | 0.032368 | 0.010935 | -0.0031559 | -0.09683 | 0.07365 | 0.051705 |
| Carotene | -0.099012 | 0.0024073 | -0.02484 | -0.05944 | -0.14851 | 0.016711 |
| Catechin | -0.1798 | 0.016084 | -0.029546 | -0.07163 | 0.063191 | 0.017143 |
| Chlorophyll a | -0.088456 | 0.06605 | -0.034996 | -0.04713 | -0.17436 | 0.007707 |
| Chlorophyll b | -0.052963 | 0.065236 | -0.039855 | 0.004072 | -0.17573 | 0.003528 |
| Chlorophyll a/b | -0.16417 | 0.02998 | 0.0033511 | -0.1531 | 0.013461 | 0.012294 |
| cis-4-hydroxy-Cinnamic acid | 0.065197 | -0.085911 | -0.10265 | -0.07649 | 0.12097 | -0.08838 |
| Citric acid | 0.0072748 | -0.0079145 | -0.29296 | 0.008538 | -0.05695 | -0.12373 |
| Cysteine | -0.042662 | -0.11582 | 0.0093369 | -0.12207 | -0.00709 | -0.10096 |
| ∆13C | 0.03741 | 0.041039 | -0.08436 | 0.001304 | 0.016692 | -0.07896 |
| D-α,α'-Trehalose | -0.071706 | -0.030393 | 0.13704 | -0.09956 | 0.17181 | 0.11239 |
| D-Cellobiose | -0.046742 | 0.052213 | 0.1432 | 0.02259 | 0.19349 | -0.00673 |
| Dehydroascorbic acid dimer | -0.13232 | 0.1306 | 0.14787 | -0.12999 | 0.11722 | -0.0299 |
| 2,5-Dihydroxymethyl-3,4-dihydroxypyrrolidine (DMDP) | 0.12104 | -0.080025 | -0.15437 | 0.080794 | -0.09011 | -0.08174 |
| Epicatechin | -0.17077 | -0.013118 | -0.045156 | -0.12137 | 0.019706 | -0.13055 |
| Erythrose | -0.052786 | -0.11484 | 0.079664 | -0.07684 | 0.16746 | 0.084729 |
| Fructose | -0.059267 | 0.032848 | -0.024985 | -0.09648 | 0.070864 | 0.15334 |
| Fumaric acid | 0.057105 | 0.13461 | -0.13517 | 0.10494 | 0.13586 | -0.10299 |
| γ-Aminobutyric acid (GABA) | 0.14429 | -0.039284 | -0.13336 | 0.13786 | -0.04382 | 0.11671 |
| Galactinol | 0.13382 | 0.14074 | -0.040938 | 0.17879 | 0.032174 | -0.01991 |
| Galactonic acid | -0.049921 | -0.14674 | 0.026309 | -0.05249 | -0.01768 | 0.16493 |
| Galactose | -0.075507 | -0.094865 | 0.040112 | -0.1068 | 0.16336 | 0.092476 |
| γ-Glutamylcystein | -0.096083 | -0.17966 | 3.10E-05 | 0.074086 | -0.19582 | -0.03094 |
| Gluconic acid-1,4-lactone | -0.13791 | 0.020389 | -0.10678 | 0.038961 | -0.00185 | -0.0933 |
| Glucose | -0.05974 | -0.03334 | 0.035785 | -0.10063 | 0.037901 | 0.17087 |
| Glucose-6-phosphate | -0.12301 | -0.010175 | 0.032152 | -0.13777 | 0.06546 | 0.15127 |
| Glutamic acid | 0.058021 | -0.12794 | -0.17549 | -0.13419 | -0.06688 | 0.02306 |
| Glutamine | 0.11818 | 0.13673 | 0.021801 | 0.14328 | -0.06234 | 0.002919 |
| Glyceric acid | -0.15008 | 0.12946 | -0.1105 | -0.02571 | 0.060445 | -0.08419 |
| Glycerol-3-phosphate | 0.0051186 | -0.14337 | 0.049536 | -0.11343 | 0.041158 | -0.1083 |
| Glycine | 0.10997 | -0.16536 | 0.013647 | -0.10789 | -0.08735 | 0.16526 |
| Glutathione (GSH) | 0.02699 | -0.19619 | 0.0069754 | -0.17409 | 0.004165 | -0.07723 |
| Glutathione disulfide (GSSG) | 0.048757 | -0.15394 | 0.10285 | -0.12796 | 0.067627 | -0.04116 |
| GSSG/GSH | 0.050369 | -0.12044 | 0.12362 | -0.02111 | -0.04766 | 0.06142 |
| Guaiacylglycerol | -0.11512 | 0.079441 | 0.085072 | -0.12989 | 0.070239 | -0.02585 |
