Supplementary Materials

Non-Additivity of the Combined Drought and Heat-Shock Response in the Leaf Metabolite Profile of Seven *Prunus* Rootstocks

Text in red marks material that is new or has been changed in the revised version.

Table S1. Effect of rootstock (main effect) on amino acid, organic acid and phenolic compound concentrations in leaf extracts (means ± SE)

Parameter	Unit	GF 677	Myrobalan 29C	Marianna 2624	Rootpac 20	Rootpac 40	Rootpac R	Garnem	Sig.
Amino acids									
Aspartate	pmol µL⁻¹	5386.7 ± 856.1^{g}	8793.1 ± 548.4^{e}	9175.6 ± 685.1^{d}	11611.3 ± 881.7^{c}	20851.9 ± 663.6^{a}	12793.0 ± 1679.3^{b}	7641.0 ± 837.9^{f}	***
Glutamate	pmol µL⁻¹	4136.1 ± 520.0^{f}	6283.7 ± 366.8^{d}	2940.2 ± 347.5^{g}	9712.5 ± 483.4^{c}	13800.6 ± 538.4^{b}	16790.4 ± 1460.5^{a}	5919.9 ± 626.4^{e}	***
Asparagine	pmol µL⁻¹	11749.4 ± 1665.6^{g}	19905.3 ± 1423.0^{e}	68688.0 ± 8925.1^{a}	23983.2 ± 3158.4^{d}	35030.9 ± 2539.9^{c}	48672.2 ± 4267.6^{b}	18461.8 ± 1958.3^{f}	***
Serine	pmol µL⁻¹	11868.7 ± 1217.7^{d}	21024.7 ± 1313.0^{c}	7302.3 ± 1033.0^{e}	27064.1 ± 2635.2^{b}	34639.3 ± 2097.9^{a}	27619.8 ± 4705.5^{b}	20114.9 ± 2496.5^{c}	***
Glutamine	pmol µL⁻¹	7522.3 ± 881.3^{f}	12516.8 ± 606.7^{d}	4807.9 ± 819.6^{g}	16732.5 ± 1041.3^{c}	22345.8 ± 934.6^{b}	27802.1 ± 1558.9^{a}	11193.4 ± 1327.2^{e}	***
Histidine	pmol µL⁻¹	2162.0 ± 123.9^{f}	4153.9 ± 121.0^{c}	1593.2 ± 243.2^{g}	5805.1 ± 363.5^{b}	6561.7 ± 201.2^{a}	3621.8 ± 832.8^{e}	3870.6 ± 415.4^{d}	***
Glycine	pmol µL⁻¹	3281.0 ± 410.9^{e}	5153.9 ± 477.4^{d}	1589.6 ± 197.6^{f}	7076.3 ± 980.0^{b}	8875.6 ± 797.3^{a}	5597.6 ± 1680.0^{c}	5797.5 ± 776.5^{c}	***
Threonine	pmol µL⁻¹	6715.7 ± 922.7^{d}	10587.4 ± 597.4^{c}	12603.1 ± 1206.1^{b}	13136.8 ± 743.2^{b}	21522.6 ± 732.4^{a}	21988.8 ± 3525.8^{a}	10008.4 ± 1158.4^{c}	***
Arginine	pmol µL⁻¹	10154.3 ± 1160.6^{f}	17379.9 ± 879.8^{de}	17579.3 ± 1501.8^{d}	22136.2 ± 2099.1^{c}	31214.7 ± 1652.3^{a}	25999.6 ± 3933.1^{b}	16215.0 ± 1704.5^{e}	***
Alanine	pmol µL⁻¹	6540.9 ± 515.3^{e}	12507.2 ± 597.4^{c}	12144.6 ± 852.0^{c}	16037.4 ± 1225.0^{b}	18158.4 ± 822.3^{a}	15272.5 ± 1744.5^{b}	11247.0 ± 1400.1^{d}	***
Tyrosine	pmol µL⁻¹	1071.0 ± 74.9^{g}	1756.3 ± 78.7^{f}	2031.3 ± 174.9^{d}	2646.9 ± 202.7^{b}	2948.8 ± 126.5^{a}	2433.9 ± 235.9^{c}	1898.6 ± 227.9^{e}	***
Cystine	pmol µL⁻¹	1421.3 ± 216.8^{e}	2311.3 ± 247.1^{d}	2602.2 ± 361.3^{c}	2610.1 ± 413.7^{c}	3596.5 ± 386.1^{a}	3289.8 ± 662.3^{b}	2231.8 ± 311.4^{d}	***
Valine	pmol µL⁻¹	788.9 ± 118.2^{e}	1310.4 ± 137.3^{d}	1428.6 ± 238.2^{cd}	1529.9 ± 227.6^{c}	2241.2 ± 213.2^{a}	1862.1 ± 332.4^{b}	1353.3 ± 158.2^{d}	***
Methionine	pmol µL⁻¹	1935.0 ± 213.9^{f}	3406.2 ± 171.9^{e}	3739.8 ± 350.7^{d}	4574.5 ± 403.4^{c}	6558.7 ± 315.5^{a}	5541.6 ± 790.7^{b}	3250.8 ± 359.8^{e}	***
Tryptophan	pmol µL⁻¹	1452.8 ± 177.4^{e}	2601.3 ± 217.6^{d}	2647.2 ± 337.6^{d}	3141.9 ± 398.6^{c}	4097.5 ± 329.0^{a}	3516.1 ± 573.8^{b}	2526.4 ± 327.4^{d}	***
Phenylalanine	pmol µL⁻¹	2399.3 ± 233.7^{f}	4250.4 ± 229.7^{d}	4433.9 ± 332.9^{d}	5682.3 ± 446.7^{c}	6795.6 ± 383.0^{a}	6279.0 ± 861.7^{b}	3852.9 ± 514.7^{e}	***
Isoleucine	pmol µL⁻¹	1524.7 ± 148.9^{e}	2693.0 ± 154.9^{d}	3012.7 ± 296.6^{c}	3480.6 ± 275.3^{b}	4148.7 ± 191.9^{a}	3578.3 ± 362.5^{b}	2574.7 ± 290.0^{d}	***
Leucine	pmol µL⁻¹	2707.7 ± 288.5^{e}	4767.0 ± 298.7^{d}	6102.5 ± 754.7^{c}	5857.8 ± 662.3^{c}	8270.8 ± 572.9^{a}	6979.3 ± 769.5^{b}	4574.8 ± 474.3^{d}	***
Lysine	pmol µL⁻¹	3962.7 ± 660.0^{e}	6366.2 ± 688.8^{d}	6774.6 ± 1178.3^{d}	7409.5 ± 1250.3^{c}	12610.9 ± 1332.1^{a}	8704.8 ± 1354.3^{b}	6667.7 ± 839.4^{d}	***
Hydroxyproline	pmol µL⁻¹	1648.5 ± 174.5^{f}	2860.6 ± 328.0^{e}	3750.7 ± 642.2^{c}	3563.0 ± 564.7^{c}	6245.5 ± 775.6^{a}	4530.6 ± 539.9^{b}	3194.4 ± 439.5^{d}	***
Sarcosine	pmol µL⁻¹	5244.4 ± 732.1^{e}	8233.3 ± 632.1^{d}	8633.5 ± 1054.6^{d}	9803.3 ± 1221.5^{c}	15895.3 ± 1237.1^{a}	14269.6 ± 2711.3^{b}	8152.9 ± 950.9^{d}	***
Organic acids									
Oxalic acid	ng µL⁻¹	4.3 ± 0.3^{f}	8.1 ± 0.3^{d}	9.8 ± 0.8^{c}	11.7 ± 0.7^{b}	13.8 ± 0.5^{a}	11.9 ± 0.9^{b}	6.8 ± 0.8^{e}	***
Propionic acid	ng µL⁻¹	10.2 ± 1.1^{f}	17.1 ± 0.8^{e}	21.0 ± 1.7^{d}	24.5 ± 1.4^{c}	38.9 ± 2.0^{a}	35.2 ± 4.9^{b}	15.8 ± 1.7^{e}	***
Tartaric acid	ng µL⁻¹	16.8 ± 1.5^{g}	30.8 ± 1.1^{e}	39.8 ± 2.8^{d}	43.7 ± 2.3^{c}	58.2 ± 2.0^{a}	54.6 ± 5.9^{b}	26.9 ± 3.0^{f}	***
Butyric acid	ng µL⁻¹	51.3 ± 3.0^{f}	91.1 ± 4.0^{d}	107.4 ± 6.4^{c}	124.8 ± 6.5^{b}	142.9 ± 5.9^{a}	125.9 ± 8.1^{b}	82.5 ± 9.7^{e}	***
Malonic acid	ng µL⁻¹	42.3 ± 2.1^{f}	80.0 ± 4.4^{e}	95.2 ± 7.6^{d}	114.4 ± 7.2^{b}	134.9 ± 7.7^{a}	106.2 ± 5.5^{c}	79.6 ± 10.0^{e}	***
Malic acid	ng µL⁻¹	15.1 ± 0.9^{f}	28.9 ± 1.9^{e}	34.2 ± 2.4^{d}	43.2 ± 2.5^{c}	57.8 ± 3.5^{a}	47.3 ± 5.1^{b}	25.9 ± 3.2^{e}	***
Lactic acid	ng µL⁻¹	71.0 ± 5.1^{g}	126.1 ± 5.2^{e}	146.0 ± 8.9^{d}	175.1 ± 10.0^{c}	231.7 ± 10.9^{a}	195.1 ± 20.0^{b}	113.4 ± 12.1^{f}	***
Citric acid	ng µL⁻¹	59.8 ± 5.3^{e}	108.7 ± 4.3^{d}	152.2 ± 14.6^{c}	149.8 ± 10.1^{c}	213.7 ± 8.9^{a}	195.7 ± 18.2^{b}	100.7 ± 11.0^{d}	***
Maleic acid	ng µL⁻¹	15.9 ± 1.4^{f}	29.2 ± 2.8^{d}	42.4 ± 3.8^{c}	47.8 ± 4.0^{b}	52.7 ± 4.7^{a}	53.7 ± 5.8^{a}	23.0 ± 2.8^{e}	***
Fumaric acid	ng µL⁻¹	17.9 ± 1.1^{e}	31.4 ± 2.4^{d}	35.6 ± 3.0^{c}	43.8 ± 3.6^{b}	59.7 ± 5.0^{a}	45.7 ± 3.8^{b}	30.9 ± 4.3^{d}	***
Succinic acid	ng µL⁻¹	83.1 ± 6.5^{e}	144.8 ± 6.7^{c}	148.6 ± 8.6^{c}	189.0 ± 12.7^{b}	216.5 ± 9.5^{a}	188.2 ± 20.7^{b}	129.4 ± 15.7^{d}	***
Phenolic compounds									
Gallic acid	µg L⁻¹	3.1 ± 0.5^{d}	4.1 ± 0.2^{c}	2.7 ± 0.2^{d}	1.7 ± 0.4^{f}	8.9 ± 0.5^{a}	6.4 ± 0.6^{b}	2.1 ± 0.4^{e}	***
Vanillic acid	µg L⁻¹	4.6 ± 0.7^{d}	6.5 ± 0.4^{c}	4.0 ± 0.2^{e}	2.3 ± 0.6^{g}	12.8 ± 0.6^{a}	9.4 ± 0.9^{b}	3.1 ± 0.6^{f}	***
trans-Caffeic acid	µg L⁻¹	4.6 ± 0.8^{c}	4.6 ± 0.3^{c}	2.6 ± 0.1^{d}	2.2 ± 0.5^{e}	9.1 ± 0.5^{a}	6.5 ± 0.6^{b}	2.2 ± 0.4^{e}	***
trans-p-Coumaric acid	µg L⁻¹	3.9 ± 0.6^{e}	6.6 ± 0.2^{c}	4.4 ± 0.2^{d}	2.2 ± 0.5^{g}	12.8 ± 0.5^{a}	9.4 ± 0.8^{b}	3.2 ± 0.6^{f}	***
Ferulic acid	µg L⁻¹	2.3 ± 0.3^{c}	2.6 ± 0.1^{a}	2.6 ± 0.1^{a}	1.1 ± 0.2^{d}	2.5 ± 0.1^{b}	2.7 ± 0.1^{a}	1.0 ± 0.2^{d}	***
Caftaric acid	µg L⁻¹	5.7 ± 0.9^{d}	8.2 ± 0.6^{c}	4.8 ± 0.3^{e}	2.9 ± 0.7^{g}	16.1 ± 0.9^{a}	12.0 ± 1.2^{b}	3.9 ± 0.8^{f}	***
Catechin	µg L⁻¹	5.2 ± 0.8^{d}	8.3 ± 0.5^{c}	5.8 ± 0.4^{d}	3.3 ± 0.7^{f}	17.0 ± 1.1^{a}	12.9 ± 1.4^{b}	4.1 ± 0.8^{e}	***
Epicatechin	µg L⁻¹	3.5 ± 0.6^{d}	5.0 ± 0.3^{c}	2.8 ± 0.1^{e}	1.8 ± 0.4^{f}	10.7 ± 0.5^{a}	7.4 ± 0.7^{b}	2.6 ± 0.5^{e}	***
Quercetin	µg L⁻¹	5.6 ± 1.2^{a}	3.9 ± 0.1^{bc}	4.2 ± 0.1^{b}	0.9 ± 0.3^{e}	3.7 ± 0.1^{c}	4.0 ± 0.1^{bc}	1.5 ± 0.3^{d}	***
Rutin	µg L⁻¹	4.9 ± 1.4^{c}	3.7 ± 0.2^{d}	2.3 ± 0.1^{e}	1.8 ± 0.4^{f}	7.2 ± 0.4^{a}	5.3 ± 0.5^{b}	1.8 ± 0.3^{f}	***
Myricetin	µg L⁻¹	3.6 ± 0.5^{c}	3.0 ± 0.2^{d}	1.9 ± 0.2^{e}	1.0 ± 0.2^{f}	6.3 ± 0.6^{a}	4.7 ± 0.5^{b}	1.5 ± 0.3^{e}	***

Values are means ± standard error (SE), rounded to one decimal place. Means within a row followed by different superscript letters differ significantly according to Duncan's multiple range test ($p < 0.05$). SE = SD/√n. Letters compare the seven rootstocks within each row (n = 12 per mean). Sig.: *** $p < 0.001$; ** $p < 0.01$; * $p < 0.05$; ns, not significant.

Table S2. Effect of treatment (main effect) on amino acid, organic acid and phenolic compound concentrations in leaf extracts (means ± SE)

Parameter	Unit	Control	Drought	Heat shock	Drought + Heat shock	Sig.
Amino acids						
Aspartate	pmol µL⁻¹	15110.6 ± 1094.2^{a}	9240.5 ± 1050.4^{c}	11528.7 ± 1157.2^{b}	7693.1 ± 1046.2^{d}	***
Glutamate	pmol µL⁻¹	6169.2 ± 838.0^{d}	9407.9 ± 1281.4^{b}	7268.3 ± 932.6^{c}	11202.4 ± 1312.2^{a}	***
Asparagine	pmol µL⁻¹	17567.2 ± 1944.2^{d}	37477.2 ± 5218.3^{b}	27223.3 ± 3462.6^{c}	47155.6 ± 6381.6^{a}	***
Serine	pmol µL⁻¹	13599.1 ± 1493.3^{d}	22889.5 ± 2141.1^{b}	16909.4 ± 1908.3^{c}	32107.0 ± 2971.8^{a}	***
Glutamine	pmol µL⁻¹	14855.2 ± 2192.0^{ab}	14446.2 ± 2031.3^{bc}	15500.9 ± 1777.9^{a}	14009.6 ± 1341.5^{c}	**
Histidine	pmol µL⁻¹	2934.4 ± 360.1^{d}	4117.1 ± 479.4^{b}	3629.0 ± 460.7^{c}	5187.1 ± 442.4^{a}	***
Glycine	pmol µL⁻¹	2625.0 ± 362.9^{d}	5807.0 ± 491.6^{b}	3822.2 ± 523.6^{c}	9101.2 ± 916.9^{a}	***
Threonine	pmol µL⁻¹	9176.2 ± 980.9^{d}	15042.0 ± 1567.7^{b}	11347.6 ± 1037.7^{c}	19613.0 ± 1920.3^{a}	***
Arginine	pmol µL⁻¹	13049.0 ± 1104.8^{d}	22072.9 ± 1696.7^{b}	16667.3 ± 1419.3^{c}	28598.7 ± 2165.9^{a}	***
Alanine	pmol µL⁻¹	9575.4 ± 748.2^{d}	13774.7 ± 786.7^{b}	11169.1 ± 813.3^{c}	17999.7 ± 1133.9^{a}	***
Tyrosine	pmol µL⁻¹	1489.1 ± 114.5^{d}	2267.0 ± 134.2^{b}	1833.1 ± 129.7^{c}	2860.4 ± 178.5^{a}	***
Cystine	pmol µL⁻¹	1278.2 ± 92.1^{d}	2626.1 ± 130.3^{b}	1939.2 ± 143.8^{c}	4478.3 ± 316.4^{a}	***
Valine	pmol µL⁻¹	691.1 ± 55.6^{d}	1714.7 ± 113.1^{b}	1199.0 ± 107.0^{c}	2403.4 ± 171.2^{a}	***
Methionine	pmol µL⁻¹	5778.1 ± 465.2^{a}	3525.0 ± 311.6^{c}	4621.3 ± 374.4^{b}	2650.8 ± 250.6^{d}	***
Tryptophan	pmol µL⁻¹	1593.1 ± 120.8^{d}	3020.8 ± 164.3^{b}	2278.1 ± 172.8^{c}	4527.0 ± 306.8^{a}	***
Phenylalanine	pmol µL⁻¹	3327.7 ± 274.5^{d}	5008.8 ± 358.1^{b}	3978.7 ± 293.1^{c}	6938.0 ± 482.7^{a}	***
Isoleucine	pmol µL⁻¹	2024.3 ± 160.5^{d}	3271.3 ± 188.2^{b}	2591.7 ± 175.3^{c}	4120.0 ± 234.4^{a}	***
Leucine	pmol µL⁻¹	3262.4 ± 236.7^{d}	6397.6 ± 441.7^{b}	4877.1 ± 410.3^{c}	7897.2 ± 522.2^{a}	***
Lysine	pmol µL⁻¹	3184.6 ± 282.9^{d}	8566.0 ± 625.6^{b}	6013.2 ± 684.0^{c}	12234.1 ± 792.5^{a}	***
Hydroxyproline	pmol µL⁻¹	1718.3 ± 128.5^{d}	4333.6 ± 420.1^{b}	2779.3 ± 245.5^{c}	5907.8 ± 460.3^{a}	***
Sarcosine	pmol µL⁻¹	5367.8 ± 444.1^{d}	11071.5 ± 842.3^{b}	7939.3 ± 772.3^{c}	15754.2 ± 1445.0^{a}	***
Organic acids						
Oxalic acid	ng µL⁻¹	12.1 ± 0.8^{a}	8.5 ± 0.7^{c}	10.2 ± 0.8^{b}	7.2 ± 0.6^{d}	***
Propionic acid	ng µL⁻¹	15.9 ± 1.7^{d}	25.8 ± 2.7^{b}	19.5 ± 1.9^{c}	31.8 ± 3.1^{a}	***
Tartaric acid	ng µL⁻¹	39.5 ± 4.1^{b}	41.4 ± 4.6^{a}	38.0 ± 3.0^{b}	35.8 ± 3.2^{c}	***
Butyric acid	ng µL⁻¹	78.4 ± 5.9^{d}	111.4 ± 6.9^{b}	93.9 ± 6.6^{c}	131.2 ± 7.6^{a}	***
Malonic acid	ng µL⁻¹	121.1 ± 7.9^{a}	83.4 ± 6.1^{c}	100.7 ± 6.8^{b}	67.8 ± 5.2^{d}	***
Malic acid	ng µL⁻¹	49.0 ± 4.1^{a}	31.4 ± 2.7^{c}	38.5 ± 3.3^{b}	25.3 ± 2.4^{d}	***
Lactic acid	ng µL⁻¹	111.8 ± 9.4^{d}	163.6 ± 12.4^{b}	132.2 ± 10.8^{c}	197.2 ± 14.6^{a}	***
Citric acid	ng µL⁻¹	183.2 ± 14.1^{a}	125.8 ± 11.3^{c}	155.4 ± 12.7^{b}	95.9 ± 9.3^{d}	***
Maleic acid	ng µL⁻¹	55.1 ± 4.9^{a}	31.3 ± 2.8^{c}	39.0 ± 3.1^{b}	25.9 ± 2.3^{d}	***
Fumaric acid	ng µL⁻¹	34.0 ± 3.3^{c}	37.6 ± 3.2^{b}	34.6 ± 2.4^{bc}	45.2 ± 5.2^{a}	***
Succinic acid	ng µL⁻¹	149.7 ± 16.0^{b}	150.8 ± 9.1^{b}	151.5 ± 11.6^{b}	176.4 ± 13.7^{a}	***
Phenolic compounds						
Gallic acid	µg L⁻¹	2.6 ± 0.5^{d}	4.7 ± 0.6^{b}	3.3 ± 0.5^{c}	5.9 ± 0.6^{a}	***
Vanillic acid	µg L⁻¹	3.9 ± 0.7^{d}	6.9 ± 0.8^{b}	5.1 ± 0.8^{c}	8.6 ± 0.9^{a}	***
trans-Caffeic acid	µg L⁻¹	2.8 ± 0.5^{d}	5.2 ± 0.5^{b}	3.7 ± 0.6^{c}	6.5 ± 0.6^{a}	***
trans-p-Coumaric acid	µg L⁻¹	4.8 ± 0.7^{d}	6.4 ± 0.9^{b}	5.5 ± 0.8^{c}	7.6 ± 1.0^{a}	***
Ferulic acid	µg L⁻¹	1.4 ± 0.2^{d}	2.4 ± 0.1^{b}	1.9 ± 0.2^{c}	2.8 ± 0.1^{a}	***
Caftaric acid	µg L⁻¹	5.6 ± 0.8^{d}	6.6 ± 0.9^{c}	8.2 ± 1.2^{b}	10.2 ± 1.4^{a}	***
Catechin	µg L⁻¹	5.9 ± 0.8^{d}	8.4 ± 1.2^{b}	7.0 ± 0.9^{c}	11.0 ± 1.5^{a}	***
Epicatechin	µg L⁻¹	3.6 ± 0.5^{d}	5.0 ± 0.8^{b}	4.5 ± 0.6^{c}	6.2 ± 0.9^{a}	***
Quercetin	µg L⁻¹	2.1 ± 0.3^{d}	4.0 ± 0.5^{b}	2.8 ± 0.3^{c}	4.7 ± 0.6^{a}	***
Rutin	µg L⁻¹	2.0 ± 0.4^{d}	4.8 ± 0.6^{b}	2.7 ± 0.5^{c}	5.9 ± 0.6^{a}	***
Myricetin	µg L⁻¹	2.8 ± 0.3^{b}	2.9 ± 0.5^{b}	3.5 ± 0.4^{a}	3.3 ± 0.7^{a}	***

Values are means ± standard error (SE), rounded to one decimal place. Means within a row followed by different superscript letters differ significantly according to Duncan's multiple range test ($p < 0.05$). SE = SD/√n. Letters compare the four treatments within each row (n = 21 per mean). Sig.: *** $p < 0.001$; ** $p < 0.01$; * $p < 0.05$; ns, not significant.

