

**Supplementary Table S3. List of the 111 MetabOxi variables considered in this study.**

Compound class	Platform	Number	Compound name
Amino acid	GC-TOF-MS	24	Alanine (Ala), Alanine, beta- (beta-Ala), Arginine (Arg), Asparagine (Asn), Asparagine -H <sub>2</sub> O (Asn-H <sub>2</sub> O), Aspartic acid (Asp), Cysteine (Cys), Glutamic acid (Glu), Glutamine (Gln), Glycine (Gly), Isoleucine (Ile), Leucine (Leu), Lysine (Lys), Methionine (Met), Ornithine (Orn), Phenylalanine (Phe), Proline (Pro), Pyroglutamic acid, Serine (Ser), Serine O-acetyl-, Threonine (Thr), Tryptophan (Trp), Tyrosine (Tyr), Valine (Val)
Organic acid	GC-TOF-MS	37	2-Piperidinecarboxylic acid, Adipic acid, 2-amino-, Ascorbic acid, Butanoic acid, 4-amino-, Butanoic acid, 4-hydroxy-, Citric acid, Erythronic acid, Fumaric acid, Galactaric acid, Galactonic acid-1,4-lactone, Gluconic acid-1,5-lactone, Gluconic acid-6-phosphate, Glutaric acid, 2-hydroxy-, Glutaric acid, 2-oxo-, Glyceric acid, Glyceric acid-3-phosphate, Isocitric acid, Maleic acid, Malic acid, Malic acid, 2-methyl-, Malonic acid, Phosphoenolpyruvic acid, Phosphoric acid, Prephenic acid, Pyruvic acid, Quinic acid, Quinic acid, 3-caffeoyl-, trans-, Quinic acid, 4-caffeoyl-, trans-, Quinic acid, 5-caffeoyl-, trans-, Quinoline-2-carboxylic acid, 4,8-dihydroxy-, Salicylic acid, Shikimic acid, Shikimic acid, 3-dehydro-, Sinapic acid, trans-, Succinic acid, Tartronic acid, Threonic acid
Sugar	GC-TOF-MS	19	Erythritol, Fructose-6-phosphate, Fucose, Galactinol, Galactosamine N-acetyl-, Glucosamine N-acetyl-, Glucose, Glucose-6-phosphate, Glycerol-3-phosphate, Inositol, myo-, Isomaltose, Maltose, Mannosamine, N-acetyl-, Melibiose, Raffinose, Ribitol, Ribose-5-phosphate, Ribulose-5-phosphate, Trehalose
	Spectrophotometer	3	Fructose (abs), Sucrose (abs), Glucose (abs)
Other known	Spectrophotometer	8	4-Hydroxyphenyl-beta-glucopyranoside, Allantoin, Guanosine, Putrescine, Secologanin, Tyramine, Urea, Uridine
Oxidative stress markers and molecular antioxidants	Spectrophotometer	4	Malondialdehyde (MDA), Polyphenols (Poly), Protein oxidation (ProtOx), Total antioxidant capacity (TAC)
Antioxidant enzyme activity	Spectrophotometer	16	Ascorbate oxidase (AO), Ascorbate peroxidase (APX), Catalase (CAT), Dehydroascorbate reductase (DHAR), Ferredoxins (Frxs), Glycolate oxidase (GOX), Glutathione peroxidase (GPX), Glutathione reductase (GR), Glutaredoxins (Grxs), Glutathione S-transferase (GST), Hydroxypyruvate reductase (HPR), Monodehydroascorbate reductase (MDHAR), Peroxidase (POX), Peroxiredoxins (Prxs), Superoxide dismutase (SOD), Thioredoxins (Trxs)

Amino acids' abbreviations (in brackets) are used in the results and discussion of the manuscript instead of their respective full names.

**Supplementary Table S4. Effect of treatment on the 111 MetabOxi variables.**

*P*-values of one-way ANOVA analyzing the effect of treatment on the levels of individual variables are reported. MetabOxi variables are listed based on the significance (*p*-value) of treatment effect. ns: not significant (Bonferroni-corrected *p*-value > 0.05).