| Heptadecanoic acid (Margaric acid) | 0.15034 | 0.0071068 | -0.10802 | 0.10179 | 0.066347 | -0.13128 |
| Isoascorbic acid | -0.060902 | -0.17656 | -0.041348 | -0.02918 | 0.074343 | 0.043272 |
| Lactic acid | -0.01889 | 0.0094146 | -0.075135 | -0.06382 | -0.0015 | 0.027177 |
| Lactose | -0.16088 | -0.10263 | 0.048842 | -0.16624 | 0.047992 | 0.07321 |
| Laminaribiose | -0.064851 | -0.069543 | 0.093457 | -0.1078 | 0.15488 | 0.10983 |
| Dodecanoic acid (Lauric acid) | 0.0015449 | 0.14552 | 0.10007 | 0.081528 | 0.12952 | 0.14901 |
| Leaf hydration | -0.059457 | 0.079805 | -0.28915 | 0.015935 | 0.043518 | 0.19587 |
| 9,12-Octadecadienoic acid (Linoleic acid) | -0.045417 | 0.014691 | -0.072542 | -0.09365 | -0.03638 | -0.19308 |
| 9,12,15-Octadecatrienoic acid (Linolenelaidic acid) | -0.12633 | -0.060966 | -0.15416 | -0.14045 | -0.14298 | 0.14523 |
| Lumichrome | 0.011247 | 0.15149 | -0.0077195 | 0.068123 | -0.0552 | -0.06807 |
| Lysine | -0.15745 | -0.056108 | -0.069853 | -0.1601 | 0.067251 | 0.092367 |
| Lyxonic acid | 0.090357 | 0.043017 | -0.11895 | 0.034344 | 0.020959 | 0.21994 |
| Lyxose | -0.11052 | -0.07804 | -0.21881 | -0.10641 | 0.01211 | 0.052324 |
| Maleamic acid-BP | 0.019002 | 0.0091669 | -0.25954 | 0.005736 | -0.18336 | -0.00636 |
| Malic acid | 0.1288 | 0.075792 | -0.11945 | 0.10995 | 0.080979 | -0.04368 |
| myo-Inositol | -0.078937 | -0.093819 | -0.10286 | -0.1145 | -0.06911 | 0.051518 |
| Tetradecanoic acid (Myristic acid) | 0.002166 | 0.11927 | 0.088819 | 0.057972 | 0.12686 | 0.18161 |
| NA181001 (MPIMP ID) | -0.033391 | -0.10952 | -0.13261 | -0.12848 | 0.066641 | 0.18884 |
| N-acetyl-Glutamic acid | 0.068285 | 0.043276 | -0.27469 | 0.007247 | -0.10962 | -0.04499 |
| N-acetyl-Neuraminic acid | 0.086835 | 0.15756 | 0.069059 | 0.12631 | 0.080433 | 0.059325 |
| Nicotinic acid | -0.13041 | 0.015617 | -0.043369 | -0.0784 | -0.03133 | 0.088564 |
| Nitrate | -0.043007 | -0.012621 | -0.13912 | -0.06549 | -0.14936 | 0.083161 |
| N-methyl trans-4-hydroxy-L-proline 2S,4R-4-hydroxy-1-methyl pyrrolidine-2-carboxylic acid A143018 | -0.052124 | 0.081733 | -0.19819 | -0.00136 | -0.1546 | -0.086 |
| Hexadecanoic acid (Palmitic acid) | 0.031533 | -0.034179 | -0.20917 | -0.10049 | 0.034072 | -0.16626 |
| Phenylalanine | 0.14037 | -0.1688 | -0.030603 | -0.12833 | -0.15455 | 0.075417 |
| Phospahte | 0.10072 | 0.082179 | 0.090543 | 0.097089 | -0.0337 | 0.13529 |
| Phosphoric acid | 0.12974 | 0.056405 | 0.018658 | 0.019455 | 0.026632 | 0.19352 |
| Phosphoric acid monomethyl ester | -0.0031708 | 0.060187 | -0.11737 | 0.10451 | -0.0566 | 0.032961 |
| Phytol | 0.0078606 | -0.14222 | -0.066866 | -0.09297 | -0.14244 | 0.01419 |
| Pidolic acid | 0.10754 | -0.13967 | -0.10895 | 0.002647 | 0.07514 | 0.034625 |
| Proline | 0.05244 | -0.21814 | -0.007625 | -0.12114 | 0.11502 | -0.04342 |
| Protein | -0.011292 | 0.046874 | -0.099684 | -0.00633 | -0.08694 | -0.12404 |
| Pyrophosphate | -0.063679 | 0.17595 | 0.013461 | -0.00157 | 0.18843 | -0.02656 |
| Pyruvic acid | -0.10467 | 0.11594 | -0.14415 | 0.007373 | -0.06748 | -0.15802 |