Table S3a. Rootstock × treatment interaction means (± SE) for amino acid concentrations in leaf extracts (pmol µL⁻¹)

Parameter	GF 677				Myrobalan 29C				Marianna 2624				Rootpac 20			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Aspartate	10257.6 ± 125.4^{i}	3630.2 ± 56.8^{o}	4349.6 ± 53.2^{n}	3309.4 ± 50.2^{o}	11584.0 ± 264.1^{gh}	8106.8 ± 126.9^{k}	8854.8 ± 108.2^{j}	6627.1 ± 201.5^{l}	12099.1 ± 147.9^{g}	8898.3 ± 214.1^{j}	9890.3 ± 154.8^{i}	5814.5 ± 139.9^{m}	16037.4 ± 196.0^{f}	11464.1 ± 179.5^{h}	11066.7 ± 266.2^{h}	7877.1 ± 189.5^{k}
Glutamate	2682.0 ± 74.7^{o}	3795.0 ± 177.5^{lmn}	3073.8 ± 204.9^{no}	6993.8 ± 327.0^{hi}	4500.2 ± 155.6^{kl}	7574.8 ± 78.3^{h}	5866.4 ± 36.1^{j}	7193.5 ± 50.6^{hi}	1766.4 ± 23.7^{p}	2846.0 ± 48.9^{o}	2368.7 ± 61.6^{op}	4779.5 ± 318.7^{k}	7738.2 ± 515.9^{h}	10081.3 ± 348.9^{f}	9123.4 ± 254.0^{g}	11907.1 ± 299.9^{e}
Asparagine	6383.4 ± 115.4^{q}	11406.0 ± 365.6^{no}	8461.9 ± 332.0^{pq}	20746.2 ± 665.0^{l}	12468.3 ± 225.3^{no}	22284.9 ± 714.3^{kl}	19908.9 ± 302.3^{l}	24959.0 ± 800.0^{jk}	29939.6 ± 179.6^{i}	83126.3 ± 2985.7^{b}	53862.9 ± 973.5^{e}	107823.1 ± 3456.1^{a}	12250.6 ± 221.4^{no}	27140.0 ± 974.8^{ij}	17211.2 ± 311.1^{m}	39331.1 ± 1960.5^{g}
Serine	7642.5 ± 225.8^{op}	12212.5 ± 581.6^{lm}	9529.1 ± 637.9^{no}	18090.8 ± 861.5^{j}	15067.2 ± 445.2^{k}	23760.1 ± 1131.5^{ghi}	19610.5 ± 1312.7^{j}	25661.0 ± 1222.1^{fgh}	4068.1 ± 120.2^{q}	6928.5 ± 330.0^{op}	5294.8 ± 354.4^{pq}	12917.7 ± 381.7^{klm}	17657.3 ± 521.7^{j}	27981.4 ± 1873.1^{f}	22243.1 ± 657.2^{i}	40374.5 ± 1922.8^{c}
Glutamine	12232.5 ± 687.5^{jk}	5546.5 ± 68.5^{op}	7385.5 ± 415.1^{no}	4924.8 ± 100.6^{pq}	14799.9 ± 831.8^{hi}	10979.9 ± 466.5^{kl}	13703.6 ± 770.2^{ij}	10584.0 ± 486.0^{klm}	2964.6 ± 125.9^{q}	2857.7 ± 131.2^{q}	3996.0 ± 224.6^{pq}	9413.5 ± 399.9^{lmn}	13347.7 ± 567.0^{ij}	21930.8 ± 1232.6^{e}	14837.1 ± 681.3^{hi}	16814.2 ± 714.3^{gh}
Histidine	2818.9 ± 88.5^{ij}	1757.2 ± 73.9^{k}	2064.9 ± 78.9^{k}	2006.9 ± 63.0^{k}	3625.7 ± 125.5^{h}	4263.8 ± 70.1^{g}	4046.7 ± 104.0^{g}	4679.5 ± 34.5^{f}	988.0 ± 41.6^{lm}	1263.5 ± 9.3^{l}	1151.2 ± 18.9^{lm}	2970.0 ± 125.0^{i}	4059.8 ± 170.8^{g}	6404.9 ± 244.8^{c}	5552.3 ± 233.6^{de}	7203.3 ± 226.2^{a}
Glycine	1679.8 ± 69.6^{q}	3693.9 ± 152.5^{o}	2493.9 ± 103.5^{p}	5256.5 ± 217.0^{ijk}	2918.7 ± 121.0^{p}	6333.7 ± 261.5^{i}	4523.0 ± 187.8^{lm}	6840.4 ± 282.4^{h}	788.0 ± 32.7^{rs}	1846.9 ± 76.3^{q}	1221.2 ± 50.7^{r}	2502.3 ± 103.7^{p}	3881.1 ± 160.9^{no}	7323.0 ± 304.0^{g}	4889.1 ± 202.6^{kl}	12212.1 ± 504.2^{c}
Threonine	4056.4 ± 151.5^{p}	6211.3 ± 581.6^{nop}	5003.2 ± 414.7^{op}	11591.8 ± 1085.3^{ijk}	8348.0 ± 311.8^{lmn}	11164.3 ± 358.0^{ijkl}	9506.0 ± 265.0^{klm}	13331.3 ± 730.6^{hi}	7157.1 ± 267.3^{mno}	12855.0 ± 407.5^{hij}	12505.9 ± 1180.8^{hij}	17894.5 ± 1227.0^{efg}	10212.1 ± 381.4^{jkl}	12864.3 ± 480.5^{hij}	12697.9 ± 605.3^{hij}	16773.1 ± 623.2^{fg}
Arginine	6909.3 ± 188.9^{o}	9111.2 ± 267.4^{mno}	8055.8 ± 264.8^{no}	16540.7 ± 1026.9^{gh}	13531.9 ± 705.8^{ijk}	18599.1 ± 336.4^{fg}	16285.9 ± 391.8^{gh}	21102.9 ± 767.0^{f}	10982.8 ± 572.9^{klm}	19591.1 ± 908.5^{f}	15697.0 ± 818.8^{hi}	24046.0 ± 1156.1^{e}	13682.4 ± 713.7^{ij}	24561.3 ± 1556.1^{e}	18712.5 ± 976.1^{fg}	31588.8 ± 1961.1^{cd}
Alanine	4970.9 ± 221.8^{n}	6721.3 ± 461.8^{mn}	5377.4 ± 68.6^{n}	9094.1 ± 624.9^{jkl}	10140.4 ± 518.7^{ijk}	13391.2 ± 450.6^{fg}	11390.1 ± 178.4^{hi}	15107.3 ± 389.3^{def}	8693.7 ± 444.7^{kl}	12425.6 ± 274.4^{gh}	11357.2 ± 580.9^{hi}	16102.0 ± 1106.4^{cde}	11673.6 ± 597.1^{ghi}	15550.2 ± 343.4^{de}	14705.3 ± 752.1^{ef}	22220.6 ± 1526.9^{a}
Tyrosine	808.2 ± 30.0^{q}	1107.1 ± 41.3^{op}	922.2 ± 34.0^{q}	1446.3 ± 53.9^{l}	1404.2 ± 52.2^{lm}	1865.2 ± 50.6^{j}	1672.6 ± 61.7^{k}	2083.3 ± 46.4^{i}	1203.9 ± 44.7^{no}	2258.0 ± 83.3^{h}	1895.6 ± 70.4^{j}	2767.7 ± 103.1^{e}	1867.2 ± 69.4^{j}	2708.0 ± 99.9^{e}	2352.1 ± 87.4^{gh}	3660.2 ± 136.4^{a}
Cystine	698.9 ± 17.1^{u}	1596.9 ± 50.8^{nop}	874.6 ± 33.9^{tu}	2514.6 ± 80.0^{j}	1255.8 ± 30.7^{qrs}	2976.5 ± 94.7^{gh}	1798.3 ± 69.8^{mn}	3214.7 ± 102.3^{g}	1076.6 ± 26.3^{rst}	2889.8 ± 180.6^{hi}	2134.7 ± 226.3^{kl}	4307.6 ± 137.1^{d}	1341.3 ± 32.8^{pqr}	2563.8 ± 99.5^{j}	1689.6 ± 41.3^{no}	4845.6 ± 154.2^{c}
Valine	295.4 ± 3.5^{p}	859.3 ± 72.6^{lmn}	657.6 ± 51.2^{mno}	1343.1 ± 113.5^{hij}	607.9 ± 7.2^{no}	1517.3 ± 18.6^{hi}	1300.8 ± 70.0^{ij}	1815.6 ± 116.6^{fg}	521.2 ± 6.2^{op}	1900.0 ± 147.9^{fg}	863.2 ± 10.2^{lmn}	2429.9 ± 205.3^{cd}	743.6 ± 8.8^{lmno}	1887.5 ± 146.9^{fg}	936.7 ± 11.1^{klm}	2551.7 ± 215.5^{c}
Methionine	3071.5 ± 219.8^{ikl}	1755.6 ± 125.6^{pq}	1662.3 ± 75.1^{pq}	1250.6 ± 56.2^{q}	4099.8 ± 165.9^{fgh}	3288.2 ± 80.4^{ijk}	3632.6 ± 87.4^{hij}	2604.4 ± 116.9^{lmno}	5120.1 ± 253.4^{d}	3307.6 ± 148.5^{ijk}	4417.7 ± 114.8^{efg}	2113.8 ± 94.9^{nop}	6301.1 ± 450.9^{c}	3951.6 ± 177.4^{ghi}	5156.0 ± 233.0^{d}	2889.4 ± 129.7^{klm}
Tryptophan	778.4 ± 21.4^{p}	1576.6 ± 59.0^{mn}	1120.9 ± 34.4^{o}	2335.5 ± 87.4^{j}	1562.3 ± 42.9^{mn}	3122.5 ± 116.9^{fgh}	2348.2 ± 72.1^{ij}	3372.3 ± 126.3^{f}	1339.4 ± 36.8^{no}	2982.2 ± 91.5^{gh}	1984.1 ± 54.5^{kl}	4282.9 ± 160.4^{d}	1798.5 ± 49.4^{lm}	3291.4 ± 101.0^{fg}	2265.6 ± 62.2^{jk}	5212.2 ± 195.1^{c}
Phenylalanine	1671.0 ± 104.3^{s}	2441.6 ± 110.8^{r}	1867.6 ± 53.5^{s}	3616.9 ± 164.1^{mnop}	3320.1 ± 115.9^{opq}	4641.0 ± 107.8^{ij}	3800.7 ± 27.1^{lmno}	5239.8 ± 188.3^{gh}	3156.6 ± 90.4^{pq}	4125.8 ± 253.8^{jklm}	4347.9 ± 158.4^{jk}	6105.2 ± 276.9^{f}	4314.8 ± 123.6^{jkl}	5435.4 ± 155.7^{g}	4906.8 ± 306.1^{hi}	8072.1 ± 366.1^{c}
Isoleucine	963.1 ± 25.2^{r}	1621.0 ± 88.2^{op}	1264.6 ± 70.6^{qr}	2250.0 ± 122.5^{lm}	1982.1 ± 51.9^{mn}	2934.6 ± 66.0^{ij}	2515.9 ± 90.5^{kl}	3339.5 ± 76.0^{fgh}	1699.3 ± 44.5^{nop}	3421.9 ± 191.1^{efg}	2636.2 ± 69.0^{ijk}	4293.4 ± 233.7^{c}	2424.7 ± 63.5^{kl}	3629.5 ± 202.7^{def}	3054.4 ± 79.9^{hi}	4813.6 ± 262.0^{b}
Leucine	1666.7 ± 51.5^{q}	2648.0 ± 117.6^{p}	2309.3 ± 75.6^{p}	4206.7 ± 250.2^{n}	3220.0 ± 99.4^{o}	5256.0 ± 64.1^{kl}	4734.0 ± 57.2^{lm}	5858.0 ± 182.1^{j}	2613.7 ± 81.0^{p}	7857.3 ± 241.8^{f}	4991.3 ± 154.4^{l}	8947.7 ± 390.3^{cd}	3198.3 ± 98.8^{o}	7307.3 ± 328.7^{g}	4374.3 ± 135.1^{mn}	8551.3 ± 446.9^{de}
Lysine	1383.6 ± 38.3^{p}	4062.9 ± 159.0^{kl}	3059.0 ± 122.1^{mno}	7345.3 ± 287.5^{i}	2727.8 ± 75.6^{no}	7745.2 ± 180.5^{hi}	6295.4 ± 251.3^{j}	8696.2 ± 220.5^{g}	2338.7 ± 64.8^{o}	8876.5 ± 354.3^{g}	3846.2 ± 106.6^{klm}	12037.0 ± 471.1^{c}	3196.8 ± 88.6^{lmno}	8982.6 ± 358.5^{g}	4027.0 ± 111.6^{kl}	13431.8 ± 525.7^{cd}
Hydroxyproline	881.6 ± 54.4^{p}	2171.8 ± 107.4^{lm}	1338.8 ± 79.6^{op}	2201.8 ± 131.0^{lm}	1612.6 ± 99.5^{no}	2842.4 ± 128.6^{jk}	2441.2 ± 54.8^{kl}	4546.1 ± 224.8^{fg}	1382.5 ± 85.3^{op}	4197.4 ± 249.7^{g}	2467.3 ± 152.2^{kl}	6955.5 ± 343.9^{c}	1691.9 ± 104.4^{mno}	4062.2 ± 241.7^{gh}	2131.4 ± 131.5^{lmn}	6366.6 ± 314.8^{d}
Sarcosine	2831.5 ± 92.0^{q}	5120.5 ± 274.3^{mnop}	3887.6 ± 222.7^{pq}	9138.0 ± 489.5^{hij}	5087.8 ± 165.2^{mnop}	9184.5 ± 280.5^{hij}	7993.8 ± 457.8^{jk}	10667.2 ± 289.4^{gh}	4361.9 ± 141.7^{op}	10312.0 ± 590.6^{ghi}	6563.2 ± 213.2^{klm}	13296.8 ± 712.3^{e}	5434.1 ± 176.5^{lmno}	11396.4 ± 652.7^{fg}	6845.4 ± 222.3^{kl}	15537.1 ± 832.3^{d}

Table S3a (continued).

Parameter	Rootpac 40				Rootpac R				Garnem			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Aspartate	24035.7 ± 293.8^{a}	19243.3 ± 301.3^{d}	21552.5 ± 337.4^{b}	18576.2 ± 446.9^{e}	20345.6 ± 493.1^{c}	7884.4 ± 123.4^{k}	15848.2 ± 524.2^{f}	7093.7 ± 170.6^{l}	11415.1 ± 139.5^{h}	5456.2 ± 66.7^{m}	9139.1 ± 143.1^{j}	4553.7 ± 71.3^{n}
Glutamate	11261.7 ± 313.5^{e}	15095.1 ± 304.1^{c}	13247.5 ± 396.9^{d}	15598.3 ± 446.9^{c}	11528.3 ± 42.5^{e}	19863.2 ± 834.4^{b}	12771.6 ± 118.1^{d}	22998.7 ± 550.7^{a}	3707.6 ± 103.2^{mn}	6599.7 ± 183.7^{i}	4426.5 ± 207.0^{klm}	8945.7 ± 418.3^{g}
Asparagine	22282.4 ± 402.7^{kl}	39352.9 ± 1413.5^{g}	33871.1 ± 701.8^{h}	44617.3 ± 1430.1^{f}	28847.7 ± 521.4^{i}	57763.5 ± 1851.5^{d}	42939.2 ± 776.0^{f}	65138.5 ± 2555.9^{c}	10798.6 ± 387.9^{op}	21267.1 ± 834.5^{l}	14307.7 ± 458.6^{n}	27473.7 ± 880.6^{ij}
Serine	26156.2 ± 772.8^{fg}	35536.4 ± 2378.8^{d}	32904.1 ± 2202.6^{e}	43960.5 ± 2093.6^{b}	13487.8 ± 103.0^{klm}	30757.7 ± 908.7^{e}	14539.5 ± 303.9^{kl}	51694.3 ± 2461.9^{a}	11114.7 ± 744.0^{mn}	23049.6 ± 713.1^{hi}	14244.7 ± 678.4^{kl}	32050.6 ± 1526.4^{e}
Glutamine	19508.0 ± 895.7^{f}	26699.0 ± 1500.6^{c}	22107.6 ± 939.2^{e}	21068.7 ± 967.4^{ef}	35104.3 ± 1973.0^{a}	24495.0 ± 1126.0^{d}	29067.4 ± 1234.9^{b}	22541.6 ± 108.0^{de}	6029.6 ± 276.9^{op}	8614.4 ± 484.2^{mn}	17409.4 ± 978.5^{g}	12720.4 ± 584.1^{ijk}
Histidine	5702.3 ± 239.9^{d}	6801.0 ± 47.1^{b}	6337.0 ± 141.6^{c}	7406.5 ± 176.3^{a}	801.9 ± 33.7^{m}	5856.4 ± 246.4^{d}	983.7 ± 37.6^{lm}	6845.0 ± 215.0^{b}	2544.1 ± 97.2^{j}	2472.7 ± 77.7^{j}	5267.0 ± 165.4^{e}	5198.4 ± 198.7^{e}
Glycine	5522.8 ± 228.9^{j}	8934.1 ± 370.9^{e}	8272.3 ± 343.4^{f}	12773.3 ± 527.4^{b}	675.6 ± 28.0^{s}	6238.8 ± 258.6^{i}	1047.0 ± 43.5^{rs}	14429.1 ± 595.7^{a}	2908.8 ± 120.8^{p}	6278.3 ± 260.6^{i}	4308.6 ± 177.9^{mn}	9694.4 ± 400.3^{d}
Threonine	18604.3 ± 479.9^{ef}	22242.6 ± 335.3^{d}	20257.2 ± 77.8^{de}	24986.2 ± 369.4^{c}	10019.9 ± 374.2^{jklm}	28234.5 ± 1054.6^{b}	12218.3 ± 1012.7^{ijk}	37482.7 ± 3509.4^{a}	5835.7 ± 483.7^{nop}	11721.8 ± 478.9^{ijk}	7244.9 ± 678.3^{mno}	15231.2 ± 984.8^{gh}
Arginine	23601.3 ± 1231.1^{e}	33486.4 ± 733.2^{c}	29767.2 ± 931.8^{d}	38003.8 ± 1218.6^{b}	12740.1 ± 664.5^{jk}	29767.5 ± 1552.7^{d}	16219.9 ± 1027.6^{gh}	45271.0 ± 2810.6^{a}	9894.9 ± 341.3^{lmn}	19394.1 ± 780.5^{f}	11933.0 ± 636.9^{jkl}	23637.8 ± 1020.2^{e}
Alanine	15635.6 ± 741.0^{de}	18038.3 ± 398.4^{b}	16861.1 ± 264.5^{bcd}	22098.7 ± 1518.5^{a}	9737.0 ± 498.0^{ijk}	16964.6 ± 867.7^{bcd}	10652.9 ± 235.3^{hij}	23735.6 ± 1631.0^{a}	6176.8 ± 136.4^{mn}	13331.8 ± 294.4^{fg}	7839.7 ± 538.7^{lm}	17639.4 ± 1212.1^{bc}
Tyrosine	2439.3 ± 90.6^{fg}	3079.2 ± 83.5^{c}	2762.1 ± 61.3^{e}	3514.6 ± 131.0^{b}	1625.2 ± 60.4^{k}	2529.6 ± 94.0^{f}	1935.9 ± 71.4^{j}	3644.8 ± 135.8^{a}	1075.7 ± 39.7^{p}	2321.7 ± 85.7^{gh}	1291.4 ± 48.1^{mn}	2905.6 ± 108.3^{d}
Cystine	2112.0 ± 51.6^{kl}	3517.2 ± 79.6^{f}	3148.6 ± 98.0^{gh}	5608.3 ± 178.5^{b}	1442.7 ± 35.3^{opq}	2640.0 ± 64.5^{ij}	2066.0 ± 80.1^{klm}	7010.4 ± 223.1^{a}	1020.1 ± 39.6st	2198.0 ± 85.3^{k}	1862.7 ± 59.3^{lmn}	3846.6 ± 122.4^{e}
Valine	1162.3 ± 13.7^{jk}	2591.4 ± 70.0^{c}	2190.4 ± 63.1^{de}	3020.9 ± 206.5^{b}	740.0 ± 8.7^{lmno}	1629.0 ± 126.8^{gh}	1442.1 ± 17.0^{hij}	3637.2 ± 307.2^{a}	767.1 ± 59.7^{lmno}	1618.3 ± 125.9^{gh}	1002.3 ± 84.7^{kl}	2025.6 ± 171.1^{ef}
Methionine	7828.4 ± 256.7^{b}	6394.0 ± 171.4^{c}	6957.3 ± 114.9^{c}	5055.2 ± 227.0^{de}	9290.2 ± 664.8^{a}	3724.7 ± 168.3^{hij}	6467.0 ± 290.4^{c}	2684.5 ± 120.5^{klmn}	4735.5 ± 249.2^{def}	2253.1 ± 106.2^{mnop}	4056.6 ± 108.7^{gh}	1958.0 ± 52.9^{op}
Tryptophan	2664.2 ± 73.2^{i}	4218.2 ± 100.3^{d}	3832.2 ± 85.2^{e}	5675.2 ± 212.5^{b}	1701.1 ± 46.7^{lm}	3132.9 ± 86.0^{fgh}	2556.8 ± 78.5^{ij}	6673.6 ± 249.9^{a}	1307.4 ± 40.1^{no}	2821.8 ± 86.6^{hi}	1839.0 ± 68.9^{lm}	4137.6 ± 154.9^{d}
Phenylalanine	5495.3 ± 154.4^{g}	6695.1 ± 130.2^{e}	6202.8 ± 117.9^{ef}	8789.0 ± 398.7^{b}	3387.2 ± 118.3^{nop}	7516.1 ± 215.3^{d}	3877.6 ± 27.6^{klmn}	10335.2 ± 468.8^{a}	1949.1 ± 121.6^{s}	4206.8 ± 262.5^{jkl}	2847.9 ± 129.2^{qr}	6407.9 ± 290.7^{ef}
Isoleucine	3365.5 ± 88.1^{efgh}	4472.0 ± 167.1^{c}	3846.3 ± 88.4^{d}	4911.0 ± 267.3^{b}	2260.1 ± 59.1^{lm}	3708.3 ± 97.0^{de}	2933.8 ± 163.8^{ij}	5411.2 ± 294.6^{a}	1475.0 ± 82.4^{pq}	3111.7 ± 173.8^{ghi}	1890.8 ± 102.9^{no}	3821.2 ± 208.0^{d}
Leucine	5241.3 ± 162.0^{kl}	9162.7 ± 265.7^{c}	8400.3 ± 217.2^{e}	10279.0 ± 257.7^{b}	4051.0 ± 125.2^{n}	6861.3 ± 203.5^{gh}	6067.7 ± 75.6^{ij}	10937.3 ± 649.9^{a}	2845.7 ± 92.9^{op}	5690.3 ± 147.2^{jk}	3262.7 ± 145.1^{o}	6500.7 ± 255.3^{hi}
Lysine	5779.5 ± 160.1^{j}	14194.2 ± 365.8^{c}	12620.5 ± 294.1^{de}	17849.2 ± 698.6^{a}	3297.5 ± 91.4^{lmn}	8399.3 ± 129.0^{gh}	7505.5 ± 214.1^{hi}	15616.8 ± 1002.7^{b}	3568.1 ± 142.4^{lmn}	7701.1 ± 307.4^{hi}	4738.9 ± 185.5^{k}	10662.6 ± 417.3^{f}
Hydroxyproline	2782.6 ± 171.7^{jk}	8074.5 ± 181.4^{b}	4910.5 ± 292.2^{f}	9214.4 ± 344.4^{a}	2115.3 ± 130.5^{lmn}	5762.2 ± 102.5^{e}	3632.9 ± 224.2^{hi}	6612.0 ± 302.5^{cd}	1561.5 ± 92.9^{o}	3224.7 ± 191.9^{ij}	2533.2 ± 125.2^{kl}	5458.3 ± 269.9^{e}
Sarcosine	9697.7 ± 315.0^{hi}	17977.8 ± 375.5^{c}	15471.4 ± 757.2^{d}	20434.4 ± 1044.4^{b}	5626.9 ± 182.8^{lmno}	13738.4 ± 446.2^{e}	8840.9 ± 506.3^{ij}	28872.3 ± 1546.6^{a}	4534.5 ± 259.7^{nop}	9770.6 ± 559.6^{hi}	5972.6 ± 319.9^{lmn}	12333.8 ± 660.7^{ef}

Values are means ± SE (n = 3), rounded to one decimal place. For each parameter (row), means followed by different superscript letters differ significantly among the 28 rootstocks × treatment combinations according to Duncan's multiple range test ($p < 0.05$). SE = SD/√n. The former Table S3 has been split by compound class (Tables S3a–S3c); the replicate-level values are given in Data S1 at the end of this document.