Compound name	Treatment	Compound name	Treatment
Raffinose	5.68E-167	Methionine	6.86E-20
Isomaltose	1.57E-154	Valine	9.01E-20
Galactinol	1.03E-153	TAC	5.38E-19
SOD	5.91E-143	CAT	6.47E-19
Adipic acid, 2-amino-	2.29E-101	Galactonic acid-1,4-lactone	1.09E-18
Allantoin	2.45E-97	Maltose	1.33E-18
Proline	6.88E-82	Shikimic acid, 3-dehydro-	3.86E-17
Secologanin	7.29E-80	Quinic acid	3.20E-15
MDA	2.43E-79	Trxs	6.30E-15
Isocitric acid	9.25E-77	Salicylic acid	7.43E-15
Alanine, beta-	3.19E-71	GR	6.29E-14
Glyceric acid-3-phosphate	2.49E-67	Shikimic acid	1.31E-13
Phosphoenolpyruvic acid	2.73E-66	Glucosamine, N-acetyl-	3.96E-13
Malonic acid	2.91E-63	Prxs	1.28E-12
Glycerol-3-phosphate	4.25E-60	Ribitol	2.12E-10
Asparagine -H2O	9.22E-60	2-Piperidinecarboxylic acid	8.03E-10
ProtOx	1.03E-59	Poly	1.58E-09
Alanine	1.31E-59	Mannosamine, N-acetyl-	3.30E-09
Ornithine	1.78E-59	Galactosamine, N-acetyl-	4.14E-09
Glutamine	9.38E-59	Maleic acid	2.29E-07
Butanoic acid, 4-amino-	1.93E-58	Prephenic acid	5.85E-07
Butanoic acid, 4-hydroxy-	2.73E-56	Gluconic acid-1,5-lactone	9.08E-07
GOX	2.36E-53	Glucose-6-phosphate	1.15E-06
Urea	3.35E-50	Succinic acid	1.60E-06
APX	5.53E-50	POX	2.62E-06
Guanosine	1.30E-49	GST	6.07E-06
Malic acid, 2-methyl-	4.22E-49	AO	1.08E-05
Citric acid	2.56E-48	Fructose-6-phosphate	0.0002
Threonine	1.59E-47	Trehalose	0.0002
Leucine	5.94E-47	DHAR	0.0011
Phenylalanine	6.89E-45	Ribose-5-phosphate 1 MEOX	0.0018
Inositol, myo-	5.23E-44	Serine, O-acetyl-	0.0018
HPR	9.86E-44	Fumaric acid	0.0117
Serine	2.89E-42	Uridine	0.0301
Pyroglutamic acid	1.05E-41	Quinoline-2-carboxylic acid,...	0.0414
Cysteine	3.55E-41	Grxs	ns
Glyceric acid	4.23E-38	Tartronic acid	ns
Glycine	6.63E-38	Ribulose-5-phosphate	ns
Isoleucine	1.04E-37	Gluconic acid-6-phosphate	ns
Fucose	3.45E-37	GPX	ns
Phosphoric acid	7.47E-34	4-Hydroxyphenyl-beta-...	ns
Glucose (abs)	2.91E-33	Ascorbic acid	ns
Frxs	1.14E-32	Asparagine	ns
Fructose (abs)	3.57E-32	Galactaric acid	ns
Erythronic acid	1.39E-31	Glutaric acid, 2-oxo-	ns
Glutamic acid	1.82E-31	Malic acid	ns
Tyrosine	1.59E-30	Melibiose	ns
Aspartic acid	7.30E-30	Putrescine	ns
Erythritol	3.62E-28	Pyruvic acid	ns
Threonic acid	5.54E-28	Quinic acid, 3-caffeoyl-, trans-	ns
Tryptophan	8.92E-28	Quinic acid, 4-caffeoyl-, trans-	ns
Arginine	1.27E-25	Quinic acid, 5-caffeoyl-, trans-	ns
Glucose	2.48E-25	Sinapic acid, trans-	ns
Lysine	2.79E-24	Sucrose (abs)	ns
MDHAR	2.83E-23	Tyramine	ns
Glutaric acid, 2-hydroxy-	1.68E-20		

**Supplementary Table S11. Ranking of the cross-validated PLSR model based on control values of the variables.**

Variables are ranked based on their rank-product value. Variables with the lowest rank-product value are the ones with the largest discriminative power.