| Quinic acid | 0.063458 | 0.088005 | -0.073601 | 0.015973 | -0.0436 | 0.083565 |
| Raffinose | 0.15215 | -0.019003 | -0.042657 | 0.094795 | 0.097368 | -0.0654 |
| Reduced ascorbate | -0.1474 | 0.048268 | -0.082562 | -0.1245 | 0.10885 | -0.064 |
| Salicylic acid | 0.093246 | 0.080557 | -0.097854 | 0.11215 | 0.10403 | -0.0341 |
| Serine | -0.093877 | 0.075638 | 0.049314 | -0.07949 | 0.006584 | -0.02115 |
| Shikimic acid | -0.13535 | -0.046017 | -0.19731 | -0.11285 | -0.17097 | -0.10448 |
| Sorbitol | -0.13243 | -0.056098 | -0.093987 | -0.07594 | 0.18552 | 0.034841 |
| Sorbose | -0.14227 | -0.1113 | -0.035737 | -0.18472 | 0.064686 | 0.041164 |
| Stearyl alcohol | -0.06747 | -0.057116 | 0.001785 | 0.046839 | -0.06155 | 0.12792 |
| Stigmasterol | 0.070633 | -0.040008 | -0.017128 | 0.075043 | 0.032479 | -0.07238 |
| Structural N | 0.0043896 | 0.05348 | 0.062912 | -0.03399 | -0.18712 | -0.04866 |
| Succinic acid | -0.12798 | -0.069034 | -0.14704 | -0.11691 | -0.07118 | -0.09177 |
| Sucrose | -0.1376 | 0.03864 | 0.076726 | -0.0981 | 0.14854 | 0.018016 |
| Sulfate | 0.0091592 | 0.0074264 | 0.17207 | 0.017068 | -0.06171 | 0.18154 |
| Total amino acid | 0.1109 | -0.12412 | -0.11056 | 0.034325 | -0.06351 | -0.01001 |
| Taxifolin | -0.0012622 | 0.11227 | 0.078161 | -0.10476 | -0.0236 | -0.13552 |
| Threonine | 0.12288 | -0.17654 | -0.088394 | 0.057906 | -0.19008 | 0.044074 |
| Total ascorbate | -0.15389 | 0.054994 | -0.068756 | -0.09759 | 0.11538 | -0.07967 |
| Total C (carbon) | -0.048949 | 0.06308 | -0.057673 | -0.04311 | -0.08485 | 0.002179 |
| total N (nitrogen) | 0.03951 | -0.037546 | -0.054532 | -0.01928 | -0.20698 | -0.077 |
| trans-4-hydroxy-Cinnamic acid | 0.021011 | -0.14074 | -0.087823 | -0.10448 | -0.01917 | -0.00187 |
| trans-Caffeic acid | -0.031717 | -0.11543 | -0.16204 | -0.13364 | -0.02478 | -0.10381 |
| trans-Ferulic acid | 0.020838 | -0.0067939 | -0.012909 | -0.13878 | 0.052974 | 0.050143 |
| trans-Sinapic acid | 0.13673 | -0.022393 | -0.11746 | 0.12218 | 0.079249 | -0.05655 |
| Tryptophan | 0.14883 | -0.16038 | -0.06055 | 0.066511 | -0.02307 | -0.04177 |
| UN-013 (Unknown compound 13) | 0.01667 | 0.22233 | 0.017378 | 0.15602 | 0.068023 | -0.07306 |
| Urea | 0.014678 | -0.054814 | -0.1677 | -0.03606 | -0.10729 | -0.08092 |

# Table S2. *P* values from Two‐Way ANOVA followed by Tukey post hoc test showing the effects of drought, climate treatment and their interaction (Drought × Climate) on parameters of mature date palm leaves during drought and recovery periods, respectively. Bold, *P* < 0.05; nd, not detectable due to low concentration. P values from Tukey post hoc test were given only when there was significant difference (*P* <0.05).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Drought phase** | | | | | | | **Recovery phase** | | | | | | |
|  |  | Factor 1 | | | Factor 2 | | | Interaction | Factor 1 | | | Factor 2 | | | Interaction |