Table S3b. Rootstock × treatment interaction means (± SE) for organic acid concentrations in leaf extracts (ng µL⁻¹)

Parameter	GF 677				Myrobalan 29C				Marianna 2624				Rootpac 20			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Oxalic acid	5.6 ± 0.6^{mno}	3.9 ± 0.1^{pq}	4.3 ± 0.1^{opq}	3.3 ± 0.1^{q}	9.5 ± 0.3^{hi}	7.6 ± 0.3^{jkl}	8.5 ± 0.0^{ijk}	6.7 ± 0.2^{lmn}	12.7 ± 0.5^{cde}	8.7 ± 0.6^{ijk}	11.2 ± 0.3^{efg}	6.4 ± 0.5^{lmn}	14.3 ± 0.8^{bc}	10.9 ± 0.3^{fgh}	12.6 ± 0.2^{cde}	8.8 ± 0.6^{ij}
Propionic acid	7.1 ± 0.2^{q}	9.7 ± 0.7^{opq}	7.9 ± 0.2^{q}	16.1 ± 0.9^{klm}	14.6 ± 0.4^{lmn}	17.3 ± 0.2^{jkl}	15.8 ± 0.1^{klm}	20.8 ± 1.5^{ij}	13.0 ± 0.8^{mno}	22.7 ± 0.7^{i}	20.4 ± 0.6^{ij}	27.9 ± 2.1^{fg}	18.5 ± 1.1^{jk}	26.3 ± 0.7^{gh}	22.9 ± 0.5^{hi}	30.3 ± 1.7^{ef}
Tartaric acid	24.4 ± 2.2^{i}	14.7 ± 0.8^{j}	14.1 ± 1.1^{j}	14.1 ± 1.3^{j}	28.8 ± 2.6^{hi}	31.1 ± 1.7^{gh}	31.3 ± 2.3^{gh}	31.9 ± 2.9^{gh}	44.2 ± 2.4^{e}	44.5 ± 3.3^{e}	45.3 ± 4.1^{e}	25.3 ± 1.4^{i}	33.9 ± 1.8^{fg}	50.7 ± 4.6^{d}	43.9 ± 3.3^{e}	46.4 ± 2.5^{de}
Butyric acid	39.9 ± 3.1^{n}	52.5 ± 0.7^{lmn}	47.3 ± 0.2^{mn}	65.3 ± 4.1^{kl}	72.2 ± 4.1^{jk}	96.5 ± 2.0^{gh}	88.5 ± 2.4^{hi}	107.1 ± 0.8^{fg}	80.9 ± 5.3^{ij}	115.8 ± 4.3^{ef}	96.9 ± 3.4^{gh}	136.0 ± 1.0^{d}	98.8 ± 4.9^{gh}	134.1 ± 5.4^{d}	113.5 ± 0.2^{ef}	152.8 ± 6.1^{bc}
Malonic acid	51.9 ± 2.0^{ijk}	37.1 ± 2.1^{l}	44.5 ± 1.8^{jkl}	35.9 ± 2.3^{l}	101.9 ± 6.7^{de}	74.3 ± 0.1^{gh}	80.0 ± 0.2^{g}	64.0 ± 1.6^{hi}	129.4 ± 8.5^{c}	87.0 ± 3.8^{fg}	101.6 ± 0.2^{de}	62.7 ± 3.6^{hi}	145.4 ± 9.5^{b}	103.3 ± 3.9^{de}	123.3 ± 2.8^{c}	85.8 ± 4.9^{fg}
Malic acid	18.4 ± 0.8^{mno}	14.1 ± 0.7^{op}	16.9 ± 0.9^{nop}	11.1 ± 0.5^{p}	38.7 ± 1.2^{fgh}	25.3 ± 0.7^{jkl}	29.4 ± 1.2^{ij}	22.1 ± 0.7^{klmn}	46.1 ± 1.4^{de}	30.7 ± 0.7^{ij}	34.9 ± 1.4^{ghi}	24.9 ± 1.7^{jklm}	55.4 ± 1.6^{c}	40.1 ± 0.6^{efgh}	43.8 ± 1.5^{ef}	33.4 ± 2.3^{hi}
Lactic acid	54.3 ± 0.9^{p}	70.8 ± 3.1^{op}	62.1 ± 2.0^{op}	96.6 ± 6.4^{mn}	107.4 ± 3.0^{lm}	130.5 ± 1.9^{ijk}	116.4 ± 1.8^{klm}	150.1 ± 7.3^{fghi}	105.5 ± 7.8^{lm}	156.2 ± 5.2^{fgh}	139.1 ± 1.4^{hij}	183.1 ± 8.9^{de}	131.5 ± 9.7^{ijk}	185.6 ± 1.8^{de}	165.6 ± 5.8^{efg}	217.7 ± 9.6^{bc}
Citric acid	88.4 ± 4.6^{opq}	51.1 ± 0.6^{t}	57.1 ± 2.1st	42.8 ± 1.9^{t}	127.1 ± 4.2^{kl}	105.8 ± 2.4^{mno}	112.6 ± 1.2^{lmn}	89.4 ± 3.3^{op}	203.4 ± 6.7^{d}	148.5 ± 9.5^{hij}	179.5 ± 2.2^{ef}	77.3 ± 6.6^{pqr}	189.8 ± 4.2^{de}	138.8 ± 9.3^{jk}	166.6 ± 2.1^{fgh}	103.8 ± 8.9^{no}
Maleic acid	22.4 ± 2.4^{mnop}	13.0 ± 1.1^{pq}	16.8 ± 0.8^{opq}	11.5 ± 0.8^{q}	43.3 ± 5.4^{fgh}	24.2 ± 0.6^{lmno}	28.2 ± 1.5^{klmn}	21.2 ± 0.9^{nopq}	60.7 ± 7.5^{cd}	36.1 ± 0.7^{hijk}	42.3 ± 2.5^{fghi}	30.4 ± 0.7^{jklmn}	67.7 ± 5.4^{bc}	40.6 ± 0.8^{ghij}	48.4 ± 1.9^{efg}	34.6 ± 1.8^{hijkl}
Fumaric acid	22.3 ± 1.6^{ijkl}	15.4 ± 0.9^{kl}	20.0 ± 0.6^{jkl}	13.8 ± 0.9^{l}	43.3 ± 4.0^{cd}	26.9 ± 1.0^{ghij}	31.1 ± 0.3^{fghi}	24.3 ± 0.4^{hijk}	25.5 ± 2.2^{hij}	36.1 ± 0.4^{defg}	30.6 ± 0.6^{fghi}	50.2 ± 4.7^{c}	60.8 ± 6.5^{b}	39.1 ± 0.2^{def}	44.4 ± 1.8^{cd}	31.0 ± 2.2^{fghi}
Succinic acid	61.2 ± 4.3^{n}	85.7 ± 4.2^{lmn}	71.8 ± 3.1^{mn}	113.5 ± 10.7^{jkl}	125.9 ± 8.8^{ijk}	136.1 ± 4.7^{ij}	139.6 ± 9.6^{hij}	177.4 ± 5.2^{efg}	184.4 ± 17.2^{efg}	141.0 ± 9.8^{hij}	152.4 ± 5.3^{ghi}	116.7 ± 4.0^{jkl}	145.4 ± 5.0^{hij}	191.6 ± 1.8^{def}	171.0 ± 9.5^{fgh}	248.1 ± 23.2^{bc}

Table S3b (continued).

Parameter	Rootpac 40				Rootpac R				Garnem			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Oxalic acid	16.1 ± 0.5^{a}	13.3 ± 0.3^{bc}	14.5 ± 0.3^{b}	11.6 ± 0.4^{def}	16.1 ± 0.6^{a}	9.9 ± 0.5^{ghi}	12.9 ± 0.5^{bcd}	8.8 ± 0.2^{ij}	10.2 ± 0.7^{fghi}	5.1 ± 0.4^{nop}	7.1 ± 1.7^{klm}	4.6 ± 0.2^{opq}
Propionic acid	31.9 ± 0.5^{c}	39.3 ± 0.8^{c}	35.3 ± 0.7^{d}	48.9 ± 2.8^{b}	16.7 ± 0.5^{kl}	46.9 ± 1.3^{b}	22.2 ± 2.0^{i}	55.1 ± 1.7^{a}	9.4 ± 0.3^{pq}	18.2 ± 0.5^{jkl}	12.0 ± 0.8^{nop}	23.7 ± 1.9^{hi}
Tartaric acid	55.3 ± 4.1^{c}	57.6 ± 5.3^{bc}	58.6 ± 3.1^{bc}	61.4 ± 4.6^{b}	72.7 ± 6.6^{a}	73.9 ± 4.0^{a}	35.9 ± 1.9^{fg}	36.1 ± 2.7^{fg}	17.4 ± 1.3^{j}	17.4 ± 1.6^{j}	37.1 ± 3.4^{f}	35.6 ± 2.7^{fg}
Butyric acid	116.9 ± 5.2^{ef}	150.7 ± 3.5^{c}	136.3 ± 3.2^{d}	167.8 ± 4.6^{a}	93.3 ± 4.1^{hi}	131.0 ± 7.6^{d}	115.4 ± 0.6^{ef}	164.0 ± 6.2^{ab}	46.6 ± 3.6^{mn}	98.8 ± 8.4^{gh}	59.6 ± 2.3^{klm}	125.1 ± 5.2^{de}
Malonic acid	168.5 ± 9.6^{a}	121.4 ± 0.3^{c}	145.1 ± 4.2^{b}	104.5 ± 4.8^{de}	125.9 ± 0.3^{c}	103.2 ± 0.3^{de}	116.1 ± 6.1^{cd}	79.7 ± 4.6^{g}	124.6 ± 8.2^{c}	57.7 ± 3.8^{ij}	94.1 ± 6.0^{ef}	41.8 ± 2.7^{kl}
Malic acid	72.7 ± 2.5^{a}	51.9 ± 2.5^{cd}	62.8 ± 3.7^{b}	43.6 ± 2.0^{ef}	70.5 ± 7.1^{a}	37.4 ± 1.1^{fgh}	53.0 ± 2.4^{c}	28.2 ± 1.3^{ijk}	40.9 ± 3.8^{efg}	20.0 ± 1.9^{lmno}	29.1 ± 1.3^{ij}	13.6 ± 0.6^{op}
Lactic acid	192.9 ± 3.7^{d}	235.9 ± 4.3^{b}	214.7 ± 6.7^{c}	283.3 ± 17.5^{a}	119.1 ± 6.0^{gkl}	233.3 ± 5.0^{bc}	146.0 ± 9.1^{ghi}	281.8 ± 8.0^{a}	72.1 ± 4.8^{op}	132.7 ± 2.2^{ijk}	81.4 ± 5.9^{no}	167.6 ± 11.4^{ef}
Citric acid	251.6 ± 8.9^{b}	206.7 ± 3.9^{cd}	222.2 ± 2.6^{c}	174.4 ± 9.0^{efg}	276.5 ± 7.1^{a}	159.4 ± 9.2^{ghi}	223.1 ± 11.5^{c}	123.7 ± 10.6^{klm}	145.6 ± 4.5^{ij}	70.3 ± 2.5^{qrs}	126.6 ± 3.9^{kl}	60.3 ± 2.0^{rst}
Maleic acid	75.2 ± 9.4^{ab}	44.4 ± 0.9^{fgh}	52.5 ± 2.4^{def}	38.5 ± 1.5^{ghijk}	81.8 ± 5.6^{a}	44.8 ± 2.7^{fgh}	56.1 ± 4.0^{de}	32.3 ± 3.0^{ijklm}	34.8 ± 1.8^{hijkl}	15.9 ± 0.9^{opq}	28.4 ± 1.4^{klmn}	12.8 ± 0.6^{pq}
Fumaric acid	41.5 ± 1.0^{cde}	62.1 ± 4.4^{b}	50.8 ± 1.4^{c}	84.5 ± 4.4^{a}	28.9 ± 2.0^{ghij}	50.1 ± 0.3^{c}	41.8 ± 2.8^{cde}	61.9 ± 3.5^{b}	16.0 ± 1.0^{kl}	33.1 ± 2.2^{efgh}	23.6 ± 3.1^{hijk}	50.7 ± 6.8^{c}
Succinic acid	180.8 ± 5.3^{efg}	216.6 ± 4.1^{d}	207.7 ± 0.4^{de}	261.0 ± 16.4^{ab}	279.0 ± 26.1^{a}	130.7 ± 4.5^{ij}	222.3 ± 7.7^{cd}	120.8 ± 8.4^{ijk}	71.4 ± 5.0^{mn}	153.8 ± 10.7^{ghi}	95.4 ± 8.9^{klm}	197.0 ± 18.4^{def}

Values are means ± SE (n = 3), rounded to one decimal place. For each parameter (row), means followed by different superscript letters differ significantly among the 28 rootstocks × treatment combinations according to Duncan's multiple range test ($p < 0.05$). SE = SD/√n. The former Table S3 has been split by compound class (Tables S3a–S3c); the replicate-level values are given in Data S1 at the end of this document.

Table S3c. Rootstock × treatment interaction means (± SE) for phenolic compound concentrations in leaf extracts (µg L⁻¹)

Parameter	GF 677				Myrobalan 29C				Marianna 2624				Rootpac 20			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Gallic acid	1.5 ± 0.1^{kl}	3.5 ± 0.4^{fgh}	2.0 ± 0.1^{jkl}	5.5 ± 0.3^{e}	3.6 ± 0.2^{fg}	4.1 ± 0.3^{f}	3.8 ± 0.1^{fg}	5.0 ± 0.3^{e}	2.1 ± 0.1^{jk}	3.0 ± 0.1^{ghi}	2.4 ± 0.1^{ij}	3.4 ± 0.1^{fgh}	0.2 ± 0.0^{n}	2.4 ± 0.1^{ij}	0.7 ± 0.1^{mn}	3.4 ± 0.2^{fgh}
Vanillic acid	2.2 ± 0.1^{n}	5.3 ± 0.8^{hij}	2.8 ± 0.2^{mn}	8.0 ± 0.6^{e}	5.0 ± 0.1^{hijk}	6.8 ± 0.1^{f}	6.4 ± 0.0^{fg}	8.0 ± 0.6^{e}	3.3 ± 0.1^{m}	4.4 ± 0.1^{jkl}	3.6 ± 0.1^{lm}	4.9 ± 0.1^{ijk}	0.2 ± 0.0^{o}	3.3 ± 0.2^{m}	1.0 ± 0.1^{o}	4.9 ± 0.5^{ijk}
trans-Caffeic acid	2.1 ± 0.2^{kl}	5.3 ± 0.8^{ef}	2.8 ± 0.4^{ij}	8.4 ± 0.5^{c}	3.3 ± 0.0^{i}	5.0 ± 0.2^{fg}	4.4 ± 0.1^{gh}	5.6 ± 0.2^{e}	2.1 ± 0.0^{kl}	2.7 ± 0.0^{ijk}	2.3 ± 0.0^{jk}	3.0 ± 0.1^{i}	0.3 ± 0.0^{n}	3.1 ± 0.1^{i}	1.0 ± 0.1^{m}	4.3 ± 0.3^{h}
trans-p-Coumaric acid	2.0 ± 0.1^{o}	4.4 ± 0.8^{kl}	2.4 ± 0.1^{no}	7.0 ± 0.5^{fg}	5.7 ± 0.1^{ij}	6.7 ± 0.1^{fgh}	6.3 ± 0.1^{ghi}	7.6 ± 0.5^{ef}	3.7 ± 0.1^{lm}	4.5 ± 0.1^{kl}	4.1 ± 0.1^{l}	5.2 ± 0.2^{jk}	4.5 ± 0.7^{kl}	0.9 ± 0.1^{p}	3.1 ± 0.1^{mn}	0.3 ± 0.0^{p}
Ferulic acid	1.1 ± 0.0^{m}	2.8 ± 0.2^{de}	1.9 ± 0.1^{j}	3.4 ± 0.1^{a}	2.1 ± 0.1^{i}	2.8 ± 0.0^{de}	2.6 ± 0.1^{ef}	3.1 ± 0.2^{bc}	2.2 ± 0.1^{hi}	2.9 ± 0.0^{cd}	2.4 ± 0.0^{gh}	3.0 ± 0.1^{bc}	0.1 ± 0.0^{o}	1.6 ± 0.0^{k}	0.5 ± 0.0^{n}	2.2 ± 0.2^{hi}
Caftaric acid	2.7 ± 0.2^{l}	3.7 ± 0.4^{kl}	6.6 ± 0.9^{ghi}	9.8 ± 0.8^{de}	5.7 ± 0.2^{hij}	7.9 ± 0.2^{fg}	8.6 ± 0.1^{ef}	10.6 ± 1.2^{d}	3.7 ± 0.1^{kl}	4.1 ± 0.1^{jkl}	5.4 ± 0.2^{ij}	6.1 ± 0.2^{hi}	6.1 ± 0.5^{hi}	4.1 ± 0.3^{jkl}	1.2 ± 0.2^{mn}	0.3 ± 0.0^{n}
Catechin	2.6 ± 0.1^{mn}	5.9 ± 0.7^{hijk}	3.2 ± 0.1^{lm}	9.0 ± 0.5^{c}	6.6 ± 0.1^{fghi}	8.3 ± 0.2^{ef}	7.4 ± 0.1^{efgh}	10.8 ± 1.2^{d}	4.3 ± 0.1^{kl}	6.4 ± 0.2^{ghij}	4.8 ± 0.1^{jkl}	7.8 ± 0.3^{efg}	6.5 ± 0.6^{ghi}	1.5 ± 0.2^{no}	4.3 ± 0.5^{kl}	0.7 ± 0.0^{o}
Epicatechin	1.8 ± 0.4^{mn}	2.8 ± 0.5^{ijklm}	3.0 ± 1.1^{ijkl}	6.3 ± 0.5^{e}	3.8 ± 0.1^{ghi}	5.4 ± 0.2^{ef}	4.8 ± 0.2^{fg}	6.2 ± 0.2^{e}	2.3 ± 0.0^{klm}	2.9 ± 0.1^{ijklm}	2.6 ± 0.1^{ijklm}	3.2 ± 0.1^{hijk}	3.8 ± 0.3^{ghij}	0.8 ± 0.1^{no}	2.5 ± 0.1^{jklm}	0.3 ± 0.0^{o}
Quercetin	0.7 ± 0.0^{kl}	8.0 ± 0.2^{b}	3.4 ± 1.2^{fg}	10.4 ± 0.2^{a}	3.5 ± 0.1^{efg}	4.0 ± 0.1^{cdefg}	3.7 ± 0.0^{cdefg}	4.5 ± 0.1^{cde}	3.6 ± 0.0^{defg}	4.6 ± 0.0^{cd}	3.9 ± 0.1^{cdefg}	4.8 ± 0.0^{c}	0.1 ± 0.0^{l}	1.0 ± 0.0^{kl}	0.3 ± 0.0^{l}	2.2 ± 0.9^{hij}
Rutin	0.3 ± 0.0^{o}	8.4 ± 0.8^{bc}	0.5 ± 0.1^{o}	10.3 ± 0.1^{a}	2.8 ± 0.1^{ijk}	3.9 ± 0.1^{h}	3.5 ± 0.1^{hi}	4.6 ± 0.4^{g}	1.8 ± 0.1^{lm}	2.5 ± 0.1^{jk}	2.1 ± 0.1^{kl}	2.8 ± 0.1^{ijk}	0.1 ± 0.0^{o}	2.7 ± 0.1^{jk}	0.8 ± 0.1^{no}	3.7 ± 0.1^{h}
Myricetin	4.2 ± 0.6^{d}	2.3 ± 0.2^{fghij}	6.2 ± 0.1^{c}	1.8 ± 0.1^{ijklm}	3.2 ± 0.1^{ef}	2.9 ± 0.1^{fgh}	4.0 ± 0.4^{de}	2.0 ± 0.0^{hijkl}	1.3 ± 0.0^{klm}	2.2 ± 0.1^{ghijk}	1.4 ± 0.0^{jklm}	2.6 ± 0.1^{fghi}	2.2 ± 0.2^{fghijk}	0.3 ± 0.0^{n}	1.2 ± 0.1^{lmn}	0.3 ± 0.0^{n}

Table S3c (continued).