Ranking	Variable	Rank-product	Ranking	Variable	Rank-product
1	Galactaric acid	32	57	Shikimic acid	3.285E+17
2	Erythritol	64	58	MDA	3.518E+17
3	Adipic acid, 2-amino-	9.841E+04	59	Malic acid, 2-methyl-	3.648E+17
4	Tryptophan	7.680E+05	60	Quinic acid	3.916E+17
5	Allantoin	2.540E+07	61	ProtOx	5.448E+17
6	Quinic acid, 3-caffeoyl-, trans-	9.526E+07	62	Aspartic acid	5.841E+17
7	Leucine	6.935E+08	63	Glutamic acid	7.339E+17
8	Glucose	3.105E+09	64	Tartronic acid	7.532E+17
9	Poly	5.225E+09	65	Phosphoenolpyruvic acid	8.209E+17
10	Quinic acid, 5-caffeoyl-, trans-	6.538E+09	66	Fumaric acid	1.385E+18
11	Mannosamine, N-acetyl-	1.201E+10	67	Glutaric acid, 2-oxo-	2.133E+18
12	Phenylalanine	7.083E+10	68	Ascorbic acid	2.523E+18
13	Glucosamine, N-acetyl-	7.814E+10	69	Glucose-6-phosphate	2.554E+18
14	Galactosamine, N-acetyl-	1.409E+11	70	Galactonic acid-1,4-lactone	3.245E+18
15	Ornithine	1.673E+11	71	GPX	3.273E+18
16	Isoleucine	1.947E+12	72	GST	3.831E+18
17	Alanine, beta-	2.347E+12	73	Urea	4.323E+18
18	Ribitol	3.661E+12	74	Glyceric acid-3-phosphate	4.719E+18
19	Proline	3.765E+12	75	Glycerol-3-phosphate	5.353E+18
20	Maltose	6.916E+12	76	Phosphoric acid	5.482E+18
21	Putrescine	1.835E+13	77	HPR	5.863E+18
22	Tyramine	2.047E+13	78	AO	5.928E+18
23	Lysine	1.282E+14	79	GR	7.333E+18
24	Isocitric acid	1.706E+14	80	Raffinose	7.334E+18
25	Arginine	1.758E+14	81	MDHAR	1.074E+19
26	SOD	1.910E+14	82	TAC	1.266E+19
27	Valine	2.109E+14	83	Serine, O-acetyl-	1.366E+19
28	Glycine	3.146E+14	84	Alanine	1.503E+19
29	Methionine	3.795E+14	85	APX	1.552E+19
30	Cysteine	6.466E+14	86	Sinapic acid, trans-	1.707E+19
31	Melibiose	8.157E+14	87	DHAR	1.761E+19
32	Threonine	1.185E+15	88	Ribose-5-phosphate 1 MEOX	2.320E+19
33	CAT	1.667E+15	89	Isomaltose	2.842E+19
34	Glucose (abs)	2.019E+15	90	Butanoic acid, 4-hydroxy-	3.388E+19
35	Shikimic acid, 3-dehydro-	4.740E+15	91	Secologanin	3.923E+19
36	Tyrosine	5.229E+15	92	Glyceric acid	5.563E+19
37	Glutaric acid, 2-hydroxy-	5.563E+15	93	Ribulose-5-phosphate	6.293E+19
38	Glutamine	6.439E+15	94	Galactinol	6.393E+19
39	Inositol, myo-	1.089E+16	95	Quinic acid, 4-caffeoyl-, trans-	6.654E+19
40	Serine	1.417E+16	96	Uridine	7.275E+19
41	Threonic acid	1.730E+16	97	Succinic acid	7.919E+19
42	2-Piperidinecarboxylic acid	2.362E+16	98	Maleic acid	8.214E+19
43	Fructose (abs)	3.322E+16	99	GOX	8.321E+19
44	Prephenic acid	4.151E+16	100	Malic acid	8.662E+19
45	Malonic acid	4.455E+16	101	Sucrose (abs)	9.320E+19
46	Prxs	4.557E+16	102	Pyruvic acid	9.451E+19
47	4-Hydroxyphenyl-beta-...	5.012E+16	103	Trehalose	1.005E+20
48	Gluconic acid-1,5-lactone	9.304E+16	104	Gluconic acid-6-phosphate	1.117E+20
49	Quinoline-2-carboxylic acid,...	1.022E+17	105	Trxs	1.151E+20
50	Asparagine -H2O	1.289E+17	106	Asparagine	1.213E+20
51	POX	1.301E+17	107	Salicylic acid	1.234E+20
52	Erythronic acid	1.814E+17	108	Grxs	1.343E+20
53	Fucose	1.885E+17	109	Butanoic acid, 4-amino-	1.393E+20
54	Pyroglutamic acid	2.491E+17	110	Fructose-6-phosphate	1.567E+20
55	Citric acid	2.720E+17	111	Frxs	1.901E+20
56	Guanosine	3.195E+17			

**Supplementary Table S12. Ranking of the cross-validated PLSR model based on drought values of the variables.**

Variables are ranked based on their rank-product value. Variables with the lowest rank-product value are the ones with the largest discriminative power.