|  |  | Drought | Tukey post hoc test between drought and control within | | Climate | Tukey post hoc test between summer and winter within | | Drought × Climate | Drought | Tukey post hoc test between drought and control within | | Climate | Tukey post hoc test (summer *vs* winter) within | | Drought × Climate |
| Classes | Parameters | Winter | Summer |  | Control | Drought | Winter | Summer |  | Control | Re-watered |
| Water status | Leaf hydration | **0.021** | 0.531 | **<0.001** | 0.657 |  |  | **0.003** | 0.309 |  |  | 0.683 |  |  | 0.243 |
| Carbon and nitrogen fractions | Total carbon (C) | 0.164 |  |  | 0.756 |  |  | 0.562 | 0.940 |  |  | 0.239 |  |  | 0.610 |
| Total nitrogen (N) | 0.501 |  |  | 0.820 |  |  | 0.547 | **0.018** | 0.271 | **0.021** | 0.627 |  |  | 0.333 |
| C/N | 0.209 |  |  | 0.691 |  |  | 0.673 | **0.011** | 0.196 | **0**.**016** | 0.617 | 0.759 | 0.343 | 0.365 |
| Soluble protein | 0.355 |  |  | 0.757 |  |  | 0.930 | 0.096 |  |  | 0.857 |  |  | 0.636 |
| Total amino acids N | **0.006** | **0.039** | **0.042** | 0.186 | 0.337 | 0.353 | 0.982 | 0.777 |  |  | 0.409 |  |  | 0.441 |
| Structural N | 0.650 |  |  | 0.837 |  |  | 0.477 | **0.045** | 0.450 | **0.035** | 0.456 | 0.825 | 0.232 | 0.301 |
| ∆13C | 0.810 |  |  | 0.209 |  |  | 0.553 | 0.450 |  |  | 0.861 |  |  | 0.636 |
| Antioxidants | Reduced ascorbate | **0.017** | 0.657 | **0.004** | **0.041** | 0.883 | **0.008** | 0.062 | 0.398 | 0.703 | 0.125 | **0.013** | **0.006** | 0.375 | 0.175 |
| Total ascorbate | **0.008** | 0.417 | **0.004** | **0.025** | 0.644 | **0.008** | 0.095 | 0.212 |  |  | 0.082 |  |  | 0.154 |
| Cysteine | 0.519 | 0.737 | 0.219 | **0.042** | **0.030** | 0.475 | 0.269 | 0.788 | **0.308** | **0.516** | **0.003** | **0.003** | 0.152 | 0.242 |
| γ-Glutamylcysteine | 0.245 | 0.593 | 0.264 | **<0.001** | **<0.001** | **0.002** | 0.672 | **0.003** | 0.231 | **0.002** | 0.057 | **0.012** | 0.839 | 0.102 |
| Total glutathione (GSH) | **0.003** | 0.067 | **0.006** | 0.075 | 0.083 | 0.418 | 0.487 | 0.093 | **0.017** | 0.900 | **<0.001** | **<0.001** | **0.003** | 0.066 |
| Oxidised glutathione (GSSG) | **<0.001** | **0.045** | **0.002** | 0.253 | 0.127 | 0.942 | 0.296 | 0.139 | 0.521 | 0.142 | **0.001** | **0.004** | **0.042** | 0.541 |
|  | GSSG/GSH | 0.002 | 0.130 | **0.002** | 0.529 | 0.174 | 0.621 | 0.191 | 0.456 |  |  | 0.751 |  |  | 0.375 |
| Pigments | Chlorophyll a | 0.060 |  |  | 0.342 |  |  | 0.610 | 0.056 |  |  | 0.228 |  |  | 0.205 |
| Chlorophyll b | 0.143 |  |  | 0.746 |  |  | 0.569 | 0.061 |  |  | 0.980 |  |  | 0.213 |
| Carotene | 0.191 |  |  | 0.135 |  |  | 0.569 | 0.145 |  |  | 0.171 |  |  | 0.239 |
| Chlorophyll a/b | **0.006** | 0.111 | **0.014** | **0.001** | **0.043** | **0.005** | 0.478 | 0.836 | 0.900 | 0.868 | **<0.001** | **0.002** | **0.003** | 0.977 |
| Anions | Nitrate | 0.578 |  |  | 0.131 |  |  | 0.057 | 0.348 |  |  | 0.061 |  |  | 0.072 |
|  | Phosphate | 0.969 | 0.188 | 0.171 | **0.014** | 0.606 | **0.004** | 0.063 | 0.99 | 0.319 | 0.319 | **0.046** | **0.016** | 0.615 | 0.164 |
|  | Sulfate | 0.705 |  |  | 0.465 |  |  | 0.421 | 0.516 | 0.269 | 0.053 | 0.748 | 0.166 | 0.095 | **0.035** |