Parameter	Rootpac 40				Rootpac R				Garnem			
	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock	Control	Drought	Heat shock	Drought + Heat shock
Gallic acid	6.9 ± 0.2^{d}	9.6 ± 0.5^{b}	7.8 ± 0.2^{c}	11.1 ± 0.3^{a}	3.7 ± 0.5^{fg}	7.2 ± 0.6^{cd}	5.4 ± 0.4^{e}	9.1 ± 0.2^{b}	0.4 ± 0.0^{n}	2.7 ± 0.4^{hij}	1.3 ± 0.4^{lm}	3.9 ± 0.2^{fg}
Vanillic acid	10.4 ± 0.2^{d}	13.6 ± 0.6^{b}	11.6 ± 0.2^{c}	15.6 ± 0.3^{a}	5.9 ± 0.7^{gh}	10.7 ± 0.9^{d}	8.1 ± 0.7^{e}	13.1 ± 0.4^{b}	0.6 ± 0.0^{o}	4.2 ± 0.5^{kl}	2.0 ± 0.6^{n}	5.7 ± 0.3^{ghi}
trans-Caffeic acid	7.2 ± 0.4^{d}	9.6 ± 0.3^{b}	8.4 ± 0.2^{c}	11.1 ± 0.4^{a}	3.9 ± 0.3^{h}	7.3 ± 0.3^{d}	5.8 ± 0.5^{e}	9.1 ± 0.2^{b}	0.4 ± 0.0^{mn}	3.0 ± 0.5^{ij}	1.6 ± 0.3^{l}	4.0 ± 0.2^{h}
trans-p-Coumaric acid	10.8 ± 0.4^{d}	13.2 ± 0.2^{b}	12.1 ± 0.3^{c}	15.1 ± 0.2^{a}	6.0 ± 0.5^{hij}	10.8 ± 0.5^{d}	8.1 ± 0.8^{e}	12.9 ± 0.5^{bc}	0.6 ± 0.0^{p}	4.4 ± 0.6^{kl}	2.1 ± 0.7^{o}	5.5 ± 0.2^{ij}
Ferulic acid	2.0 ± 0.1^{ij}	2.7 ± 0.0^{def}	2.2 ± 0.0^{hi}	2.9 ± 0.0^{cd}	2.2 ± 0.1^{hi}	2.9 ± 0.1^{cd}	2.5 ± 0.1^{fg}	3.2 ± 0.1^{ab}	0.2 ± 0.0^{o}	1.3 ± 0.0^{l}	1.0 ± 0.3^{m}	1.6 ± 0.1^{k}
Caftaric acid	12.9 ± 0.3^{c}	13.9 ± 0.4^{c}	17.2 ± 1.2^{b}	20.3 ± 0.4^{a}	7.3 ± 1.2^{fgh}	10.1 ± 0.5^{d}	13.3 ± 1.3^{c}	17.2 ± 0.5^{b}	0.8 ± 0.0^{n}	2.5 ± 0.7^{lm}	5.0 ± 0.6^{ijk}	7.2 ± 0.4^{fgh}
Catechin	13.2 ± 0.3^{c}	17.9 ± 1.4^{b}	14.7 ± 0.3^{c}	22.0 ± 0.9^{a}	7.4 ± 1.1^{efgh}	13.6 ± 1.4^{c}	11.1 ± 0.2^{d}	19.4 ± 0.9^{b}	0.8 ± 0.0^{o}	5.2 ± 0.8^{ijk}	3.2 ± 0.2^{lm}	7.3 ± 0.8^{efgh}
Epicatechin	8.5 ± 0.7^{d}	11.3 ± 0.3^{b}	10.2 ± 0.3^{c}	12.6 ± 0.4^{a}	4.3 ± 0.3^{fgh}	8.7 ± 0.3^{d}	6.3 ± 0.9^{e}	10.3 ± 0.2^{bc}	0.5 ± 0.0^{o}	3.4 ± 0.6^{hijk}	1.9 ± 0.1^{lm}	4.4 ± 0.1^{fgh}
Quercetin	3.1 ± 0.0^{gh}	4.0 ± 0.0^{cdefg}	3.4 ± 0.1^{fg}	4.2 ± 0.1^{cdef}	3.3 ± 0.1^{fg}	4.2 ± 0.0^{cdef}	3.8 ± 0.1^{cdefg}	4.6 ± 0.0^{cd}	0.2 ± 0.0^{l}	2.0 ± 0.0^{ij}	1.3 ± 0.5^{jk}	2.4 ± 0.1^{hi}
Rutin	5.7 ± 0.1^{f}	7.9 ± 0.3^{cd}	6.4 ± 0.1^{e}	8.9 ± 0.3^{b}	3.2 ± 0.5^{hij}	6.0 ± 0.5^{ef}	4.6 ± 0.2^{g}	7.5 ± 0.2^{d}	0.3 ± 0.0^{o}	2.3 ± 0.4^{kl}	1.3 ± 0.3^{mn}	3.2 ± 0.2^{hij}
Myricetin	4.5 ± 0.1^{d}	6.7 ± 0.8^{bc}	4.9 ± 0.1^{d}	9.1 ± 0.4^{a}	2.6 ± 0.4^{fghi}	4.9 ± 0.5^{d}	4.0 ± 0.1^{de}	7.2 ± 0.4^{b}	1.8 ± 0.3^{ijklm}	0.9 ± 0.3^{mn}	3.0 ± 0.5^{fg}	0.3 ± 0.0^{n}

Values are means ± SE (n = 3), rounded to one decimal place. For each parameter (row), means followed by different superscript letters differ significantly among the 28 rootstocks × treatment combinations according to Duncan's multiple range test ($p < 0.05$). SE = SD/√n. The former Table S3 has been split by compound class (Tables S3a–S3c); the replicate-level values are given in Data S1 at the end of this document.

Table S4. Partition of the treatment and rootstock × treatment effects into the components of the 2 × 2 factorial of drought (D) and heat shock (H): F-values, p-values and Benjamini–Hochberg-adjusted p-values (p adj., across the 43 compounds) for each compound. R, rootstock. Error df = 54.

Compound	D (df = 1)		H (df = 1)		D × H (df = 1)			R × D (df = 6)		R × H (df = 6)		R × D × H (df = 6)		
	F	p	F	p	F	p	p adj.	F	p	F	p	F	p	p adj.
Amino acids														
Aspartate	4141.59	<0.001	1156.69	<0.001	181.98	<0.001	<0.001	174.57	<0.001	22.59	<0.001	26.59	<0.001	<0.001
Glutamate	1379.67	<0.001	224.53	<0.001	12.97	<0.001	0.002	102.64	<0.001	4.31	0.001	11.45	<0.001	<0.001
Asparagine	3070.02	<0.001	722.96	<0.001	0.00	0.975	0.975	285.67	<0.001	51.26	<0.001	10.16	<0.001	<0.001
Serine	1330.87	<0.001	348.32	<0.001	77.45	<0.001	<0.001	72.71	<0.001	10.80	<0.001	15.59	<0.001	<0.001
Glutamine	11.81	0.001	0.14	0.707	3.83	0.055	0.077	45.34	<0.001	32.35	<0.001	17.26	<0.001	<0.001
Histidine	877.61	<0.001	363.76	<0.001	16.47	<0.001	<0.001	262.91	<0.001	57.01	<0.001	9.84	<0.001	<0.001
Glycine	4805.67	<0.001	1354.16	<0.001	295.20	<0.001	<0.001	278.27	<0.001	71.55	<0.001	83.89	<0.001	<0.001
Threonine	419.75	<0.001	95.56	<0.001	12.10	0.001	0.003	52.24	<0.001	2.81	0.019	1.89	0.099	0.158
Arginine	1111.94	<0.001	260.57	<0.001	21.40	<0.001	<0.001	53.72	<0.001	7.49	<0.001	8.23	<0.001	<0.001
Alanine	566.95	<0.001	157.78	<0.001	32.27	<0.001	<0.001	20.73	<0.001	4.05	0.002	2.13	0.065	0.111
Tyrosine	3487.13	<0.001	940.47	<0.001	66.53	<0.001	<0.001	99.50	<0.001	26.67	<0.001	16.94	<0.001	<0.001
Cystine	3069.08	<0.001	1283.08	<0.001	288.25	<0.001	<0.001	39.87	<0.001	55.93	<0.001	50.21	<0.001	<0.001
Valine	953.99	<0.001	275.22	<0.001	6.28	0.015	0.023	14.91	<0.001	13.96	<0.001	10.49	<0.001	<0.001
Methionine	665.16	<0.001	153.79	<0.001	2.98	0.090	0.114	34.85	<0.001	4.74	<0.001	3.64	0.004	0.008
Tryptophan	2128.77	<0.001	756.17	<0.001	106.19	<0.001	<0.001	30.80	<0.001	29.21	<0.001	23.22	<0.001	<0.001
Phenylalanine	1345.40	<0.001	415.96	<0.001	102.08	<0.001	<0.001	73.33	<0.001	7.93	<0.001	5.03	<0.001	<0.001
Isoleucine	1013.28	<0.001	263.81	<0.001	10.41	0.002	0.005	15.65	<0.001	6.36	<0.001	3.22	0.009	0.017
Leucine	2174.58	<0.001	556.69	<0.001	0.76	0.387	0.427	49.16	<0.001	22.16	<0.001	16.14	<0.001	<0.001
Lysine	2784.58	<0.001	873.12	<0.001	14.58	<0.001	<0.001	34.87	<0.001	28.07	<0.001	21.05	<0.001	<0.001
Hydroxyproline	1864.44	<0.001	392.45	<0.001	14.89	<0.001	<0.001	52.24	<0.001	9.27	<0.001	11.30	<0.001	<0.001
Sarcosine	1381.17	<0.001	397.71	<0.001	33.69	<0.001	<0.001	54.15	<0.001	27.84	<0.001	25.55	<0.001	<0.001
Organic acids														
Oxalic acid	278.64	<0.001	66.01	<0.001	2.21	0.143	0.176	6.82	<0.001	0.89	0.508	1.54	0.184	0.247
Propionic acid	649.91	<0.001	122.31	<0.001	7.69	0.008	0.014	65.70	<0.001	2.21	0.056	1.69	0.141	0.196
Tartaric acid	0.07	0.794	35.34	<0.001	11.63	0.001	0.003	15.09	<0.001	120.22	<0.001	10.03	<0.001	<0.001
Butyric acid	473.70	<0.001	120.05	<0.001	1.75	0.191	0.222	11.22	<0.001	1.63	0.157	0.62	0.715	0.755
Malonic acid	417.09	<0.001	109.17	<0.001	1.87	0.177	0.211	11.85	<0.001	2.33	0.045	0.97	0.453	0.573
Malic acid	354.17	<0.001	101.65	<0.001	7.07	0.010	0.018	12.66	<0.001	2.43	0.037	0.57	0.749	0.767
Lactic acid	539.83	<0.001	115.13	<0.001	6.97	0.011	0.019	25.63	<0.001	1.92	0.094	0.98	0.451	0.573
Citric acid	638.59	<0.001	155.83	<0.001	0.20	0.660	0.692	24.80	<0.001	4.76	<0.001	3.66	0.004	0.008
Maleic acid	224.40	<0.001	76.36	<0.001	19.27	<0.001	<0.001	4.97	<0.001	2.80	0.019	0.61	0.720	0.755
Fumaric acid	41.53	<0.001	14.11	<0.001	10.39	0.002	0.005	40.06	<0.001	14.80	<0.001	0.81	0.568	0.668
Succinic acid	11.65	0.001	12.92	<0.001	9.81	0.003	0.006	52.51	<0.001	9.54	<0.001	0.39	0.880	0.880
Phenolic compounds														
Gallic acid	540.87	<0.001	97.04	<0.001	8.16	0.006	0.012	15.29	<0.001	3.35	0.007	0.78	0.588	0.668
Vanillic acid	890.45	<0.001	171.45	<0.001	6.32	0.015	0.023	20.85	<0.001	3.93	0.002	2.00	0.082	0.136
trans-Caffeic acid	1054.68	<0.001	218.32	<0.001	5.48	0.023	0.034	34.47	<0.001	7.05	<0.001	5.40	<0.001	<0.001
trans-p-Coumaric acid	271.87	<0.001	68.15	<0.001	4.76	0.033	0.048	73.42	<0.001	10.85	<0.001	1.86	0.105	0.161
Ferulic acid	1138.61	<0.001	192.34	<0.001	3.55	0.065	0.085	32.33	<0.001	6.08	<0.001	2.44	0.037	0.066
Caftaric acid	61.63	<0.001	251.32	<0.001	6.82	0.012	0.019	9.04	<0.001	50.00	<0.001	0.78	0.590	0.668
Catechin	269.95	<0.001	84.53	<0.001	15.50	<0.001	<0.001	51.03	<0.001	12.89	<0.001	0.88	0.518	0.637
Epicatechin	124.65	<0.001	52.81	<0.001	0.68	0.412	0.443	32.68	<0.001	7.82	<0.001	1.72	0.134	0.192
Quercetin	249.22	<0.001	40.12	<0.001	0.01	0.928	0.950	55.18	<0.001	6.79	<0.001	0.73	0.630	0.695
Rutin	1126.84	<0.001	99.05	<0.001	3.74	0.058	0.079	142.72	<0.001	2.14	0.064	1.76	0.126	0.186
Myricetin	0.31	0.582	24.51	<0.001	1.63	0.207	0.235	65.19	<0.001	7.74	<0.001	8.36	<0.001	<0.001

D × H tests departure from additivity averaged over rootstocks; R × D × H tests whether that departure differs among rootstocks. D, H and D × H partition the treatment sum of squares (3 df) and R × D, R × H and R × D × H the rootstock × treatment sum of squares (18 df) of Table 1.

Table S5. Additivity contrast I = (D+H) − D − H + C for the 301 compound × rootstock combinations. C, D, H and D+H are the cell means (n = 3) of the control, drought, heat-shock and drought + heat-shock treatments in the units of the compound (amino acids, pmol µL⁻¹; organic acids, ng µL⁻¹; phenolic compounds, µg L⁻¹). SE = √(4 × MSE/3); t-test with 54 df; p adj., Benjamini–Hochberg-adjusted p across the 301 contrasts. Direction: S, synergistic (I > 0); A, antagonistic (I < 0), given where p adj. < 0.05. The last two columns give the contrast on ln-transformed data (multiplicative null hypothesis) and its adjusted p.

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
Aspartate	GF 677	10257.6	3630.2	4349.6	3309.4	5587.1	399.0	4787.1	6387.1	+0.54	14.00	<0.001	<0.001	S	+0.765	<0.001
	Myrobalan 29C	11584.0	8106.8	8854.8	6627.1	1249.5	399.0	449.5	2049.5	+0.11	3.13	0.003	0.011	S	+0.066	0.099
	Marianna 2624	12099.1	8898.3	9890.3	5814.5	-875.0	399.0	-1674.9	-74.96	-0.07	-2.19	0.033	0.084	–	-0.224	<0.001
	Rootpac 20	16037.4	11464.1	11066.7	7877.1	1383.7	399.0	583.7	2183.7	+0.09	3.47	0.001	0.005	S	-0.004	0.964
	Rootpac 40	24035.7	19243.3	21552.5	18576.2	1816.1	399.0	1016.1	2616.1	+0.08	4.55	<0.001	<0.001	S	+0.074	0.061
	Rootpac R	20345.6	7884.4	15848.2	7093.7	3706.6	399.0	2906.6	4506.6	+0.18	9.29	<0.001	<0.001	S	+0.144	<0.001
	Garnem	11415.1	5456.2	9139.1	4553.7	1373.6	399.0	573.6	2173.6	+0.12	3.44	0.001	0.005	S	+0.042	0.390
Glutamate	GF 677	2682.0	3795.0	3073.8	6993.8	2807.1	510.9	1782.8	3831.4	+1.05	5.49	<0.001	<0.001	S	+0.479	<0.001
	Myrobalan 29C	4500.2	7574.8	5866.4	7193.5	-1747.5	510.9	-2771.8	-723.2	-0.39	-3.42	0.001	0.006	A	-0.318	<0.001
	Marianna 2624	1766.4	2846.0	2368.7	4779.5	1331.2	510.9	306.8	2355.5	+0.75	2.61	0.012	0.036	S	+0.221	0.001
	Rootpac 20	7738.2	10081.3	9123.4	11907.1	440.6	510.9	-583.7	1464.9	+0.06	0.86	0.392	0.579	–	-0.001	0.995
	Rootpac 40	11261.7	15095.1	13247.5	15598.3	-1482.6	510.9	-2506.9	-458.2	-0.13	-2.90	0.005	0.019	A	-0.130	0.066
	Rootpac R	11528.3	19863.2	12771.6	22998.7	1892.2	510.9	867.9	2916.6	+0.16	3.70	<0.001	0.003	S	+0.045	0.664
	Garnem	3707.6	6599.7	4426.5	8945.7	1627.2	510.9	602.9	2651.5	+0.44	3.18	0.002	0.010	S	+0.127	0.073
Asparagine	GF 677	6383.4	11406.0	8461.9	20746.2	7261.6	1902.5	3447.4	11075.9	+1.14	3.82	<0.001	0.002	S	+0.318	<0.001
	Myrobalan 29C	12468.3	22284.9	19908.9	24959.0	-4766.4	1902.5	-8580.7	-952.2	-0.38	-2.51	0.015	0.045	A	-0.355	<0.001
	Marianna 2624	29939.6	83126.3	53862.9	107823.1	773.5	1902.5	-3040.8	4587.7	+0.03	0.41	0.686	0.827	–	-0.327	<0.001
	Rootpac 20	12250.6	27140.0	17211.2	39331.1	7230.6	1902.5	3416.3	11044.8	+0.59	3.80	<0.001	0.002	S	+0.030	0.575
	Rootpac 40	22282.4	39352.9	33871.1	44617.3	-6324.3	1902.5	-10138.6	-2510.1	-0.28	-3.32	0.002	0.007	A	-0.293	<0.001
	Rootpac R	28847.7	57763.5	42939.2	65138.5	-6716.4	1902.5	-10530.7	-2902.1	-0.23	-3.53	<0.001	0.004	A	-0.278	<0.001
	Garnem	10798.6	21267.1	14307.7	27473.7	2697.5	1902.5	-1116.7	6511.8	+0.25	1.42	0.162	0.315	–	-0.025	0.664
Serine	GF 677	7642.5	12212.5	9529.1	18090.8	3991.7	1776.0	431.1	7552.3	+0.52	2.25	0.029	0.075	–	+0.176	0.014
	Myrobalan 29C	15067.2	23760.1	19610.5	25661.0	-2642.5	1776.0	-6203.1	918.1	-0.18	-1.49	0.143	0.286	–	-0.183	0.010
	Marianna 2624	4068.1	6928.5	5294.8	12917.7	4762.5	1776.0	1201.9	8323.1	+1.17	2.68	0.010	0.031	S	+0.364	<0.001
	Rootpac 20	17657.3	27981.4	22243.1	40374.5	7807.2	1776.0	4246.7	11367.8	+0.44	4.40	<0.001	<0.001	S	+0.138	0.062
	Rootpac 40	26156.2	35536.4	32904.1	43960.5	1676.3	1776.0	-1884.3	5236.8	+0.06	0.94	0.349	0.531	–	-0.011	0.958
	Rootpac R	13487.8	30757.7	14539.5	51694.3	19884.9	1776.0	16324.3	23445.5	+1.47	11.20	<0.001	<0.001	S	+0.443	<0.001
	Garnem	11114.7	23049.6	14244.7	32050.6	5871.0	1776.0	2310.4	9431.6	+0.53	3.31	0.002	0.007	S	+0.078	0.390
Glutamine	GF 677	12232.5	5546.5	7385.5	4924.8	4225.2	1462.8	1292.4	7158.0	+0.35	2.89	0.006	0.020	S	+0.385	<0.001
	Myrobalan 29C	14799.9	10979.9	13703.6	10584.0	700.4	1462.8	-2232.4	3633.2	+0.05	0.48	0.634	0.794	–	+0.040	0.832
	Marianna 2624	2964.6	2857.7	3996.0	9413.5	5524.4	1462.8	2591.6	8457.2	+1.86	3.78	<0.001	0.002	S	+0.895	<0.001
	Rootpac 20	13347.7	21930.8	14837.1	16814.2	-6606.0	1462.8	-9538.8	-3673.2	-0.49	-4.52	<0.001	<0.001	A	-0.370	<0.001
	Rootpac 40	19508.0	26699.0	22107.6	21068.7	-8229.9	1462.8	-11162.7	-5297.1	-0.42	-5.63	<0.001	<0.001	A	-0.361	<0.001
	Rootpac R	35104.3	24495.0	29067.4	22541.6	4083.5	1462.8	1150.7	7016.3	+0.12	2.79	0.007	0.024	S	+0.106	0.407
	Garnem	6029.6	8614.4	17409.4	12720.4	-7273.8	1462.8	-10206.6	-4341.0	-1.21	-4.97	<0.001	<0.001	A	-0.668	<0.001
Histidine	GF 677	2818.9	1757.2	2064.9	2006.9	1003.8	244.8	513.1	1494.6	+0.36	4.10	<0.001	<0.001	S	+0.446	<0.001
	Myrobalan 29C	3625.7	4263.8	4046.7	4679.5	-5.27	244.8	-496.0	485.5	-0.00	-0.02	0.983	0.993	–	-0.017	0.901