Ranking	Variable	Rank-product	Ranking	Variable	Rank-product
1	DHAR	1	57	Isoleucine	4.223E+17
2	MDA	1024	58	Shikimic acid, 3-dehydro	4.297E+17
3	MDHAR	5.905E+04	59	Poly	6.439E+17
4	TAC	1.806E+07	60	Trehalose	7.698E+17
5	AO	3.931E+07	61	Alanine	8.122E+17
6	Secologanin	7.007E+08	62	Salicylic acid	8.377E+17
7	Threonic acid	1.161E+09	63	Putrescine	1.282E+18
8	Melibiose	1.182E+09	64	Threonine	1.400E+18
9	Malic acid, 2-methyl-	2.021E+09	65	Asparagine	1.419E+18
10	POX	3.873E+09	66	Tyrosine	1.612E+18
11	APX	7.987E+09	67	Erythritol	1.942E+18
12	ProtOx	4.037E+11	68	GST	2.083E+18
13	Prxs	4.782E+11	69	Ribitol	2.299E+18
14	Sinapic acid, trans-	8.574E+11	70	Guanosine	2.840E+18
15	Ornithine	1.238E+12	71	Galactosamine, N-acetyl-	3.640E+18
16	Sucrose (abs)	1.769E+12	72	HPR	4.209E+18
17	Glycerol-3-phosphate	2.493E+12	73	Ribulose-5-phosphate	4.276E+18
18	Quinoline-2-carboxylic acid, ...	7.738E+12	74	Butanoic acid, 4-amino-	4.313E+18
19	Urea	8.311E+12	75	Maltose	4.695E+18
20	Fucose	1.190E+13	76	Glutaric acid, 2-hydroxy	5.339E+18
21	Asparagine -H2O	1.652E+13	77	Phenylalanine	6.131E+18
22	Succinic acid	1.718E+13	78	Malic acid	8.896E+18
23	Glucose-6-phosphate	4.693E+13	79	Glucose	9.927E+18
24	Gluconic acid-6-phosphate	1.575E+14	80	Phosphoenolpyruvic acid	1.073E+19
25	Allantoin	1.731E+14	81	Adipic acid, 2-amino-	1.092E+19
26	Isomaltose	3.598E+14	82	Aspartic acid	1.173E+19
27	Cysteine	6.777E+14	83	Pyruvic acid	1.176E+19
28	GR	9.803E+14	84	Quinic acid, 4-caffeoyl-, trans-	1.288E+19
29	Quinic acid, 3-caffeoyl-, trans-	1.218E+15	85	Serine	1.342E+19
30	Tryptophan	1.736E+15	86	GPX	1.354E+19
31	Citric acid	2.187E+15	87	Raffinose	1.379E+19
32	Erythronic acid	2.946E+15	88	Glucosamine, N-acetyl-	1.401E+19
33	Lysine	3.096E+15	89	SOD	1.404E+19
34	Ascorbic acid	4.122E+15	90	Grxs	1.507E+19
35	Glyceric acid-3-phosphate	4.379E+15	91	Galactinol	1.659E+19
36	CAT	4.814E+15	92	Fructose-6-phosphate	1.701E+19
37	Ribose-5-phosphate 1 MEOX	6.932E+15	93	2-Piperidinecarboxylic acid	2.004E+19
38	Maleic acid	8.405E+15	94	Glucose (abs)	2.117E+19
39	Fructose (abs)	9.914E+15	95	Pyroglutamic acid	2.224E+19
40	Methionine	1.124E+16	96	Prephenic acid	2.291E+19
41	4-Hydroxyphenyl-beta-...	1.228E+16	97	Shikimic acid	2.321E+19
42	Galactonic acid-1,4-lactone	1.891E+16	98	Arginine	2.539E+19
43	Isocitric acid	2.478E+16	99	Leucine	2.552E+19
44	Malonic acid	2.650E+16	100	Butanoic acid, 4-hydroxy	2.632E+19
45	Inositol, myo-	3.045E+16	101	Mannosamine, N-acetyl-	2.720E+19
46	Fumaric acid	3.990E+16	102	Serine, O-acetyl-	3.619E+19
47	Phosphoric acid	8.299E+16	103	Glutamine	3.710E+19
48	Uridine	9.960E+16	104	Galactaric acid	3.756E+19
49	Quinic acid	1.269E+17	105	Glutamic acid	4.550E+19
50	Gluconic acid-1,5-lactone	1.402E+17	106	Proline	4.595E+19
51	Tyramine	1.929E+17	107	Quinic acid, 5-caffeoyl-, trans-	4.781E+19
52	Alanine, beta-	2.168E+17	108	Glutaric acid, 2-oxo-	5.609E+19
53	Frxs	2.400E+17	109	Glyceric acid	6.157E+19
54	Trxs	3.421E+17	110	Glycine	1.000E+20
55	Tartronic acid	3.581E+17	111	Valine	1.374E+20
56	GOX	3.795E+17			