| Monosaccharides | Glucose | 0.527 |  |  | 0.310 |  |  | 0.478 | **0.031** | **0.011** | 0.640 | **0.004** | 0.254 | **0.004** | 0.111 |
| Fructose | 0.171 |  |  | 0.814 |  |  | 0.337 | 0.094 | 0.082 | 0.518 | **0.026** | 0.255 | **0.041** | 0.414 |
| Galactose | 0.983 | 0.978 | 0.954 | **0.023** | 0.090 | 0.106 | 0.952 | **0.007** | **0.015** | 0.134 | **0.005** | 0.091 | **0.015** | 0.437 |
| Erythrose | 0.938 | 0.702 | 0.623 | **0.024** | **0.042** | 0.214 | 0.537 | **0.029** | 0.072 | 0.164 | 0.072 | 0.256 | 0.148 | 0.748 |
| Sorbose | 0.412 | 0.911 | 0.209 | **<0.001** | **0.019** | **<0.001** | 0.331 | **0.030** | **0.012** | 0.589 | **<0.001** | **<0.001** | **<0.001** | 0.131 |
| Xylose | 0.794 | **0.021** | **0.009** | **<0.001** | 0.813 | **<0.001** | **0.001** | 0.570 | 0.566 | 0.818 | **0.047** | 0.180 | 0.125 | 0.807 |
| Disaccharides | Sucrose | **0.002** | **0.005** | 0.096 | **0.005** | **0.008** | 0.139 | 0.331 | 0.055 |  |  | 0.078 |  |  | 0.642 |
| Lactose | 0.181 | 0.288 | 0.396 | **<0.001** | **<0.001** | **<0.001** | 0.876 | 0.176 | 0.081 | 0.889 | **<0.001** | **0.004** | **<0.001** | 0.242 |
| β-D- Galactopyranosyl -1,3-arabinose | 0.003 | **0.040** | **0.018** | 0.317 | 0.602 | 0.368 | 0.785 | 0.974 |  |  | 0.092 |  |  | 0.198 |
| D-Cellobiose | 0.109 |  |  | 0.892 |  |  | 0.680 | **0.044** | 0.606 | **0.021** | 0.077 | 0.740 | **0.039** | 0.173 |
| D-α,α-Trehalose | 0.103 |  |  | 0.126 |  |  | 0.219 | 0.050 | 0.097 | 0.237 | **0.026** | 0.146 | 0.074 | 0.712 |
| Laminaribiose | 0.388 |  |  | 0.094 |  |  | 0.466 | 0.066 | 0.100 | 0.316 | **0.014** | 0.117 | **0.043** | 0.626 |
| Trisaccharides | 6-Kestose | 0.922 |  |  | 0.811 |  |  | 0.618 | **0.005** | **0.007** | 0.146 | 0.432 | 0.844 | 0.220 | 0.297 |
| Raffinose | **0.020** | 0.210 | **0.033** | **<0.001** | **0.036** | **0.004** | 0.492 | **0.041** | 0.607 | **0.019** | **0.023** | 0.459 | **0.016** | 0.163 |
| Organic acids and derivate | Pyruvic acid | **0.001** | 0.422 | **<0.001** | 0.598 | 0.149 | **0.035** | **0.015** | 0.224 |  |  | 0.531 |  |  | 0.563 |
| Citric acid | 0.707 |  |  | 0.617 |  |  | 0.052 | 0.303 |  |  | 0.708 |  |  | 0.962 |
| Fumaric acid | 0.169 |  |  | **0.011** |  |  | 0.527 | 0.054 | 0.656 | **0.004** | **0.004** | 0.636 | **<0.001** | **0.015** |
| Succinic acid | 0.123 | 0.211 | **0.004** | **0.006** | 0.480 | **<0.001** | 0.165 | **0.015** | **0.048** | 0.107 | **0.007** | **0.023** | 0.081 | 0.763 |
| Malic acid | 0.468 | 0.471 | 0.759 | **<0.001** | **0.004** | **0.010** | 0.767 | 0.388 | 0.936 | 0.199 | **0.011** | 0.186 | **0.018** | 0.331 |
| Quinic acid | 0.824 |  |  | 0.077 |  |  | 0.521 | 0.553 |  |  | 0.859 |  |  | 0.732 |
| Shikimic acid | 0.184 |  |  | **<0.001** |  |  | **0.004** | **0.016** | **0.010** | 0.407 | **0.024** | **0.010** | 0.496 | 0.166 |
| Dehydroascorbic acid (DHA) dimer | 0.001 | **0.003** | 0.059 | 0.088 | 0.065 | 0.571 | 0.341 | 0.468 | 0.937 | 0.274 | **0.007** | **0.010** | 0.156 | 0.403 |