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	988.0	1263.5	1151.2	2970.0	1543.4	244.8	1052.6	2034.1	+1.56	6.31	<0.001	<0.001	S	+0.699	<0.001
	Rootpac 20	4059.8	6404.9	5552.3	7203.3	-694.1	244.8	-1184.9	-203.3	-0.17	-2.84	0.006	0.022	A	-0.195	0.002
	Rootpac 40	5702.3	6801.0	6337.0	7406.5	-29.16	244.8	-519.9	461.6	-0.01	-0.12	0.906	0.940	–	-0.022	0.855
	Rootpac R	801.9	5856.4	983.7	6845.0	806.8	244.8	316.0	1297.5	+1.01	3.30	0.002	0.007	S	-0.048	0.624
	Garnem	2544.1	2472.7	5267.0	5198.4	2.78	244.8	-488.0	493.5	+0.00	0.01	0.991	0.994	–	+0.014	0.932
Glycine	GF 677	1679.8	3693.9	2493.9	5256.5	748.5	322.9	101.1	1396.0	+0.45	2.32	0.024	0.065	–	-0.042	0.058
	Myrobalan 29C	2918.7	6333.7	4523.0	6840.4	-1097.7	322.9	-1745.1	-450.3	-0.38	-3.40	0.001	0.006	A	-0.361	<0.001
	Marianna 2624	788.0	1846.9	1221.2	2502.3	222.2	322.9	-425.2	869.6	+0.28	0.69	0.494	0.689	–	-0.134	<0.001
	Rootpac 20	3881.1	7323.0	4889.1	12212.1	3881.1	322.9	3233.7	4528.5	+1.00	12.02	<0.001	<0.001	S	+0.281	<0.001
	Rootpac 40	5522.8	8934.1	8272.3	12773.3	1089.7	322.9	442.3	1737.2	+0.20	3.37	0.001	0.006	S	-0.046	0.033
	Rootpac R	675.6	6238.8	1047.0	14429.1	7819.0	322.9	7171.5	8466.4	+11.57	24.21	<0.001	<0.001	S	+0.400	<0.001
	Garnem	2908.8	6278.3	4308.6	9694.4	2016.3	322.9	1368.9	2663.7	+0.69	6.24	<0.001	<0.001	S	+0.042	0.062
Threonine	GF 677	4056.4	6211.3	5003.2	11591.8	4433.8	1824.9	775.2	8092.4	+1.09	2.43	0.018	0.052	–	+0.419	0.002
	Myrobalan 29C	8348.0	11164.3	9506.0	13331.3	1009.1	1824.9	-2649.5	4667.7	+0.12	0.55	0.583	0.756	–	+0.045	0.859
	Marianna 2624	7157.1	12855.0	12505.9	17894.5	-309.4	1824.9	-3968.0	3349.3	-0.04	-0.17	0.866	0.918	–	-0.224	0.132
	Rootpac 20	10212.1	12864.3	12697.9	16773.1	1423.0	1824.9	-2235.6	5081.6	+0.14	0.78	0.439	0.626	–	+0.048	0.849
	Rootpac 40	18604.3	22242.6	20257.2	24986.2	1090.7	1824.9	-2567.9	4749.3	+0.06	0.60	0.553	0.729	–	+0.031	0.932
	Rootpac R	10019.9	28234.5	12218.3	37482.7	7049.8	1824.9	3391.2	10708.4	+0.70	3.86	<0.001	0.002	S	+0.083	0.711
	Garnem	5835.7	11721.8	7244.9	15231.2	2100.2	1824.9	-1558.4	5758.8	+0.36	1.15	0.255	0.419	–	+0.045	0.859
Arginine	GF 677	6909.3	9111.2	8055.8	16540.7	6283.0	1662.7	2949.6	9616.4	+0.91	3.78	<0.001	0.002	S	+0.440	<0.001
	Myrobalan 29C	13531.9	18599.1	16285.9	21102.9	-250.2	1662.7	-3583.6	3083.3	-0.02	-0.15	0.881	0.921	–	-0.062	0.576
	Marianna 2624	10982.8	19591.1	15697.0	24046.0	-259.3	1662.7	-3592.7	3074.1	-0.02	-0.16	0.877	0.921	–	-0.152	0.058
	Rootpac 20	13682.4	24561.3	18712.5	31588.8	1997.4	1662.7	-1336.0	5330.9	+0.15	1.20	0.235	0.395	–	-0.061	0.576
	Rootpac 40	23601.3	33486.4	29767.2	38003.8	-1648.4	1662.7	-4981.9	1685.0	-0.07	-0.99	0.326	0.511	–	-0.108	0.228
	Rootpac R	12740.1	29767.5	16219.9	45271.0	12023.7	1662.7	8690.3	15357.1	+0.94	7.23	<0.001	<0.001	S	+0.178	0.023
	Garnem	9894.9	19394.1	11933.0	23637.8	2205.6	1662.7	-1127.8	5539.1	+0.22	1.33	0.190	0.347	–	+0.012	0.958
Alanine	GF 677	4970.9	6721.3	5377.4	9094.1	1966.2	1225.6	-490.9	4423.4	+0.40	1.60	0.114	0.243	–	+0.222	0.024
	Myrobalan 29C	10140.4	13391.2	11390.1	15107.3	466.3	1225.6	-1990.8	2923.5	+0.05	0.38	0.705	0.836	–	+0.002	0.995
	Marianna 2624	8693.7	12425.6	11357.2	16102.0	1013.0	1225.6	-1444.1	3470.2	+0.12	0.83	0.412	0.599	–	-0.012	0.964
	Rootpac 20	11673.6	15550.2	14705.3	22220.6	3638.6	1225.6	1181.4	6095.7	+0.31	2.97	0.004	0.017	S	+0.122	0.302
	Rootpac 40	15635.6	18038.3	16861.1	22098.7	2834.8	1225.6	377.6	5292.0	+0.18	2.31	0.025	0.065	–	+0.121	0.302
	Rootpac R	9737.0	16964.6	10652.9	23735.6	5855.1	1225.6	3397.9	8312.3	+0.60	4.78	<0.001	<0.001	S	+0.242	0.014
	Garnem	6176.8	13331.8	7839.7	17639.4	2644.7	1225.6	187.5	5101.8	+0.43	2.16	0.035	0.090	–	+0.042	0.815
Tyrosine	GF 677	808.2	1107.1	922.2	1446.3	225.2	80.88	63.01	387.3	+0.28	2.78	0.007	0.024	S	+0.135	<0.001
	Myrobalan 29C	1404.2	1865.2	1672.6	2083.3	-50.24	80.88	-212.4	111.9	-0.04	-0.62	0.537	0.718	–	-0.064	0.037
	Marianna 2624	1203.9	2258.0	1895.6	2767.7	-182.0	80.88	-344.2	-19.90	-0.15	-2.25	0.028	0.075	–	-0.251	<0.001
	Rootpac 20	1867.2	2708.0	2352.1	3660.2	467.3	80.88	305.1	629.4	+0.25	5.78	<0.001	<0.001	S	+0.070	0.021
	Rootpac 40	2439.3	3079.2	2762.1	3514.6	112.6	80.88	-49.58	274.7	+0.05	1.39	0.170	0.321	–	+0.006	0.933
	Rootpac R	1625.2	2529.6	1935.9	3644.8	804.5	80.88	642.3	966.6	+0.50	9.95	<0.001	<0.001	S	+0.190	<0.001
	Garnem	1075.7	2321.7	1291.4	2905.6	368.2	80.88	206.1	530.3	+0.34	4.55	<0.001	<0.001	S	+0.042	0.233
Cystine	GF 677	698.9	1596.9	874.6	2514.6	742.0	185.6	369.8	1114.2	+1.06	4.00	<0.001	0.001	S	+0.231	0.005
	Myrobalan 29C	1255.8	2976.5	1798.3	3214.7	-304.4	185.6	-676.6	67.77	-0.24	-1.64	0.107	0.230	–	-0.281	<0.001

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	1076.6	2889.8	2134.7	4307.6	359.8	185.6	-12.40	731.9	+0.33	1.94	0.058	0.135	–	-0.271	<0.001
	Rootpac 20	1341.3	2563.8	1689.6	4845.6	1933.5	185.6	1561.3	2305.6	+1.44	10.42	<0.001	<0.001	S	+0.406	<0.001
	Rootpac 40	2112.0	3517.2	3148.6	5608.3	1054.5	185.6	682.4	1426.7	+0.50	5.68	<0.001	<0.001	S	+0.067	0.573
	Rootpac R	1442.7	2640.0	2066.0	7010.4	3747.1	185.6	3374.9	4119.3	+2.60	20.19	<0.001	<0.001	S	+0.618	<0.001
	Garnem	1020.1	2198.0	1862.7	3846.6	806.0	185.6	433.8	1178.1	+0.79	4.34	<0.001	<0.001	S	-0.043	0.750
Valine	GF 677	295.4	859.3	657.6	1343.1	121.5	190.9	-261.1	504.2	+0.41	0.64	0.527	0.715	–	-0.348	<0.001
	Myrobalan 29C	607.9	1517.3	1300.8	1815.6	-394.7	190.9	-777.3	-12.04	-0.65	-2.07	0.043	0.107	–	-0.583	<0.001
	Marianna 2624	521.2	1900.0	863.2	2429.9	187.9	190.9	-194.7	570.5	+0.36	0.98	0.329	0.511	–	-0.259	0.009
	Rootpac 20	743.6	1887.5	936.7	2551.7	471.0	190.9	88.39	853.7	+0.63	2.47	0.017	0.049	S	+0.070	0.647
	Rootpac 40	1162.3	2591.4	2190.4	3020.9	-598.7	190.9	-981.4	-216.1	-0.52	-3.14	0.003	0.011	A	-0.483	<0.001
	Rootpac R	740.0	1629.0	1442.1	3637.2	1306.2	190.9	923.6	1688.9	+1.77	6.84	<0.001	<0.001	S	+0.135	0.240
	Garnem	767.1	1618.3	1002.3	2025.6	172.1	190.9	-210.5	554.8	+0.22	0.90	0.371	0.560	–	-0.043	0.815
Methionine	GF 677	3071.5	1755.6	1662.3	1250.6	904.3	433.3	35.60	1773.0	+0.29	2.09	0.042	0.104	–	+0.275	0.014
	Myrobalan 29C	4099.8	3288.2	3632.6	2604.4	-216.6	433.3	-1085.3	652.1	-0.05	-0.50	0.619	0.788	–	-0.115	0.419
	Marianna 2624	5120.1	3307.6	4417.7	2113.8	-491.4	433.3	-1360.1	377.3	-0.10	-1.13	0.262	0.426	–	-0.302	0.006
	Rootpac 20	6301.1	3951.6	5156.0	2889.4	82.84	433.3	-785.8	951.5	+0.01	0.19	0.849	0.915	–	-0.115	0.419
	Rootpac 40	7828.4	6394.0	6957.3	5055.2	-467.7	433.3	-1336.4	401.0	-0.06	-1.08	0.285	0.454	–	-0.119	0.401
	Rootpac R	9290.2	3724.7	6467.0	2684.5	1783.0	433.3	914.3	2651.7	+0.19	4.12	<0.001	<0.001	S	+0.032	0.886
	Garnem	4735.5	2253.1	4056.6	1958.0	383.8	433.3	-484.9	1252.4	+0.08	0.89	0.380	0.569	–	+0.014	0.964
Tryptophan	GF 677	778.4	1576.6	1120.9	2335.5	416.4	210.8	-6.26	839.1	+0.53	1.98	0.053	0.127	–	+0.029	0.843
	Myrobalan 29C	1562.3	3122.5	2348.2	3372.3	-536.1	210.8	-958.8	-113.4	-0.34	-2.54	0.014	0.042	A	-0.330	<0.001
	Marianna 2624	1339.4	2982.2	1984.1	4282.9	655.9	210.8	233.2	1078.6	+0.49	3.11	0.003	0.012	S	-0.031	0.830
	Rootpac 20	1798.5	3291.4	2265.6	5212.2	1453.8	210.8	1031.1	1876.5	+0.81	6.90	<0.001	<0.001	S	+0.228	0.003
	Rootpac 40	2664.2	4218.2	3832.2	5675.2	288.9	210.8	-133.8	711.6	+0.11	1.37	0.176	0.329	–	-0.068	0.528
	Rootpac R	1701.1	3132.9	2556.8	6673.6	2685.0	210.8	2262.3	3107.7	+1.58	12.74	<0.001	<0.001	S	+0.348	<0.001
	Garnem	1307.4	2821.8	1839.0	4137.6	784.3	210.8	361.6	1207.0	+0.60	3.72	<0.001	0.003	S	+0.042	0.743
Phenylalanine	GF 677	1671.0	2441.6	1867.6	3616.9	978.7	334.7	307.6	1649.7	+0.59	2.92	0.005	0.019	S	+0.279	<0.001
	Myrobalan 29C	3320.1	4641.0	3800.7	5239.8	118.2	334.7	-552.9	789.2	+0.04	0.35	0.725	0.850	–	-0.016	0.933
	Marianna 2624	3156.6	4125.8	4347.9	6105.2	788.1	334.7	117.1	1459.2	+0.25	2.35	0.022	0.061	–	+0.074	0.449
	Rootpac 20	4314.8	5435.4	4906.8	8072.1	2044.7	334.7	1373.6	2715.8	+0.47	6.11	<0.001	<0.001	S	+0.269	<0.001
	Rootpac 40	5495.3	6695.1	6202.8	8789.0	1386.4	334.7	715.4	2057.5	+0.25	4.14	<0.001	<0.001	S	+0.149	0.058
	Rootpac R	3387.2	7516.1	3877.6	10335.2	2328.9	334.7	1657.8	2999.9	+0.69	6.96	<0.001	<0.001	S	+0.181	0.018
	Garnem	1949.1	4206.8	2847.9	6407.9	1302.2	334.7	631.2	1973.3	+0.67	3.89	<0.001	0.002	S	+0.042	0.743
Isoleucine	GF 677	963.1	1621.0	1264.6	2250.0	327.6	230.7	-134.9	790.0	+0.34	1.42	0.161	0.315	–	+0.058	0.641
	Myrobalan 29C	1982.1	2934.6	2515.9	3339.5	-128.9	230.7	-591.4	333.6	-0.07	-0.56	0.579	0.756	–	-0.109	0.253
	Marianna 2624	1699.3	3421.9	2636.2	4293.4	-65.44	230.7	-527.9	397.0	-0.04	-0.28	0.778	0.887	–	-0.212	0.009
	Rootpac 20	2424.7	3629.5	3054.4	4813.6	554.4	230.7	91.89	1016.8	+0.23	2.40	0.020	0.055	–	+0.051	0.693
	Rootpac 40	3365.5	4472.0	3846.3	4911.0	-41.76	230.7	-504.2	420.7	-0.01	-0.18	0.857	0.915	–	-0.042	0.750
	Rootpac R	2260.1	3708.3	2933.8	5411.2	1029.2	230.7	566.7	1491.7	+0.46	4.46	<0.001	<0.001	S	+0.117	0.208
	Garnem	1475.0	3111.7	1890.8	3821.2	293.7	230.7	-168.8	756.1	+0.20	1.27	0.208	0.369	–	-0.043	0.746
Leucine	GF 677	1666.7	2648.0	2309.3	4206.7	916.0	349.2	215.8	1616.2	+0.55	2.62	0.011	0.035	S	+0.135	0.020
	Myrobalan 29C	3220.0	5256.0	4734.0	5858.0	-912.0	349.2	-1612.2	-211.8	-0.28	-2.61	0.012	0.036	A	-0.279	<0.001

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	2613.7	7857.3	4991.3	8947.7	-1287.3	349.2	-1987.5	-587.2	-0.49	-3.69	<0.001	0.003	A	-0.518	<0.001
	Rootpac 20	3198.3	7307.3	4374.3	8551.3	68.00	349.2	-632.2	768.2	+0.02	0.19	0.846	0.915	–	-0.157	0.007
	Rootpac 40	5241.3	9162.7	8400.3	10279.0	-2042.7	349.2	-2742.8	-1342.5	-0.39	-5.85	<0.001	<0.001	A	-0.357	<0.001
	Rootpac R	4051.0	6861.3	6067.7	10937.3	2059.3	349.2	1359.2	2759.5	+0.51	5.90	<0.001	<0.001	S	+0.059	0.424
	Garnem	2845.7	5690.3	3262.7	6500.7	393.3	349.2	-306.8	1093.5	+0.14	1.13	0.265	0.429	–	-0.004	0.982
Lysine	GF 677	1383.6	4062.9	3059.0	7345.3	1607.1	581.7	440.8	2773.4	+1.16	2.76	0.008	0.025	S	-0.200	0.007
	Myrobalan 29C	2727.8	7745.2	6295.4	8696.2	-2616.5	581.7	-3782.8	-1450.2	-0.96	-4.50	<0.001	<0.001	A	-0.720	<0.001
	Marianna 2624	2338.7	8876.5	3846.2	12037.0	1653.0	581.7	486.7	2819.2	+0.71	2.84	0.006	0.022	S	-0.193	0.010
	Rootpac 20	3196.8	8982.6	4027.0	13431.8	3618.9	581.7	2452.7	4785.2	+1.13	6.22	<0.001	<0.001	S	+0.172	0.024
	Rootpac 40	5779.5	14194.2	12620.5	17849.2	-3186.1	581.7	-4352.4	-2019.9	-0.55	-5.48	<0.001	<0.001	A	-0.553	<0.001
	Rootpac R	3297.5	8399.3	7505.5	15616.8	3009.6	581.7	1843.3	4175.9	+0.91	5.17	<0.001	<0.001	S	-0.206	0.006
	Garnem	3568.1	7701.1	4738.9	10662.6	1790.6	581.7	624.3	2956.8	+0.50	3.08	0.003	0.013	S	+0.042	0.743
Hydroxyproline	GF 677	881.6	2171.8	1338.8	2201.8	-427.2	351.9	-1132.8	278.4	-0.48	-1.21	0.230	0.391	–	-0.405	<0.001
	Myrobalan 29C	1612.6	2842.4	2441.2	4546.1	875.1	351.9	169.5	1580.7	+0.54	2.49	0.016	0.047	S	+0.051	0.750
	Marianna 2624	1382.5	4197.4	2467.3	6955.5	1673.3	351.9	967.7	2378.9	+1.21	4.75	<0.001	<0.001	S	-0.073	0.630
	Rootpac 20	1691.9	4062.2	2131.4	6366.6	1865.0	351.9	1159.4	2570.6	+1.10	5.30	<0.001	<0.001	S	+0.220	0.032
	Rootpac 40	2782.6	8074.5	4910.5	9214.4	-987.9	351.9	-1693.5	-282.3	-0.36	-2.81	0.007	0.023	A	-0.437	<0.001
	Rootpac R	2115.3	5762.2	3632.9	6612.0	-667.8	351.9	-1373.4	37.78	-0.32	-1.90	0.063	0.143	–	-0.405	<0.001
	Garnem	1561.5	3224.7	2533.2	5458.3	1262.0	351.9	556.4	1967.6	+0.81	3.59	<0.001	0.004	S	+0.043	0.815
Sarcosine	GF 677	2831.5	5120.5	3887.6	9138.0	2961.5	962.4	1031.9	4891.0	+1.05	3.08	0.003	0.013	S	+0.265	0.003
	Myrobalan 29C	5087.8	9184.5	7993.8	10667.2	-1423.4	962.4	-3352.9	506.1	-0.28	-1.48	0.145	0.289	–	-0.300	<0.001
	Marianna 2624	4361.9	10312.0	6563.2	13296.8	783.5	962.4	-1146.0	2713.1	+0.18	0.81	0.419	0.607	–	-0.154	0.101
	Rootpac 20	5434.1	11396.4	6845.4	15537.1	2729.3	962.4	799.8	4658.8	+0.50	2.84	0.006	0.022	S	+0.080	0.510
	Rootpac 40	9697.7	17977.8	15471.4	20434.4	-3317.1	962.4	-5246.6	-1387.6	-0.34	-3.45	0.001	0.005	A	-0.340	<0.001
	Rootpac R	5626.9	13738.4	8840.9	28872.3	11919.9	962.4	9990.4	13849.4	+2.12	12.39	<0.001	<0.001	S	+0.291	<0.001
	Garnem	4534.5	9770.6	5972.6	12333.8	1125.1	962.4	-804.4	3054.6	+0.25	1.17	0.248	0.412	–	-0.043	0.781
Oxalic acid	GF 677	5.56	3.88	4.34	3.32	0.651	1.04	-1.44	2.74	+0.12	0.62	0.535	0.718	–	+0.080	0.788
	Myrobalan 29C	9.48	7.62	8.54	6.67	-0.013	1.04	-2.10	2.08	-0.00	-0.01	0.990	0.994	–	-0.030	0.947
	Marianna 2624	12.71	8.68	11.20	6.45	-0.729	1.04	-2.82	1.36	-0.06	-0.70	0.487	0.682	–	-0.173	0.426
	Rootpac 20	14.27	10.92	12.64	8.81	-0.473	1.04	-2.56	1.62	-0.03	-0.45	0.652	0.798	–	-0.101	0.717
	Rootpac 40	16.07	13.27	14.46	11.59	-0.066	1.04	-2.16	2.02	-0.00	-0.06	0.950	0.972	–	-0.031	0.947
	Rootpac R	16.13	9.86	12.87	8.79	2.20	1.04	0.108	4.29	+0.14	2.11	0.040	0.099	–	+0.114	0.664
	Garnem	10.22	5.13	7.12	4.57	2.53	1.04	0.443	4.62	+0.25	2.43	0.018	0.052	–	+0.314	0.079
Propionic acid	GF 677	7.10	9.74	7.88	16.10	5.58	2.30	0.960	10.19	+0.79	2.42	0.019	0.053	–	+0.399	<0.001
	Myrobalan 29C	14.57	17.28	15.76	20.79	2.33	2.30	-2.29	6.95	+0.16	1.01	0.316	0.498	–	+0.101	0.516
	Marianna 2624	12.99	22.66	20.40	27.86	-2.20	2.30	-6.82	2.42	-0.17	-0.96	0.344	0.528	–	-0.251	0.029
	Rootpac 20	18.54	26.34	22.94	30.25	-0.475	2.30	-5.09	4.14	-0.03	-0.21	0.837	0.915	–	-0.080	0.647
	Rootpac 40	31.93	39.31	35.33	48.85	6.14	2.30	1.52	10.76	+0.19	2.67	0.010	0.032	S	+0.113	0.438
	Rootpac R	16.71	46.92	22.17	55.05	2.68	2.30	-1.93	7.30	+0.16	1.17	0.249	0.412	–	-0.116	0.424
	Garnem	9.38	18.19	12.00	23.65	2.84	2.30	-1.78	7.45	+0.30	1.23	0.223	0.384	–	+0.014	0.964
Tartaric acid	GF 677	24.38	14.69	14.15	14.13	9.68	3.15	3.35	16.00	+0.40	3.07	0.003	0.013	S	+0.497	<0.001
	Myrobalan 29C	28.77	31.15	31.31	31.94	-1.75	3.15	-8.07	4.58	-0.06	-0.55	0.582	0.756	–	-0.068	0.401