| Isoascorbic acid | 0.415 | 0.117 | 0.649 | 0.006 | 0.283 | **0.005** | 0.153 | 0.612 |  |  | 0.777 |  |  | 0.626 |
| Lactic acid | 0.615 |  |  | 0.992 |  |  | 0.585 | 0.909 |  |  | 0.820 |  |  | 0.719 |
| 3-Hydroxymethylglutaric acid (Meglutol) | 0.678 |  |  | 0.808 |  |  | 0.092 | 0.588 |  |  | 0.096 |  |  | 0.208 |
| Sugar acids | Galactonic acid | 0.107 | **0.016** | 0.810 | **0.009** | 0.552 | **0.002** | 0.055 | 0.180 |  |  | 0.361 |  |  | 0.103 |
| Glyceric acid | **<0.001** | 0.082 | **<0.001** | **0.033** | 0.629 | **0.001** | **0.007** | 0.555 |  |  | 0.476 |  |  | 0.391 |
| Lyxonic acid | 0.961 | 0.507 | 0.551 | **0.008** | **0.013** | 0.165 | 0.375 | 0.942 |  |  | 0.584 |  |  | 0.186 |
| Alcohols | Sorbitol | 0.175 | 0.983 | 0.058 | **0.008** | 0.300 | **0.006** | 0.166 | 0.314 |  |  | 0.227 |  |  | 0.359 |
| myo-Inositol | 0.736 |  |  | 0.053 |  |  | 0.414 | 0.720 | 0.175 | 0.382 | **0.003** | 0.212 | **0.003** | 0.120 |
| Galactinol | 0.329 | 0.139 | 0.901 | **<0.001** | **<0.001** | **<0.001** | 0.252 | **0.026** | 0.804 | **0.005** | **<0.001** | **<0.001** | **<0.001** | 0.053 |
| Phosphates | Phosphoric acid | 0.808 | 0.099 | 0.051 | **0.005** | 0.729 | **<0.001** | **0.014** | 0.494 |  |  | 0.726 |  |  | 0.174 |
| Phosphoric acid monomethyl ester | 0.308 |  |  | 0.104 |  |  | 0.496 | 0.953 | 0.507 | 0.456 | **0.022** | **0.018** | 0.325 | 0.322 |
| Pyrophosphate | **0.027** | 0.182 | 0.060 | 0.465 | 0.414 | 0.829 | 0.668 | 0.286 |  |  | 0.414 |  |  | 0.191 |
| Glucose-6-phosphate | **0.028** | 0.134 | 0.088 | **0.011** | **0.049** | 0.077 | 0.870 | 0.115 | **0.036** | 0.940 | **0.002** | 0.132 | **0.002** | 0.139 |
| Glycerol-3-phosphate | 0.075 |  |  | 0.068 |  |  | 0.654 | 0.979 | 0.316 | 0.333 | **0.005** | **0.003** | 0.249 | 0.169 |
| Amino acids | Alanine | **0.008** | **0.014** | 0.167 | **<0.001** | **0.002** | **0.028** | 0.380 | 0.384 | 0.771 | 0.137 | **<0.001** | **0.005** | **<0.001** | 0.206 |
| β-Alanine | **<0.001** | **0.003** | **<0.001** | 0.609 | 0.874 | 0.381 | 0.464 | 0.745 |  |  | 0.130 |  |  | 0.119 |
| Glycine | **<0.001** | 0.054 | **<0.001** | 0.660 | 0.47 3 | 0.188 | 0.154 | 0.088 | 0.745 | **0.010** | **0.006** | 0.556 | **0.002** | **0.036** |
| Serine | **0.011** | **0.015** | 0.215 | 0.110 | 0.076 | 0.630 | 0.339 | 0.300 | 0.150 | 0.998 | **0.029** | **0.020** | 0.386 | 0.302 |
| Glutamic acid | 0.089 |  |  | 0.971 |  |  | 0.307 | 0.069 | 0.260 | 0.133 | **<0.001** | **0.015** | **0.011** | 0.775 |
| Glutamine | 0.810 | 0.728 | 0.994 | **<0.001** | **0.001** | **<0.001** | 0.802 | 0.973 | 0.730 | 0.766 | 0.001 | **0.006** | **0.038** | 0.650 |
| Proline | **<0.001** | 0.004 | 0.006 | 0.159 | 0.345 | 0.284 | 0.926 | 0.553 | 0.893 | 0.335 | **0.007** | **0.011** | 0.145 | 0.436 |
| Arginine | **0.006** | **0.041** | **0.046** | **0.011** | 0.059 | 0.067 | 0.964 | 0.623 |  |  | 0.082 |  |  | 0.457 |
| γ-Aminobutyric acid (GABA) | **0.012** | **0.014** | 0.238 | **0.002** | **0.004** | 0.096 | 0.307 | 0.459 | 0.580 | 0.120 | **<0.001** | **<0.001** | 0.117 | 0.138 |
| Aspartic acid | 0.770 |  |  | 0.796 |  |  | 0.993 | 0.545 |  |  | 0.498 |  |  | 0.911 |
| Threonine | **<0.001** | **0.004** | **0.003** | 0.476 | 0.700 | 0.532 | 0.864 | **0.017** | 0.683 | **0.004** | 0.115 | **0.013** | 0.793 | 0.055 |
| Lysine | 0.068 | 0.967 | **0.012** | **<0.001** | 0.093 | **<0.001** | 0.061 | 0.064 | **0.036** | 0.606 | **<0.001** | **0.011** | **<0.001** | 0.234 |
| Tryptophan | **<0.001** | **<0.001** | **<0.001** | **0.036** | 0.239 | 0.063 | 0.600 | 0.706 |  |  | 0.151 |  |  | 0.683 |
| Phenylalanine | **<0.001** | **0.008** | **<0.001** | 0.156 | 0.798 | 0.083 | 0.281 | **0.002** | 0.168 | **0.001** | **<0.001** | **0.028** | **<0.001** | 0.107 |
| Other nitrogen compounds | N-acetyl-Glutamic acid | 0.587 | 0.088 | 0.324 | **0.027** | **0.006** | 0.783 | 0.061 | 0.309 |  |  | 0.827 |  |  | 0.616 |
| Pyroglutamic acid | **0.007** | 0.055 | **0.039** | 0.378 | 0.588 | 0.477 | 0.903 | 0.581 |  |  | 0.350 |  |  | 0.734 |
| N-acetyl-Ornithine | 0.191 | 0.811 | 0.111 | **<0.001** | **<0.001** | **<0.001** | 0.325 | 0.763 | 0.658 | 0.986 | **<0.001** | **0.001** | **0.007** | 0.744 |
| N-acetyl-Neuraminic acid | 0.530 | 0.577 | 0.740 | **<0.001** | **0.013** | **0.008** | 0.872 | 0.653 | 0.641 | 0.865 | **0.001** | **0.007** | **0.024** | 0.834 |
| Lumichrome | 0.084 |  |  | 0.184 |  |  | 0.698 | 0.682 |  |  | 0.110 |  |  | 0.926 |
| Maleamic acid | 0.883 |  |  | 0.672 |  |  | 0.118 | **0.040** | 0.387 | **0.038** | 0.895 | 0.548 | 0.469 | 0.350 |
| Urea | 0.520 |  |  | 0.884 |  |  | 0.218 | 0.083 |  |  | 0.481 |  |  | 0.896 |
| N-methyl trans-4-hydroxy-L-proline (2S,4R)-4-hydroxy-1-methyl pyrrolidine-2-carboxylic acid (A143018) | 0.164 |  |  | 0.812 |  |  | 0.105 | **0.030** | 0.174 | 0.072 | 0.931 | 0.748 | 0.861 | 0.0729 |
| Fatty acids and fatty alcohol | 5,8,11,14-Eicosatetraenoic acid (Arachidonic acid, C20:4) | **0.004** | 0.054 | **0.021** | 0353 | 0.659 | 0.380 | 0.754 | 0.108 | **0.012** | 0.692 | 0.965 | 0.118 | 0.136 | **0.036** |
| 9,12,15-Octadecatrienoic acid (α-Linolenic acid, C18:3) | 0.770 | 0.300 | 0.154 | **0.003** | 0.261 | **0.002** | 0.087 | **<0.001** |  |  | **<0.001** |  |  | **<0.001** |
| 9,12-Octadecadienoic acid (Linoleic acid, C18:2) | 0.452 |  |  | 0.359 |  |  | 0.920 | **0.038** | **0.004** | 0.830 | **0.028** | **0.002** | 0.914 | **0.020** |
| 5-Hydroxypentanoic acid (C5:0) | 0.081 | 0.566 | 0.058 | **0.008** | 0.185 | **0.011** | 0.324 | **0.020** |  |  | **<0.001** |  |  | 0.727 |
| Hexanoic acid (caproic acid, C6:0) | 0.363 |  |  | 0.658 |  |  | 0.626 | 0.382 |  |  | 0.094 |  |  | 0.866 |
| Dodecanoic acid (Lauric acid, C12:0) | 0.264 |  |  | 0.394 |  |  | 0.760 | **0.016** | **0.039** | 0.139 | **0.046** | 0.067 | 0.274 | 0.637 |
| Tetradecanoic acid (Myristic acid, C14:0) | 0.202 |  |  | 0.542 |  |  | 0.488 | **0.003** | **0.004** | 0.159 | 0.155 | 0.051 | 0.925 | 0.197 |