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	44.23	44.45	45.35	25.28	-20.29	3.15	-26.61	-13.97	-0.46	-6.43	<0.001	<0.001	A	-0.581	<0.001
	Rootpac 20	33.95	50.73	43.88	46.43	-14.24	3.15	-20.56	-7.91	-0.42	-4.51	<0.001	<0.001	A	-0.337	<0.001
	Rootpac 40	55.34	57.64	58.55	61.43	0.577	3.15	-5.75	6.90	+0.01	0.18	0.856	0.915	–	+0.007	0.964
	Rootpac R	72.70	73.85	35.90	36.08	-0.969	3.15	-7.29	5.36	-0.01	-0.31	0.760	0.876	–	-0.019	0.879
	Garnem	17.43	17.41	37.09	35.61	-1.46	3.15	-7.79	4.86	-0.08	-0.46	0.644	0.795	–	-0.034	0.743
Butyric acid	GF 677	39.93	52.53	47.34	65.25	5.32	8.54	-11.79	22.43	+0.13	0.62	0.536	0.718	–	+0.037	0.851
	Myrobalan 29C	72.20	96.51	88.47	107.1	-5.68	8.54	-22.79	11.44	-0.08	-0.67	0.509	0.696	–	-0.101	0.481
	Marianna 2624	80.91	115.8	96.94	136.0	4.17	8.54	-12.94	21.28	+0.05	0.49	0.627	0.790	–	-0.022	0.933
	Rootpac 20	98.80	134.1	113.5	152.8	4.02	8.54	-13.09	21.13	+0.04	0.47	0.639	0.795	–	-0.010	0.970
	Rootpac 40	116.9	150.7	136.3	167.8	-2.26	8.54	-19.37	14.86	-0.02	-0.26	0.793	0.897	–	-0.047	0.812
	Rootpac R	93.33	131.0	115.4	164.0	10.99	8.54	-6.12	28.10	+0.12	1.29	0.203	0.362	–	+0.013	0.964
	Garnem	46.58	98.81	59.56	125.1	13.34	8.54	-3.77	30.45	+0.29	1.56	0.124	0.255	–	-0.009	0.972
Malonic acid	GF 677	51.88	37.12	44.46	35.86	6.16	9.14	-12.16	24.48	+0.12	0.67	0.503	0.694	–	+0.119	0.419
	Myrobalan 29C	101.9	74.32	80.02	63.97	11.51	9.14	-6.81	29.83	+0.11	1.26	0.213	0.371	–	+0.087	0.612
	Marianna 2624	129.4	87.02	101.6	62.74	3.48	9.14	-14.85	21.80	+0.03	0.38	0.705	0.836	–	-0.091	0.576
	Rootpac 20	145.4	103.3	123.3	85.76	4.52	9.14	-13.80	22.84	+0.03	0.49	0.623	0.788	–	-0.027	0.927
	Rootpac 40	168.5	121.4	145.1	104.5	6.45	9.14	-11.87	24.77	+0.04	0.71	0.483	0.680	–	-0.005	0.984
	Rootpac R	125.9	103.2	116.1	79.68	-13.64	9.14	-31.96	4.68	-0.11	-1.49	0.141	0.286	–	-0.177	0.164
	Garnem	124.6	57.74	94.12	41.83	14.59	9.14	-3.73	32.91	+0.12	1.60	0.116	0.243	–	-0.042	0.846
Malic acid	GF 677	18.42	14.09	16.93	11.07	-1.53	4.34	-10.23	7.17	-0.08	-0.35	0.726	0.850	–	-0.155	0.302
	Myrobalan 29C	38.75	25.31	29.36	22.14	6.21	4.34	-2.49	14.92	+0.16	1.43	0.158	0.311	–	+0.144	0.356
	Marianna 2624	46.11	30.67	34.93	24.94	5.44	4.34	-3.26	14.15	+0.12	1.25	0.215	0.372	–	+0.067	0.743
	Rootpac 20	55.43	40.15	43.77	33.41	4.94	4.34	-3.77	13.64	+0.09	1.14	0.261	0.426	–	+0.049	0.833
	Rootpac 40	72.75	51.94	62.77	43.55	1.58	4.34	-7.12	10.29	+0.02	0.37	0.716	0.846	–	-0.026	0.933
	Rootpac R	70.55	37.42	52.97	28.24	8.40	4.34	-0.305	17.10	+0.12	1.93	0.058	0.135	–	-0.004	0.995
	Garnem	40.94	20.04	29.06	13.64	5.49	4.34	-3.22	14.19	+0.13	1.26	0.212	0.370	–	-0.042	0.859
Lactic acid	GF 677	54.34	70.79	62.06	96.63	18.12	13.30	-8.54	44.78	+0.33	1.36	0.179	0.330	–	+0.177	0.119
	Myrobalan 29C	107.4	130.5	116.4	150.1	10.67	13.30	-15.99	37.33	+0.10	0.80	0.426	0.613	–	+0.057	0.743
	Marianna 2624	105.5	156.2	139.1	183.1	-6.67	13.30	-33.33	19.99	-0.06	-0.50	0.618	0.788	–	-0.124	0.344
	Rootpac 20	131.5	185.6	165.6	217.7	-2.03	13.30	-28.69	24.63	-0.02	-0.15	0.879	0.921	–	-0.078	0.626
	Rootpac 40	192.9	235.9	214.7	283.3	25.63	13.30	-1.03	52.29	+0.13	1.93	0.059	0.136	–	+0.073	0.652
	Rootpac R	119.1	233.3	146.0	281.8	21.57	13.30	-5.09	48.24	+0.18	1.62	0.111	0.236	–	-0.014	0.964
	Garnem	72.11	132.7	81.36	167.6	25.58	13.30	-1.08	52.25	+0.35	1.92	0.060	0.136	–	+0.109	0.419
Citric acid	GF 677	88.38	51.06	57.06	42.79	23.05	12.23	-1.48	47.57	+0.26	1.88	0.065	0.146	–	+0.257	0.017
	Myrobalan 29C	127.1	105.8	112.6	89.42	-1.86	12.23	-26.38	22.67	-0.01	-0.15	0.880	0.921	–	-0.049	0.798
	Marianna 2624	203.4	148.5	179.5	77.29	-47.30	12.23	-71.82	-22.78	-0.23	-3.87	<0.001	0.002	A	-0.532	<0.001
	Rootpac 20	189.8	138.8	166.6	103.8	-11.89	12.23	-36.41	12.63	-0.06	-0.97	0.335	0.517	–	-0.164	0.167
	Rootpac 40	251.6	206.7	222.2	174.4	-2.93	12.23	-27.45	21.59	-0.01	-0.24	0.811	0.912	–	-0.049	0.796
	Rootpac R	276.5	159.4	223.1	123.7	17.64	12.23	-6.88	42.16	+0.06	1.44	0.155	0.307	–	-0.041	0.834
	Garnem	145.6	70.30	126.6	60.28	8.97	12.23	-15.55	33.49	+0.06	0.73	0.466	0.659	–	-0.014	0.964
Maleic acid	GF 677	22.40	12.99	16.77	11.53	4.17	6.52	-8.90	17.24	+0.19	0.64	0.525	0.715	–	+0.164	0.419
	Myrobalan 29C	43.35	24.20	28.23	21.16	12.08	6.52	-0.993	25.15	+0.28	1.85	0.069	0.155	–	+0.281	0.094

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	60.68	36.11	42.29	30.38	12.66	6.52	-0.408	25.74	+0.21	1.94	0.057	0.135	–	+0.176	0.387
	Rootpac 20	67.73	40.55	48.40	34.65	13.43	6.52	0.356	26.50	+0.20	2.06	0.044	0.108	–	+0.172	0.395
	Rootpac 40	75.25	44.40	52.55	38.55	16.85	6.52	3.77	29.92	+0.22	2.58	0.013	0.038	S	+0.203	0.281
	Rootpac R	81.82	44.76	56.07	32.33	13.31	6.52	0.238	26.38	+0.16	2.04	0.046	0.112	–	+0.047	0.879
	Garnem	34.76	15.90	28.44	12.82	3.24	6.52	-9.83	16.31	+0.09	0.50	0.621	0.788	–	-0.014	0.970
Fumaric acid	GF 677	22.30	15.41	20.00	13.75	0.640	5.80	-10.98	12.26	+0.03	0.11	0.913	0.944	–	-0.011	0.982
	Myrobalan 29C	43.31	26.91	31.12	24.31	9.59	5.80	-2.03	21.21	+0.22	1.65	0.104	0.225	–	+0.222	0.248
	Marianna 2624	25.54	36.10	30.56	50.24	9.12	5.80	-2.50	20.74	+0.36	1.57	0.122	0.252	–	+0.135	0.568
	Rootpac 20	60.75	39.14	44.40	30.99	8.20	5.80	-3.43	19.82	+0.13	1.41	0.163	0.315	–	+0.065	0.832
	Rootpac 40	41.50	62.13	50.84	84.48	13.01	5.80	1.39	24.63	+0.31	2.24	0.029	0.075	–	+0.106	0.682
	Rootpac R	28.86	50.11	41.76	61.95	-1.06	5.80	-12.69	10.56	-0.04	-0.18	0.855	0.915	–	-0.161	0.449
	Garnem	15.96	33.12	23.63	50.75	9.95	5.80	-1.67	21.58	+0.62	1.72	0.092	0.203	–	+0.034	0.933
Succinic acid	GF 677	61.21	85.74	71.83	113.5	17.10	20.13	-23.26	57.45	+0.28	0.85	0.399	0.586	–	+0.110	0.616
	Myrobalan 29C	125.9	136.1	139.6	177.4	27.52	20.13	-12.83	67.88	+0.22	1.37	0.177	0.329	–	+0.161	0.390
	Marianna 2624	184.4	141.0	152.4	116.7	7.68	20.13	-32.68	48.03	+0.04	0.38	0.704	0.836	–	-0.003	0.995
	Rootpac 20	145.4	191.6	171.0	248.1	30.97	20.13	-9.38	71.32	+0.21	1.54	0.130	0.264	–	+0.089	0.711
	Rootpac 40	180.8	216.6	207.7	261.0	17.63	20.13	-22.73	57.98	+0.10	0.88	0.385	0.574	–	+0.044	0.879
	Rootpac R	279.0	130.7	222.3	120.8	46.77	20.13	6.41	87.12	+0.17	2.32	0.024	0.065	–	+0.137	0.485
	Garnem	71.39	153.8	95.39	197.0	19.16	20.13	-21.19	59.51	+0.27	0.95	0.345	0.528	–	-0.043	0.886
Gallic acid	GF 677	1.53	3.52	1.95	5.47	1.52	0.523	0.474	2.57	+1.00	2.91	0.005	0.019	S	+0.203	0.531
	Myrobalan 29C	3.56	4.10	3.79	5.02	0.676	0.523	-0.373	1.73	+0.19	1.29	0.202	0.361	–	+0.135	0.725
	Marianna 2624	2.14	3.03	2.41	3.41	0.110	0.523	-0.939	1.16	+0.05	0.21	0.834	0.915	–	+0.000	1.000
	Rootpac 20	0.203	2.45	0.714	3.41	0.453	0.523	-0.596	1.50	+2.23	0.87	0.391	0.579	–	-0.909	<0.001
	Rootpac 40	6.92	9.60	7.83	11.10	0.581	0.523	-0.468	1.63	+0.08	1.11	0.271	0.435	–	+0.023	0.970
	Rootpac R	3.75	7.21	5.37	9.13	0.297	0.523	-0.752	1.35	+0.08	0.57	0.573	0.753	–	-0.127	0.743
	Garnem	0.410	2.71	1.27	3.88	0.314	0.523	-0.735	1.36	+0.77	0.60	0.550	0.729	–	-0.638	0.006
Vanillic acid	GF 677	2.19	5.27	2.76	8.00	2.16	0.575	1.01	3.31	+0.99	3.76	<0.001	0.002	S	+0.205	0.391
	Myrobalan 29C	4.99	6.84	6.37	7.98	-0.247	0.575	-1.40	0.905	-0.05	-0.43	0.669	0.812	–	-0.098	0.750
	Marianna 2624	3.26	4.39	3.63	4.89	0.133	0.575	-1.02	1.28	+0.04	0.23	0.818	0.915	–	+0.001	1.000
	Rootpac 20	0.153	3.29	0.963	4.90	0.797	0.575	-0.355	1.95	+5.19	1.39	0.171	0.322	–	-1.441	<0.001
	Rootpac 40	10.38	13.56	11.57	15.56	0.802	0.575	-0.350	1.95	+0.08	1.40	0.169	0.321	–	+0.030	0.958
	Rootpac R	5.86	10.67	8.12	13.05	0.125	0.575	-1.03	1.28	+0.02	0.22	0.828	0.915	–	-0.126	0.664
	Garnem	0.594	4.17	2.05	5.68	0.051	0.575	-1.10	1.20	+0.09	0.09	0.930	0.956	–	-0.802	<0.001
trans-Caffeic acid	GF 677	2.11	5.28	2.78	8.39	2.44	0.420	1.60	3.28	+1.16	5.81	<0.001	<0.001	S	+0.205	0.226
	Myrobalan 29C	3.28	4.98	4.44	5.65	-0.491	0.420	-1.33	0.350	-0.15	-1.17	0.247	0.412	–	-0.177	0.323
	Marianna 2624	2.09	2.72	2.34	3.05	0.075	0.420	-0.767	0.916	+0.04	0.18	0.859	0.915	–	-0.000	1.000
	Rootpac 20	0.317	3.15	0.953	4.34	0.554	0.420	-0.288	1.40	+1.75	1.32	0.193	0.349	–	-0.775	<0.001
	Rootpac 40	7.23	9.62	8.40	11.12	0.335	0.420	-0.507	1.18	+0.05	0.80	0.429	0.614	–	-0.008	0.984
	Rootpac R	3.88	7.33	5.75	9.05	-0.143	0.420	-0.984	0.698	-0.04	-0.34	0.735	0.854	–	-0.178	0.318
	Garnem	0.410	2.98	1.56	3.96	-0.170	0.420	-1.01	0.672	-0.41	-0.40	0.687	0.827	–	-0.980	<0.001
trans-p-Coumaric acid	GF 677	2.02	4.38	2.38	6.96	2.22	0.618	0.984	3.46	+1.10	3.60	<0.001	0.004	S	+0.319	0.269
	Myrobalan 29C	5.69	6.72	6.29	7.62	0.295	0.618	-0.945	1.53	+0.05	0.48	0.635	0.794	–	+0.021	0.970

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	3.72	4.53	4.14	5.24	0.287	0.618	-0.952	1.53	+0.08	0.46	0.644	0.795	–	+0.038	0.958
	Rootpac 20	4.50	0.910	3.09	0.250	0.744	0.618	-0.496	1.98	+0.17	1.20	0.234	0.395	–	-0.925	<0.001
	Rootpac 40	10.81	13.21	12.15	15.06	0.513	0.618	-0.726	1.75	+0.05	0.83	0.410	0.599	–	+0.014	0.984
	Rootpac R	5.97	10.85	8.11	12.87	-0.111	0.618	-1.35	1.13	-0.02	-0.18	0.858	0.915	–	-0.131	0.743
	Garnem	0.574	4.39	2.11	5.54	-0.382	0.618	-1.62	0.857	-0.67	-0.62	0.539	0.718	–	-0.888	<0.001
Ferulic acid	GF 677	1.08	2.80	1.87	3.38	-0.211	0.151	-0.514	0.092	-0.20	-1.39	0.169	0.321	–	-0.359	0.055
	Myrobalan 29C	2.11	2.81	2.59	3.09	-0.191	0.151	-0.494	0.112	-0.09	-1.26	0.211	0.370	–	-0.112	0.699
	Marianna 2624	2.16	2.89	2.36	3.05	-0.042	0.151	-0.345	0.261	-0.02	-0.28	0.784	0.890	–	-0.036	0.933
	Rootpac 20	0.150	1.57	0.488	2.15	0.250	0.151	-0.053	0.553	+1.67	1.66	0.104	0.225	–	-0.883	<0.001
	Rootpac 40	2.02	2.72	2.20	2.91	0.005	0.151	-0.298	0.308	+0.00	0.03	0.973	0.989	–	-0.021	0.964
	Rootpac R	2.18	2.87	2.53	3.18	-0.047	0.151	-0.350	0.256	-0.02	-0.31	0.756	0.875	–	-0.047	0.901
	Garnem	0.154	1.31	0.954	1.59	-0.518	0.151	-0.821	-0.215	-3.37	-3.43	0.001	0.005	A	-1.515	<0.001
Caftaric acid	GF 677	2.72	3.66	6.59	9.76	2.24	1.03	0.168	4.30	+0.82	2.17	0.035	0.088	–	+0.119	0.743
	Myrobalan 29C	5.67	7.94	8.57	10.63	-0.213	1.03	-2.28	1.85	-0.04	-0.21	0.837	0.915	–	-0.133	0.711
	Marianna 2624	3.71	4.12	5.37	6.09	0.308	1.03	-1.76	2.38	+0.08	0.30	0.766	0.880	–	+0.020	0.970
	Rootpac 20	6.11	4.07	1.18	0.290	1.15	1.03	-0.920	3.22	+0.19	1.11	0.271	0.435	–	-0.991	<0.001
	Rootpac 40	12.87	13.90	17.20	20.32	2.09	1.03	0.020	4.16	+0.16	2.02	0.048	0.115	–	+0.094	0.815
	Rootpac R	7.28	10.11	13.28	17.21	1.09	1.03	-0.974	3.16	+0.15	1.06	0.294	0.465	–	-0.084	0.838
	Garnem	0.775	2.48	5.01	7.18	0.469	1.03	-1.60	2.54	+0.61	0.46	0.651	0.798	–	-0.684	0.002
Catechin	GF 677	2.59	5.95	3.18	8.97	2.43	1.05	0.331	4.54	+0.94	2.32	0.024	0.065	–	+0.216	0.244
	Myrobalan 29C	6.60	8.26	7.43	10.76	1.67	1.05	-0.429	3.78	+0.25	1.60	0.116	0.243	–	+0.135	0.547
	Marianna 2624	4.32	6.38	4.80	7.81	0.944	1.05	-1.16	3.05	+0.22	0.90	0.372	0.560	–	+0.095	0.711
	Rootpac 20	6.48	1.50	4.31	0.720	1.39	1.05	-0.710	3.50	+0.21	1.33	0.190	0.347	–	-0.298	0.072
	Rootpac 40	13.24	17.91	14.72	22.04	2.65	1.05	0.547	4.75	+0.20	2.53	0.015	0.043	S	+0.106	0.664
	Rootpac R	7.38	13.61	11.08	19.37	2.05	1.05	-0.051	4.16	+0.28	1.96	0.056	0.132	–	-0.068	0.815
	Garnem	0.840	5.18	3.22	7.33	-0.221	1.05	-2.32	1.88	-0.26	-0.21	0.834	0.915	–	-0.976	<0.001
Epicatechin	GF 677	1.76	2.79	3.03	6.34	2.27	0.756	0.758	3.79	+1.29	3.01	0.004	0.015	S	+0.374	0.180
	Myrobalan 29C	3.80	5.42	4.78	6.19	-0.222	0.756	-1.74	1.29	-0.06	-0.29	0.770	0.882	–	-0.099	0.832
	Marianna 2624	2.31	2.87	2.62	3.25	0.074	0.756	-1.44	1.59	+0.03	0.10	0.923	0.951	–	+0.000	1.000
	Rootpac 20	3.76	0.763	2.54	0.293	0.746	0.756	-0.770	2.26	+0.20	0.99	0.328	0.511	–	-0.563	0.026
	Rootpac 40	8.54	11.30	10.16	12.62	-0.301	0.756	-1.82	1.22	-0.04	-0.40	0.692	0.830	–	-0.070	0.891
	Rootpac R	4.32	8.68	6.30	10.26	-0.409	0.756	-1.93	1.11	-0.09	-0.54	0.591	0.763	–	-0.199	0.576
	Garnem	0.456	3.44	1.94	4.42	-0.507	0.756	-2.02	1.01	-1.11	-0.67	0.505	0.695	–	-1.162	<0.001
Quercetin	GF 677	0.707	8.02	3.43	10.43	-0.318	0.631	-1.58	0.946	-0.45	-0.50	0.616	0.788	–	-1.144	0.006
	Myrobalan 29C	3.45	4.01	3.72	4.49	0.216	0.631	-1.05	1.48	+0.06	0.34	0.734	0.854	–	+0.039	0.970
	Marianna 2624	3.59	4.57	3.93	4.76	-0.151	0.631	-1.42	1.11	-0.04	-0.24	0.812	0.912	–	-0.049	0.964
	Rootpac 20	0.137	1.02	0.321	2.19	0.981	0.631	-0.283	2.25	+7.18	1.56	0.126	0.257	–	-0.250	0.711
	Rootpac 40	3.09	3.99	3.38	4.16	-0.128	0.631	-1.39	1.14	-0.04	-0.20	0.840	0.915	–	-0.049	0.964
	Rootpac R	3.33	4.16	3.76	4.60	0.014	0.631	-1.25	1.28	+0.00	0.02	0.983	0.993	–	-0.020	0.984
	Garnem	0.222	2.00	1.34	2.35	-0.766	0.631	-2.03	0.498	-3.44	-1.21	0.230	0.391	–	-1.319	0.001
Rutin	GF 677	0.292	8.44	0.501	10.35	1.69	0.466	0.760	2.63	+5.81	3.64	<0.001	0.003	S	-0.330	0.101
	Myrobalan 29C	2.78	3.87	3.49	4.57	-0.003	0.466	-0.937	0.931	-0.00	-0.01	0.995	0.995	–	-0.068	0.849

Compound	Rootstock	C	D	H	D+H	I	SE	95% CI lower	95% CI upper	I / C	t	p	p adj.	Direction	I (ln scale)	p adj. (ln)
	Marianna 2624	1.77	2.50	2.07	2.81	0.017	0.466	-0.917	0.952	+0.01	0.04	0.970	0.989	–	-0.035	0.946
	Rootpac 20	0.137	2.65	0.804	3.66	0.344	0.466	-0.590	1.28	+2.52	0.74	0.464	0.658	–	-1.459	<0.001
	Rootpac 40	5.70	7.87	6.44	8.92	0.316	0.466	-0.618	1.25	+0.06	0.68	0.500	0.694	–	+0.005	0.995
	Rootpac R	3.17	6.05	4.55	7.52	0.083	0.466	-0.851	1.02	+0.03	0.18	0.860	0.915	–	-0.157	0.568
	Garnem	0.340	2.31	1.29	3.18	-0.068	0.466	-1.00	0.866	-0.20	-0.15	0.884	0.921	–	-0.939	<0.001
Myricetin	GF 677	4.16	2.34	6.20	1.76	-2.61	0.601	-3.81	-1.41	-0.63	-4.34	<0.001	<0.001	A	-0.696	0.009
	Myrobalan 29C	3.20	2.88	3.97	1.97	-1.68	0.601	-2.88	-0.472	-0.52	-2.79	0.007	0.024	A	-0.586	0.029
	Marianna 2624	1.29	2.20	1.43	2.61	0.260	0.601	-0.944	1.46	+0.20	0.43	0.667	0.812	–	+0.062	0.927
	Rootpac 20	2.23	0.331	1.16	0.280	1.02	0.601	-0.181	2.23	+0.46	1.70	0.094	0.207	–	+0.487	0.079
	Rootpac 40	4.51	6.74	4.87	9.11	2.01	0.601	0.810	3.22	+0.45	3.35	0.001	0.006	S	+0.239	0.510
	Rootpac R	2.56	4.90	4.03	7.16	0.776	0.601	-0.428	1.98	+0.30	1.29	0.202	0.361	–	-0.099	0.838
	Garnem	1.76	0.889	2.99	0.306	-1.81	0.601	-3.02	-0.610	-1.03	-3.02	0.004	0.015	A	-1.483	<0.001

Table S6. Sensitivity of mean separation to the multiple-comparison procedure: grouping letters of the main-effect means according to Duncan's multiple range test and Tukey's honestly significant difference test ($p < 0.05$). Rootstock means, n = 12; treatment means, n = 21. Within a compound and a test, means sharing a letter do not differ; letter a denotes the highest mean. GF, GF 677; My, Myrobalan 29C; Ma, Marianna 2624; R20, Rootpac 20; R40, Rootpac 40; RR, Rootpac R; Ga, Garnem; C, control; D, drought; H, heat shock; D+H, drought + heat shock.