| Heptadecanoic acid (Margaric acid, C17:0) | 0.078 | 0.285 | 0.142 | **<0.001** | **0.013** | **0.005** | 0.764 | 0.564 | 0.204 | **0.046** | **0.006** | 0.636 | **0.002** | **0.025** |
| Hexadecanoic acid (Palmitic acid, C16:0) | 0.802 |  |  | 0.358 |  |  | 0.547 | 0.573 | 0.298 | 0.076 | **0.013** | **0.002** | 0.665 | 0.051 |
| Stearyl alcohol | 0.747 |  |  | 0.069 |  |  | 0.635 | nd |  |  | nd |  |  | nd |
| Phenolics | 4-hydroxy-Benzoic acid | **0.012** | 0.093 | **0.046** | **0.002** | **0.033** | **0.015** | 0.802 | nd |  |  | nd |  |  | nd |
| cis-4-hydroxy-Cinmic acid | **0.018** |  |  | 0.384 |  |  | 0.670 | 0.983 | 0.103 | 0.098 | 0.149 | **0.009** | 0.532 | **0.025** |
| trans-4-hydroxy-Cinnamic acid | 0.214 | **0.045** | 0.143 | 0.439 | 0.750 | 0.361 | 0.381 | 0.683 | 0.986 | 0.576 | **0.032** | 0.170 | 0.083 | 0.700 |
| trans-Sinapic acid | 0.282 | 0.354 | 0.547 | **0.002** | **0.014** | **0.029** | 0.814 | **0.039** | 0.493 | **0.025** | **0.004** | 0.141 | **0.007** | 0.232 |
| trans-Caffeic acid | 0.778 |  |  | 0.122 |  |  | 0.393 | 0.356 | 0.230 | 0.924 | **0.004** | **0.007** | 0.104 | 0.429 |
| Salicylic acid | 0.957 | 0.952 | 0.987 | **0.017** | 0.078 | 0.084 | 0.975 | 1.000 | 0.159 | 0.159 | **0.010** | 0.556 | **0.004** | 0.052 |
| Guaiacylglycerol | **0.017** | 0.103 | 0.064 | 0.094 | 0.186 | 0.279 | 0.858 | 0.532 | 0.973 | 0.362 | **0.002** | **0.006** | 0.069 | 0.501 |
| Arbutin | 0.494 |  |  | 0.765 |  |  | 0.747 | 0.300 |  |  | 0.283 |  |  | 0.605 |
| Catechin | **0.004** | 0.067 | **0.014** | **<0.001** | **0.012** | **0.002** | 0.602 | 0.405 |  |  | 0.162 |  |  | 0.905 |
| Epicatechin | **0.010** | 0.237 | **0.011** | **<0.001** | **0.016** | **<0.001** | 0.279 | 0.985 | 0.410 | 0.424 | **0.011** | **0.008** | 0.274 | 0.255 |
| Taxifolin | 0.137 |  |  | 0.475 |  |  | 0.072 | 0.210 | 0.171 | 0.685 | **0.019** | **0.025** | 0.221 | 0.483 |
| Vitamins | α-Tocopherol | 0.794 |  |  | 0.157 |  |  | 0.579 | **0.025** | 0.211 | **0.045** | 0.815 | 0.788 | 0.575 | 0.552 |
| Nicotinic acid | 0.063 | 0.214 | 0.148 | **0.021** | 0.114 | 0.075 | 0.876 | 0.725 | 0.381 | 0.699 | **0.019** | 0.235 | **0.030** | 0.373 |
| Sterols | β-Sitosterol | 0.911 |  |  | 0.932 |  |  | 0.960 | 0.183 |  |  | 0.893 |  |  | 0.280 |
| Stigmasterol | 0.202 |  |  | 0.230 |  |  | 0.610 | 0.633 |  |  | 0.071 |  |  | 0.296 |
| Others | Phytol | **0.042** | 0.154 | 0.127 | 0.304 | 0.433 | 0.498 | 0.939 | 0.095 | 0.060 | 0.638 | **0.019** | 0.280 | **0.023** | 0.293 |
| 2,5-Dihydroxymethyl-3,4-dihydroxypyrrolidine (DMDP) | 0.048 | 0.214 | 0.105 | 0.077 | 0.279 | 0.142 | 0.772 | 0.306 |  |  | 0.057 |  |  | 0.402 |
| Gluconic acid-1,4-lactone | 0.073 | 0.470 | 0.067 | **0.039** | 0.348 | **0.043** | 0.405 | 0.338 |  |  | 0.236 |  |  | 0.129 |
| NA181001 (unknown) | 0.669 |  |  | 0.098 |  |  | 0.694 | **0.014** | **0.003** | 0.741 | **<0.001** | 0.120 | **<0.001** | **0.037** |
| UN-013 (unknown) | **0.012** | 0.336 | **0.009** | **0.002** | **0.003** | 0.152 | 0.187 | 0.695 | 0.465 | 0.207 | **<0.001** | **0.002** | **<0.001** | 0.163 |