Compound	Rootstock means: Duncan							Rootstock means: Tukey							Treatment means: Duncan				Treatment means: Tukey			
	GF	My	Ma	R20	R40	RR	Ga	GF	My	Ma	R20	R40	RR	Ga	C	D	H	D+H	C	D	H	D+H
Amino acids																						
Aspartate	g	e	d	c	a	b	f	f	d	d	c	a	b	e	a	c	b	d	a	c	b	d
Glutamate	f	d	g	c	b	a	e	e	d	f	c	b	a	d	d	b	c	a	d	b	c	a
Asparagine	g	e	a	d	c	b	f	f	e	a	d	c	b	e	d	b	c	a	d	b	c	a
Serine	d	c	e	b	a	b	c	d	c	e	b	a	b	c	d	b	c	a	d	b	c	a
Glutamine	f	d	g	c	b	a	e	e	d	f	c	b	a	d	ab	bc	a	c	ab	b	a	b
Histidine	f	c	g	b	a	e	d	e	c	f	b	a	d	d	d	b	c	a	d	b	c	a
Glycine	e	d	f	b	a	c	c	e	d	f	b	a	c	c	d	b	c	a	d	b	c	a
Threonine	d	c	b	b	a	a	c	d	c	b	b	a	a	c	d	b	c	a	d	b	c	a
Arginine	f	de	d	c	a	b	e	e	d	d	c	a	b	d	d	b	c	a	d	b	c	a
Alanine	e	c	c	b	a	b	d	d	c	c	b	a	b	c	d	b	c	a	d	b	c	a
Tyrosine	g	f	d	b	a	c	e	g	f	d	b	a	c	e	d	b	c	a	d	b	c	a
Cystine	e	d	c	c	a	b	d	e	d	c	c	a	b	d	d	b	c	a	d	b	c	a
Valine	e	d	cd	c	a	b	d	e	d	cd	c	a	b	cd	d	b	c	a	d	b	c	a
Methionine	f	e	d	c	a	b	e	f	de	d	c	a	b	e	a	c	b	d	a	c	b	d
Tryptophan	e	d	d	c	a	b	d	e	d	d	c	a	b	d	d	b	c	a	d	b	c	a
Phenylalanine	f	d	d	c	a	b	e	f	d	d	c	a	b	e	d	b	c	a	d	b	c	a
Isoleucine	e	d	c	b	a	b	d	e	d	c	b	a	b	d	d	b	c	a	d	b	c	a
Leucine	e	d	c	c	a	b	d	e	d	c	c	a	b	d	d	b	c	a	d	b	c	a
Lysine	e	d	d	c	a	b	d	e	d	d	c	a	b	d	d	b	c	a	d	b	c	a
Hydroxyproline	f	e	c	c	a	b	d	f	e	c	cd	a	b	de	d	b	c	a	d	b	c	a
Sarcosine	e	d	d	c	a	b	d	e	d	d	c	a	b	d	d	b	c	a	d	b	c	a
Organic acids																						
Oxalic acid	f	d	c	b	a	b	e	f	d	c	b	a	b	e	a	c	b	d	a	c	b	d
Propionic acid	f	e	d	c	a	b	e	f	e	d	c	a	b	e	d	b	c	a	d	b	c	a
Tartaric acid	g	e	d	c	a	b	f	g	e	d	c	a	b	f	b	a	b	c	ab	a	bc	c
Butyric acid	f	d	c	b	a	b	e	e	d	c	b	a	b	d	d	b	c	a	d	b	c	a
Malonic acid	f	e	d	b	a	c	e	e	d	c	b	a	b	d	a	c	b	d	a	c	b	d
Malic acid	f	e	d	c	a	b	e	e	d	c	b	a	b	d	a	c	b	d	a	c	b	d
Lactic acid	g	e	d	c	a	b	f	f	e	d	c	a	b	e	d	b	c	a	d	b	c	a
Citric acid	e	d	c	c	a	b	d	e	d	c	c	a	b	d	a	c	b	d	a	c	b	d
Maleic acid	f	d	c	b	a	a	e	d	c	b	ab	a	a	c	a	c	b	d	a	c	b	d
Fumaric acid	e	d	c	b	a	b	d	d	c	c	b	a	b	c	c	b	bc	a	b	b	b	a
Succinic acid	e	c	c	b	a	b	d	d	c	c	b	a	b	c	b	b	b	a	b	b	b	a
Phenolic compounds																						
Gallic acid	d	c	d	f	a	b	e	d	c	d	e	a	b	e	d	b	c	a	d	b	c	a
Vanillic acid	d	c	e	g	a	b	f	d	c	d	f	a	b	e	d	b	c	a	d	b	c	a
trans-Caffeic acid	c	c	d	e	a	b	e	c	c	d	d	a	b	d	d	b	c	a	d	b	c	a
trans-p-Coumaric acid	e	c	d	g	a	b	f	d	c	d	f	a	b	e	d	b	c	a	d	b	c	a
Ferulic acid	c	a	a	d	b	a	d	c	a	ab	d	b	a	d	d	b	c	a	d	b	c	a

Compound	Rootstock means: Duncan							Rootstock means: Tukey							Treatment means: Duncan				Treatment means: Tukey			
	GF	My	Ma	R20	R40	RR	Ga	GF	My	Ma	R20	R40	RR	Ga	C	D	H	D+H	C	D	H	D+H
Caftaric acid	d	c	e	g	a	b	f	d	c	de	f	a	b	ef	d	c	b	a	d	c	b	a
Catechin	d	c	d	f	a	b	e	de	c	d	f	a	b	ef	d	b	c	a	d	b	c	a
Epicatechin	d	c	e	f	a	b	e	d	c	de	f	a	b	ef	d	b	c	a	d	b	c	a
Quercetin	a	bc	b	e	c	bc	d	a	b	b	c	b	b	c	d	b	c	a	d	b	c	a
Rutin	c	d	e	f	a	b	f	b	c	d	de	a	b	e	d	b	c	a	d	b	c	a
Myricetin	c	d	e	f	a	b	e	c	c	d	e	a	b	de	b	b	a	a	c	bc	a	ab

Pairwise differences declared significant: rootstock means, Duncan 843 and Tukey 800 of 903 (43 compounds × 21 pairs); treatment means, Duncan 247 and Tukey 242 of 258 (43 compounds × 6 pairs).

Table S7. Residual diagnostics of the factorial model for each compound. Shapiro–Wilk test of the residuals (W and p) on the original and on the ln scale; Levene's test of homogeneity of variance among the 28 rootstock × treatment cells (median-centred); Spearman correlation between the absolute residuals and the fitted values (ρ and p); and number of standardized residuals (residual ÷ √MSE) larger than 3 in absolute value (of 84).

Compound	Shapiro–Wilk W	Shapiro–Wilk p	Shapiro–Wilk p (ln scale)	Levene p	Spearman ρ	Spearman p	|std. residual| > 3
Amino acids							
Aspartate	0.945	0.001	<0.001	0.840	+0.36	<0.001	1
Glutamate	0.967	0.029	0.085	0.787	+0.33	0.002	0
Asparagine	0.933	<0.001	0.075	0.462	+0.30	0.005	1
Serine	0.989	0.726	<0.001	0.525	+0.45	<0.001	0
Glutamine	0.977	0.129	<0.001	0.320	+0.52	<0.001	0
Histidine	0.983	0.356	0.002	0.706	+0.43	<0.001	0
Glycine	0.969	0.043	<0.001	0.607	+0.18	0.102	0
Threonine	0.873	<0.001	0.055	0.193	+0.27	0.011	2
Arginine	0.950	0.003	0.022	0.556	+0.37	<0.001	0
Alanine	0.975	0.104	0.001	0.652	+0.38	<0.001	0
Tyrosine	0.953	0.004	<0.001	0.991	+0.40	<0.001	1
Cystine	0.949	0.002	<0.001	0.918	+0.30	0.006	0
Valine	0.933	<0.001	<0.001	0.670	+0.49	<0.001	0
Methionine	0.961	0.011	<0.001	0.548	+0.43	<0.001	1
Tryptophan	0.986	0.484	<0.001	0.485	+0.37	<0.001	0
Phenylalanine	0.991	0.815	0.016	0.970	+0.56	<0.001	0
Isoleucine	0.961	0.013	<0.001	0.819	+0.45	<0.001	0
Leucine	0.928	<0.001	<0.001	0.873	+0.33	0.003	1
Lysine	0.952	0.003	<0.001	0.177	+0.31	0.004	0
Hydroxyproline	0.986	0.478	<0.001	0.992	+0.61	<0.001	0
Sarcosine	0.948	0.002	<0.001	0.501	+0.51	<0.001	0
Organic acids							
Oxalic acid	0.952	0.004	<0.001	0.860	+0.19	0.076	1
Propionic acid	0.964	0.020	0.019	0.706	+0.42	<0.001	0
Tartaric acid	0.987	0.586	<0.001	0.915	+0.12	0.270	0
Butyric acid	0.990	0.778	0.264	0.822	+0.17	0.117	0
Malonic acid	0.979	0.196	0.035	0.910	+0.29	0.008	0
Malic acid	0.920	<0.001	0.382	0.286	+0.47	<0.001	1
Lactic acid	0.989	0.711	0.360	0.747	+0.25	0.022	0
Citric acid	0.961	0.011	0.062	0.772	+0.37	<0.001	0
Maleic acid	0.931	<0.001	0.633	0.301	+0.58	<0.001	0
Fumaric acid	0.936	<0.001	0.363	0.191	+0.32	0.003	0
Succinic acid	0.963	0.015	<0.001	0.526	+0.27	0.013	0
Phenolic compounds							
Gallic acid	0.957	0.007	<0.001	0.923	+0.38	<0.001	0
Vanillic acid	0.962	0.015	<0.001	0.840	+0.01	0.909	0
trans-Caffeic acid	0.970	0.045	<0.001	0.917	+0.01	0.953	1
trans-p-Coumaric acid	0.959	0.010	<0.001	0.881	-0.19	0.088	1
Ferulic acid	0.943	0.001	<0.001	0.808	-0.07	0.525	1
Caftaric acid	0.955	0.005	<0.001	0.890	+0.13	0.231	0
Catechin	0.972	0.060	<0.001	0.630	+0.16	0.138	0
Epicatechin	0.926	<0.001	<0.001	0.785	+0.30	0.005	1
Quercetin	0.648	<0.001	<0.001	0.109	+0.10	0.378	3
Rutin	0.924	<0.001	0.001	0.319	+0.22	0.043	1
Myricetin	0.915	<0.001	<0.001	0.440	+0.44	<0.001	1

Normality rejected ($p < 0.05$) for 31 of 43 compounds on the original scale and 34 on the ln scale; Levene $p < 0.05$ for 0 compounds; significant positive Spearman correlation for 32 compounds; 18 of 3612 standardized residuals exceeded 3 in absolute value.

Table S8. Principal component analysis of the 28 standardized rootstock × treatment means: (a) scores and (b) loadings (eigenvectors multiplied by the square root of the eigenvalue) on the first three components. Variance explained: PC1 56.8%, PC2 19.0%, PC3 9.7%.

(a) Scores

Rootstock	Treatment	PC1	PC2	PC3
GF 677	C	-7.35	-0.63	-0.62
GF 677	D	-4.98	-3.79	-3.11
GF 677	D+H	-1.89	-4.85	-4.22
GF 677	H	-6.50	-2.38	-1.64
Garnem	C	-6.77	1.27	1.35
Garnem	D	-2.05	-2.65	1.57
Garnem	D+H	1.47	-3.50	2.41
Garnem	H	-4.57	0.11	0.79
Marianna 2624	C	-4.78	2.67	-0.39
Marianna 2624	D	-0.87	-1.13	0.71
Marianna 2624	D+H	1.69	-3.41	1.63
Marianna 2624	H	-2.86	0.74	0.26
Myrobalan 29C	C	-3.41	0.93	-1.01
Myrobalan 29C	D	-0.63	-1.72	-0.68
Myrobalan 29C	D+H	0.75	-2.56	-0.73
Myrobalan 29C	H	-1.74	-0.73	-1.09
Rootpac 20	C	-2.91	4.16	2.05
Rootpac 20	D	0.53	0.54	3.64
Rootpac 20	D+H	3.66	-2.08	5.20
Rootpac 20	H	-1.95	2.29	3.23
Rootpac 40	C	3.11	5.26	-1.53
Rootpac 40	D	8.18	1.76	-1.49
Rootpac 40	D+H	11.60	0.13	-1.49
Rootpac 40	H	6.11	3.15	-1.17
Rootpac R	C	-1.28	6.56	-1.09
Rootpac R	D	5.20	0.25	-0.88
Rootpac R	D+H	11.49	-3.46	0.21
Rootpac R	H	0.76	3.07	-1.90

(b) Loadings

Compound	PC1	PC2	PC3
Amino acids			
Aspartate	0.35	0.89	-0.13
Glutamate	0.89	0.14	-0.01
Asparagine	0.52	-0.18	0.15
Serine	0.89	-0.15	0.18
Glutamine	0.58	0.53	-0.03
Histidine	0.72	-0.02	0.33
Glycine	0.80	-0.32	0.24
Threonine	0.95	-0.07	0.04
Arginine	0.99	-0.13	0.18
Alanine	0.93	-0.10	0.35
Tyrosine	0.91	-0.09	0.40
Cystine	0.88	-0.39	0.19
Valine	0.91	-0.34	0.18
Methionine	0.19	0.98	-0.07
Tryptophan	0.93	-0.30	0.25
Phenylalanine	0.96	-0.13	0.26
Isoleucine	0.94	-0.14	0.31
Leucine	0.93	-0.17	0.21
Lysine	0.92	-0.30	0.13
Hydroxyproline	0.91	-0.22	0.15
Sarcosine	0.96	-0.24	0.10
Organic acids			
Oxalic acid	0.32	0.94	0.08
Propionic acid	0.98	0.03	0.07
Tartaric acid	0.59	0.62	0.09
Butyric acid	0.93	0.06	0.32
Malonic acid	0.23	0.92	0.12
Malic acid	0.29	0.96	0.00
Lactic acid	0.98	0.05	0.21

Compound	PC1	PC2	PC3
Citric acid	0.29	0.95	-0.06
Maleic acid	0.18	0.95	0.04
Fumaric acid	0.80	0.22	0.15
Succinic acid	0.57	0.46	0.17
Phenolic compounds			
Gallic acid	0.90	-0.02	-0.45
Vanillic acid	0.89	-0.02	-0.47
trans-Caffeic acid	0.83	-0.12	-0.53
trans-p-Coumaric acid	0.83	0.13	-0.52
Ferulic acid	0.51	-0.39	-0.53
Caftaric acid	0.79	0.12	-0.53
Catechin	0.86	0.08	-0.47
Epicatechin	0.82	0.11	-0.52
Quercetin	0.19	-0.47	-0.71
Rutin	0.67	-0.24	-0.58
Myricetin	0.56	0.10	-0.53

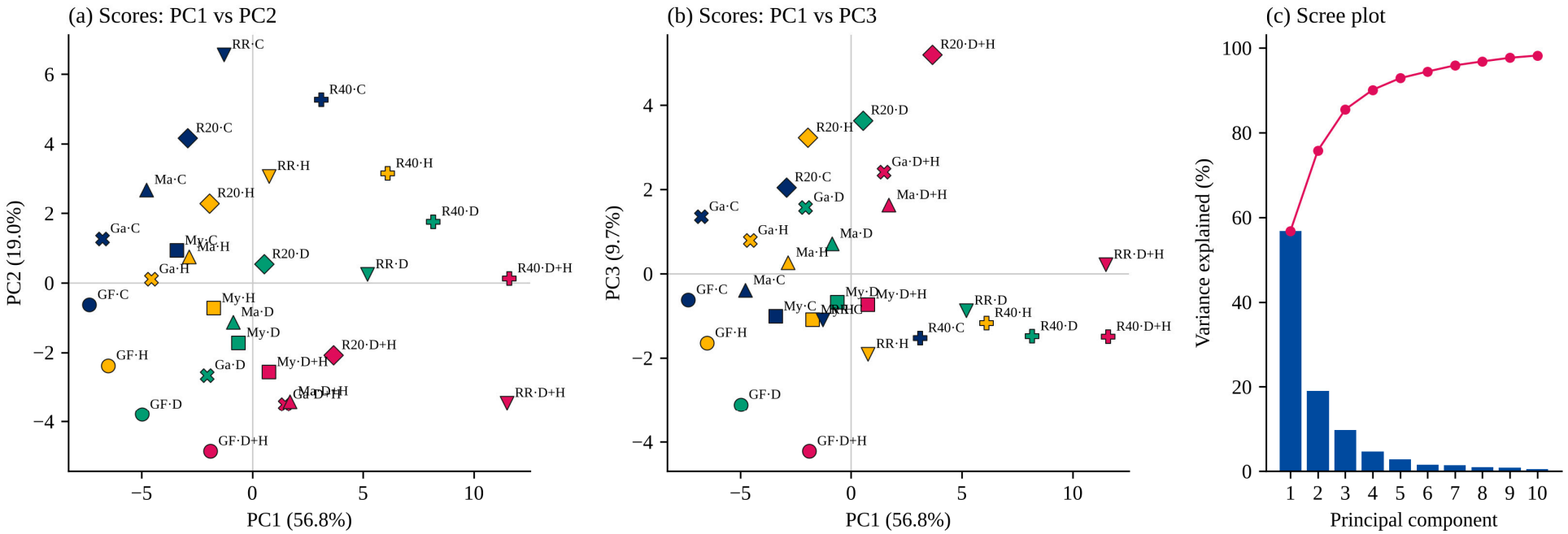


Figure S1. Principal component analysis of the 28 rootstock × treatment means (43 standardized compounds). (a) Scores on PC1 and PC2 and (b) on PC1 and PC3, with each point labeled by rootstock and treatment; symbols denote rootstocks and colors treatments. (c) Scree plot: variance explained by the first ten components (bars) and cumulative variance (line). GF, GF 677; My, Myrobalan 29C; Ma, Marianna 2624; R20, Rootpac 20; R40, Rootpac 40; RR, Rootpac R; Ga, Garnem; C, control; D, drought; H, heat shock; D+H, drought + heat shock. Scores and loadings are listed in Table S8.

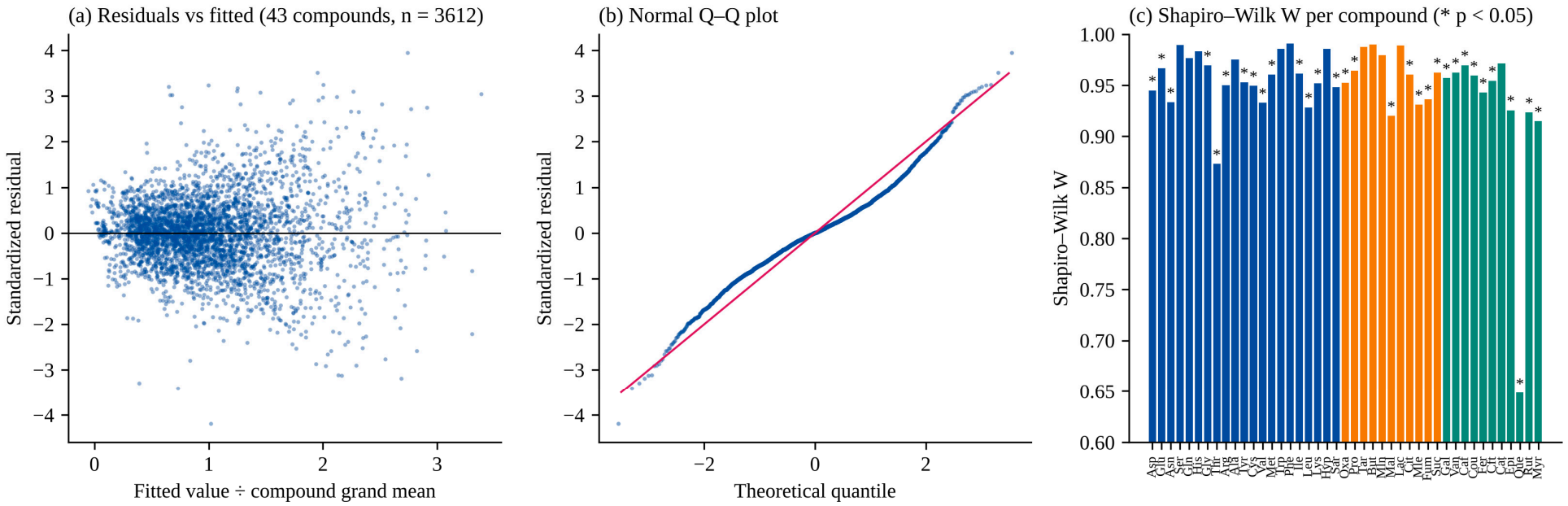


Figure S2. Residual diagnostics of the factorial model (block + rootstock × treatment), pooled over the 43 compounds. (a) Standardized residuals (residual ÷ √MSE of the compound) against fitted values expressed relative to the grand mean of the compound. (b) Normal quantile–quantile plot of the standardized residuals. (c) Shapiro–Wilk W of the residuals of each compound; asterisks mark $p < 0.05$. Compound abbreviations are as defined in Figure 3 of the article; numerical values are given in Table S7.

Table S9. Sensitivity of the non-additivity results to hypothetical treatment-dependent differences in extraction recovery. Observed concentrations were divided by the recovery ratio in the treatments indicated (a ratio of 1.25 means a recovery 25% higher than in the remaining treatments; 1 is the reported analysis). For each ratio the 301 additivity contrasts, the Benjamini–Hochberg adjustment and the rootstock × drought × heat shock (R × D × H) and drought × heat shock (D × H) tests were recalculated.

Recovery ratio	Non-additive contrasts (BH p < 0.05)	Synergistic	Antagonistic	Original 104 retained, same sign	Original contrasts with reversed sign	Amino acids	Organic acids	Phenolic compounds	Compounds with significant R × D × H	Compounds with significant D × H
(i) Drought-exposed tissue (D, D+H)										
0.80	107	91	16	88	0	82	8	17	23	32
0.90	109	87	22	98	0	87	8	14	23	31
1.00	104	78	26	104	0	86	6	12	24	30
1.11	100	72	28	96	0	82	7	11	24	28
1.25	95	65	30	89	0	78	7	10	24	24
(ii) Heat-exposed tissue (H, D+H)										
0.80	121	107	14	83	0	87	14	20	29	35
0.90	106	89	17	89	0	82	9	15	28	33
1.00	104	78	26	104	0	86	6	12	24	30
1.11	94	62	32	84	0	75	9	10	24	25
1.25	84	53	31	68	0	67	12	5	27	22
(iii) Combined treatment only (D+H)										
0.80	228	224	4	82	6	121	56	51	35	43
0.90	151	140	11	89	0	96	27	28	28	39
1.00	104	78	26	104	0	86	6	12	24	30
1.11	73	33	40	59	0	62	4	7	27	17
1.25	120	15	105	41	6	72	23	25	29	35

Of 301 contrasts (43 compounds × 7 rootstocks) and 43 compounds. The rows for a ratio of 1.00 reproduce the reported results (Section 2.8, Table 2). Results for the full range 0.5–2 (601 values) are shown in Figure S3 and are reproduced by Code S1.

Table S10. Recovery ratios at which each of the 104 non-additive contrasts ceases to be significant (Benjamini–Hochberg-adjusted $p < 0.05$) with its original sign, for the three scenarios of Table S9. The contrast remains significant with its original sign for all ratios between the lower and upper limits; ≤0.50 and ≥2.00 indicate that it did so over the whole range examined. I/C, contrast scaled to the control mean.

Compound	Rootstock	Direction	I/C	(i) Drought-exposed		(ii) Heat-exposed		(iii) Combined only	
				Lower	Upper	Lower	Upper	Lower	Upper
Aspartate	GF 677	synergistic	+0.54	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	≥2.00
Aspartate	Myrobalan 29C	synergistic	+0.11	0.87	≥2.00	0.91	≥2.00	≤0.50	1.04
Aspartate	Rootpac 20	synergistic	+0.09	0.90	≥2.00	0.90	≥2.00	≤0.50	1.05
Aspartate	Rootpac 40	synergistic	+0.08	0.55	≥2.00	0.80	≥2.00	≤0.50	1.05
Aspartate	Rootpac R	synergistic	+0.18	≤0.50	≥2.00	0.77	≥2.00	≤0.50	1.71
Aspartate	Garnem	synergistic	+0.12	0.76	≥2.00	0.93	≥2.00	≤0.50	1.09
Glutamate	GF 677	synergistic	+1.05	≤0.50	≥2.00	≤0.50	1.87	≤0.50	1.33
Glutamate	Myrobalan 29C	antagonistic	-0.39	0.57	≥2.00	0.78	≥2.00	0.93	≥2.00
Glutamate	Marianna 2624	synergistic	+0.75	≤0.50	1.09	≤0.50	1.04	≤0.50	1.02
Glutamate	Rootpac 40	antagonistic	-0.13	0.87	≥2.00	0.92	≥2.00	0.98	≥2.00
Glutamate	Rootpac R	synergistic	+0.16	≤0.50	1.39	≤0.50	1.07	≤0.50	1.03
Glutamate	Garnem	synergistic	+0.44	≤0.50	1.35	≤0.50	1.10	≤0.50	1.04
Asparagine	GF 677	synergistic	+1.14	≤0.50	≥2.00	≤0.50	1.34	≤0.50	1.17
Asparagine	Myrobalan 29C	antagonistic	-0.38	0.99	≥2.00	0.99	≥2.00	1.00	≥2.00
Asparagine	Rootpac 20	synergistic	+0.59	≤0.50	1.51	≤0.50	1.15	≤0.50	1.07
Asparagine	Rootpac 40	antagonistic	-0.28	0.86	≥2.00	0.89	≥2.00	0.96	≥2.00
Asparagine	Rootpac R	antagonistic	-0.23	0.85	≥2.00	0.92	≥2.00	0.97	≥2.00
Serine	Marianna 2624	synergistic	+1.17	≤0.50	1.17	≤0.50	1.08	≤0.50	1.03
Serine	Rootpac 20	synergistic	+0.44	≤0.50	1.59	≤0.50	1.27	≤0.50	1.09
Serine	Rootpac R	synergistic	+1.47	≤0.50	≥2.00	≤0.50	1.83	≤0.50	1.47
Serine	Garnem	synergistic	+0.53	≤0.50	1.36	≤0.50	1.11	≤0.50	1.05
Glutamine	GF 677	synergistic	+0.35	0.78	≥2.00	0.85	≥2.00	≤0.50	1.11
Glutamine	Marianna 2624	synergistic	+1.86	≤0.50	1.56	≤0.50	1.94	≤0.50	1.31
Glutamine	Rootpac 20	antagonistic	-0.49	≤0.50	≥2.00	0.51	≥2.00	0.83	≥2.00
Glutamine	Rootpac 40	antagonistic	-0.42	≤0.50	≥2.00	≤0.50	≥2.00	0.81	≥2.00
Glutamine	Rootpac R	synergistic	+0.12	0.87	≥2.00	0.94	≥2.00	≤0.50	1.02
Glutamine	Garnem	antagonistic	-1.21	0.61	≥2.00	≤0.50	≥2.00	0.76	≥2.00
Histidine	GF 677	synergistic	+0.36	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.31
Histidine	Marianna 2624	synergistic	+1.56	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.57
Histidine	Rootpac 20	antagonistic	-0.17	0.92	≥2.00	0.95	≥2.00	0.99	≥2.00
Histidine	Rootpac R	synergistic	+1.01	≤0.50	1.40	≤0.50	1.04	≤0.50	1.03
Glycine	Myrobalan 29C	antagonistic	-0.38	0.81	≥2.00	0.91	≥2.00	0.96	≥2.00
Glycine	Rootpac 20	synergistic	+1.00	≤0.50	≥2.00	≤0.50	1.86	≤0.50	1.37
Glycine	Rootpac 40	synergistic	+0.20	≤0.50	1.11	≤0.50	1.08	≤0.50	1.03
Glycine	Rootpac R	synergistic	+11.57	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	≥2.00
Glycine	Garnem	synergistic	+0.69	≤0.50	1.83	≤0.50	1.34	≤0.50	1.16
Threonine	Rootpac R	synergistic	+0.70	≤0.50	1.75	≤0.50	1.13	≤0.50	1.08
Arginine	GF 677	synergistic	+0.91	≤0.50	≥2.00	≤0.50	1.70	≤0.50	1.19
Arginine	Rootpac R	synergistic	+0.94	≤0.50	≥2.00	≤0.50	1.43	≤0.50	1.23
Alanine	Rootpac 20	synergistic	+0.31	≤0.50	1.17	≤0.50	1.13	≤0.50	1.03
Alanine	Rootpac R	synergistic	+0.60	≤0.50	≥2.00	≤0.50	1.34	≤0.50	1.15

Compound	Rootstock	Direction	I/C	(i) Drought-exposed		(ii) Heat-exposed		(iii) Combined only	
				Lower	Upper	Lower	Upper	Lower	Upper
Tyrosine	GF 677	synergistic	+0.28	≤0.50	1.18	≤0.50	1.07	≤0.50	1.02
Tyrosine	Rootpac 20	synergistic	+0.25	≤0.50	1.50	≤0.50	1.29	≤0.50	1.08
Tyrosine	Rootpac R	synergistic	+0.50	≤0.50	≥2.00	≤0.50	1.63	≤0.50	1.21
Tyrosine	Garnem	synergistic	+0.34	≤0.50	1.61	≤0.50	1.13	≤0.50	1.06
Cystine	GF 677	synergistic	+1.06	≤0.50	1.78	≤0.50	1.26	≤0.50	1.13
Cystine	Rootpac 20	synergistic	+1.44	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.48
Cystine	Rootpac 40	synergistic	+0.50	≤0.50	1.49	≤0.50	1.38	≤0.50	1.12
Cystine	Rootpac R	synergistic	+2.60	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.96
Cystine	Garnem	synergistic	+0.79	≤0.50	1.35	≤0.50	1.26	≤0.50	1.10
Valine	Rootpac 20	synergistic	+0.63	≤0.50	1.01	≤0.50	1.00	≤0.50	1.00
Valine	Rootpac 40	antagonistic	-0.52	0.87	≥2.00	0.90	≥2.00	0.96	≥2.00
Valine	Rootpac R	synergistic	+1.77	≤0.50	≥2.00	≤0.50	1.87	≤0.50	1.36
Methionine	Rootpac R	synergistic	+0.19	0.64	≥2.00	0.85	≥2.00	≤0.50	1.48
Tryptophan	Myrobalan 29C	antagonistic	-0.34	0.97	≥2.00	0.99	≥2.00	0.99	≥2.00
Tryptophan	Marianna 2624	synergistic	+0.49	≤0.50	1.18	≤0.50	1.07	≤0.50	1.03
Tryptophan	Rootpac 20	synergistic	+0.81	≤0.50	≥2.00	≤0.50	1.57	≤0.50	1.24
Tryptophan	Rootpac R	synergistic	+1.58	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.53
Tryptophan	Garnem	synergistic	+0.60	≤0.50	1.40	≤0.50	1.15	≤0.50	1.07
Phenylalanine	GF 677	synergistic	+0.59	≤0.50	1.37	≤0.50	1.14	≤0.50	1.04
Phenylalanine	Rootpac 20	synergistic	+0.47	≤0.50	≥2.00	≤0.50	1.91	≤0.50	1.19
Phenylalanine	Rootpac 40	synergistic	+0.25	≤0.50	1.59	≤0.50	1.36	≤0.50	1.07
Phenylalanine	Rootpac R	synergistic	+0.69	≤0.50	≥2.00	≤0.50	1.34	≤0.50	1.18
Phenylalanine	Garnem	synergistic	+0.67	≤0.50	1.42	≤0.50	1.18	≤0.50	1.08
Isoleucine	Rootpac R	synergistic	+0.46	≤0.50	1.57	≤0.50	1.27	≤0.50	1.09
Leucine	GF 677	synergistic	+0.55	≤0.50	1.09	≤0.50	1.05	≤0.50	1.02
Leucine	Myrobalan 29C	antagonistic	-0.28	0.96	≥2.00	0.97	≥2.00	0.99	≥2.00
Leucine	Marianna 2624	antagonistic	-0.49	0.82	≥2.00	0.91	≥2.00	0.95	≥2.00
Leucine	Rootpac 40	antagonistic	-0.39	0.62	≥2.00	0.68	≥2.00	0.90	≥2.00
Leucine	Rootpac R	synergistic	+0.51	≤0.50	1.57	≤0.50	1.39	≤0.50	1.13
Lysine	GF 677	synergistic	+1.16	≤0.50	1.10	≤0.50	1.06	≤0.50	1.03
Lysine	Myrobalan 29C	antagonistic	-0.96	0.65	≥2.00	0.74	≥2.00	0.88	≥2.00
Lysine	Marianna 2624	synergistic	+0.71	≤0.50	1.13	≤0.50	1.03	≤0.50	1.02
Lysine	Rootpac 20	synergistic	+1.13	≤0.50	≥2.00	≤0.50	1.35	≤0.50	1.22
Lysine	Rootpac 40	antagonistic	-0.55	0.74	≥2.00	0.78	≥2.00	0.91	≥2.00
Lysine	Rootpac R	synergistic	+0.91	≤0.50	1.36	≤0.50	1.28	≤0.50	1.12
Lysine	Garnem	synergistic	+0.50	≤0.50	1.26	≤0.50	1.08	≤0.50	1.04
Hydroxyproline	Myrobalan 29C	synergistic	+0.54	≤0.50	1.01	≤0.50	1.01	≤0.50	1.00
Hydroxyproline	Marianna 2624	synergistic	+1.21	≤0.50	1.60	≤0.50	1.25	≤0.50	1.14
Hydroxyproline	Rootpac 20	synergistic	+1.10	≤0.50	≥2.00	≤0.50	1.37	≤0.50	1.21
Hydroxyproline	Rootpac 40	antagonistic	-0.36	0.93	≥2.00	0.97	≥2.00	0.99	≥2.00
Hydroxyproline	Garnem	synergistic	+0.81	≤0.50	1.34	≤0.50	1.19	≤0.50	1.08
Sarcosine	GF 677	synergistic	+1.05	≤0.50	1.38	≤0.50	1.19	≤0.50	1.07
Sarcosine	Rootpac 20	synergistic	+0.50	≤0.50	1.18	≤0.50	1.05	≤0.50	1.03
Sarcosine	Rootpac 40	antagonistic	-0.34	0.82	≥2.00	0.88	≥2.00	0.95	≥2.00
Sarcosine	Rootpac R	synergistic	+2.12	≤0.50	≥2.00	≤0.50	≥2.00	≤0.50	1.56

Compound	Rootstock	Direction	I/C	(i) Drought-exposed		(ii) Heat-exposed		(iii) Combined only	
				Lower	Upper	Lower	Upper	Lower	Upper
Propionic acid	Rootpac 40	synergistic	+0.19	≤0.50	1.10	≤0.50	1.05	≤0.50	1.01
Tartaric acid	GF 677	synergistic	+0.40	0.73	≥2.00	0.57	≥2.00	≤0.50	1.14
Tartaric acid	Marianna 2624	antagonistic	-0.46	≤0.50	≥2.00	≤0.50	≥2.00	0.66	≥2.00
Tartaric acid	Rootpac 20	antagonistic	-0.42	≤0.50	≥2.00	≤0.50	≥2.00	0.87	≥2.00
Citric acid	Marianna 2624	antagonistic	-0.23	≤0.50	1.45	≤0.50	1.23	0.80	≥2.00
Maleic acid	Rootpac 40	synergistic	+0.22	0.88	≥2.00	0.94	≥2.00	≤0.50	1.02
Gallic acid	GF 677	synergistic	+1.00	≤0.50	1.26	≤0.50	1.07	≤0.50	1.04
Vanillic acid	GF 677	synergistic	+0.99	≤0.50	1.63	≤0.50	1.18	≤0.50	1.10
trans-Caffeic acid	GF 677	synergistic	+1.16	≤0.50	≥2.00	≤0.50	1.35	≤0.50	1.21
trans-p-Coumaric acid	GF 677	synergistic	+1.10	≤0.50	1.50	≤0.50	1.20	≤0.50	1.10
Ferulic acid	Garnem	antagonistic	-3.37	0.77	≥2.00	0.86	≥2.00	0.91	≥2.00
Catechin	Rootpac 40	synergistic	+0.20	≤0.50	1.04	≤0.50	1.01	≤0.50	1.00
Epicatechin	GF 677	synergistic	+1.29	≤0.50	1.16	≤0.50	1.20	≤0.50	1.06
Rutin	GF 677	synergistic	+5.81	≤0.50	1.91	≤0.50	1.06	≤0.50	1.05
Myricetin	GF 677	antagonistic	-0.63	≤0.50	≥2.00	≤0.50	1.36	0.58	≥2.00
Myricetin	Myrobalan 29C	antagonistic	-0.52	≤0.50	≥2.00	≤0.50	1.13	0.86	≥2.00
Myricetin	Rootpac 40	synergistic	+0.45	≤0.50	1.47	≤0.50	1.15	≤0.50	1.06
Myricetin	Garnem	antagonistic	-1.03	≤0.50	≥2.00	≤0.50	1.15	≤0.50	≥2.00

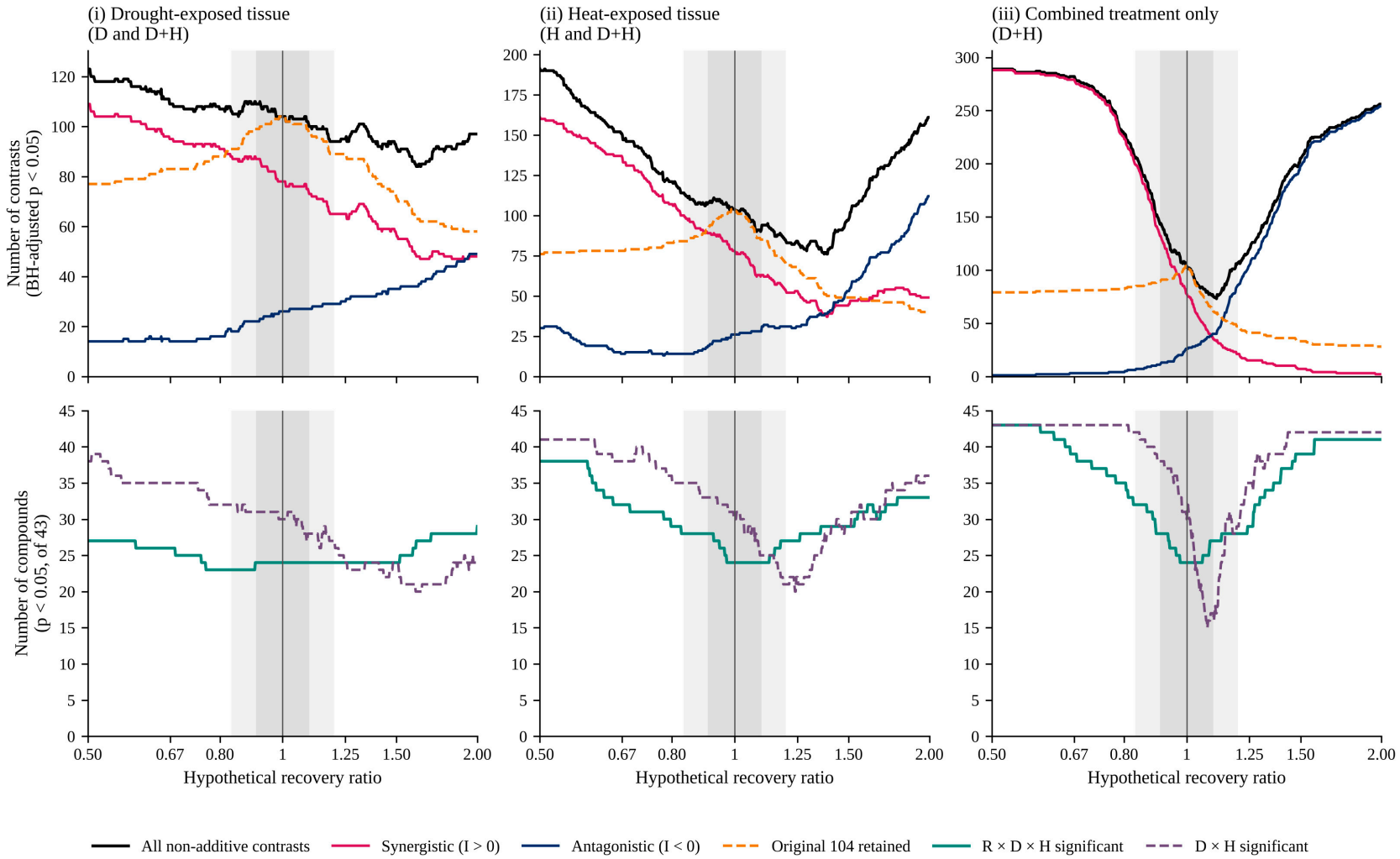


Figure S3. Sensitivity of the non-additivity results to hypothetical treatment-dependent differences in extraction recovery. Observed concentrations were divided by a recovery ratio (0.5–2, logarithmic axis) applied (i) to the drought-exposed tissue (drought and drought + heat-shock treatments; this case also represents a difference in tissue composition such as dry matter per unit fresh mass), (ii) to the heat-exposed tissue (heat-shock and drought + heat-shock treatments), or (iii) to the drought + heat-shock treatment alone. Upper panels: number of contrasts significant after Benjamini–Hochberg adjustment (of 301), split into synergistic and antagonistic, and number of the 104 originally significant contrasts that remain significant with the same sign. Lower panels: number of compounds (of 43) with a significant rootstock × drought × heat shock (R × D × H) or drought × heat shock (D × H) interaction. Shaded bands mark ratios between 0.91 and 1.10 (dark) and between 0.83 and 1.20 (light); the vertical line marks the reported analysis.

Data S1. Replicate-level concentrations in the leaf extracts for all 84 samples (7 rootstocks × 4 treatments × 3 blocks) and 43 compounds, as reported by the analytical laboratory. Each row is one experimental unit (a composite sample of five plants). Treatment: C, control; D, drought; H, heat shock; D+H, drought + heat shock. Values are given to seven significant digits. Data S1a–S1c share the columns Rootstock, Treatment and Block and together form the complete data set analyzed in the article; they can be copied into comma-separated files and analyzed with Code S1. Re-running Code S1 on these values reproduces all reported classifications and counts, including the sensitivity analysis (Tables S9 and S10); because of the rounding to seven digits, a few F-values may differ from those reported by up to 0.02.

Data S1a. Concentrations of amino acids in the leaf extracts (pmol µL⁻¹).

Rootstock	Treatment	Block	Aspartate	Glutamate	Asparagine	Serine	Glutamine	Histidine	Glycine	Threonine	Arginine	Alanine	Tyrosine	Cystine	Valine	Methionine	Tryptophan	Phenylalanine	Isoleucine	Leucine	Lysine	Hydroxyproline	Sarcosine
GF 677	C	1	10431.42	2782.76	6169.23	7819.76	12255.74	2988.262	1789.23	4117.93	6537.88	4536.677	862.8215	665.76	293.46	2982.047	748.98	1647.818	921.99	1587	1434.45	844.9979	2711.22
GF 677	C	2	10327.11	2727.105	6415.999	7194.179	13411.46	2689.436	1699.768	4282.647	7034.759	5266.95	802.424	722.6825	290.5254	2743.483	766.3563	1503.14	1008.934	1650	1308.505	811.198	3012.165
GF 677	C	3	10014.17	2536.207	6564.85	7913.597	11030.17	2779.084	1550.529	3768.73	7155.303	5108.941	759.2829	708.2288	302.1464	3488.995	820.0013	1862.035	958.487	1763	1407.952	988.6476	2771.192
GF 677	D	1	3741.98	4095.3	10921.12	11169.99	5410.141	1753.663	3983.114	6030.423	8816.048	6884.946	1169.518	1663.488	771.8398	1704.434	1571.366	2355.288	1749.314	2464	4041.31	2383.45	5586.027
GF 677	D	2	3592.301	3808.629	11174.49	12286.99	5626.547	1886.941	3633.396	5306.772	8872.575	7426.791	1122.738	1630.219	802.7133	1568.079	1681.362	2308.182	1661.848	2613	4348.45	2097.436	5139.145
GF 677	D	3	3556.378	3481.005	12122.44	13180.59	5602.937	1630.906	3465.309	7296.811	9645.08	5852.204	1029.176	1497.14	1003.392	1994.188	1477.084	2661.476	1451.93	2867	3798.832	2034.513	4636.403
GF 677	H	1	4423.334	3157.98	8215.42	9133.3	7399.525	2164.45	2634.359	4795.374	7815.617	5337.267	986.96	897.5391	580.2687	1527.671	1184.024	1762.95	1399.876	2159	3040.082	1279.069	4150.455
GF 677	H	2	4379.1	3379.039	8051.112	8676.635	8097.3	2121.161	2555.328	4411.744	7767.081	5283.895	908.0032	918.362	638.2956	1671.73	1065.621	1939.245	1231.891	2370	3279.336	1240.697	4067.446
GF 677	H	3	4246.4	2684.283	9119.116	10777.29	6659.572	1909.045	2291.892	5802.402	8584.742	5511.015	871.6831	807.7852	754.3493	1787.375	1112.982	1900.46	1161.897	2399	2857.677	1496.511	3444.878
GF 677	D+H	1	3251.45	7547.278	19864.2	16546.42	4869.127	2127.492	5668.003	11254.22	14808.16	9315.497	1527.821	2619.395	1206.367	1346.85	2327.709	3488.954	2428.075	3883	7306.366	2103.588	9968.78
GF 677	D+H	2	3267.334	7018.968	20325.05	18201.07	4785.15	1914.742	5170.352	9903.71	16451.87	10048.63	1466.709	2567.007	1254.622	1252.571	2490.648	3419.175	2306.672	4038	7861.65	2040.48	9171.278
GF 677	D+H	3	3409.392	6415.186	22049.26	19524.78	5120.11	1978.567	4931.162	13617.6	18362.12	7918.173	1344.483	2357.456	1568.277	1152.365	2188.046	3942.518	2015.302	4699	6867.984	2461.198	8274.087
Garnem	C	1	11608.6	3846.887	10857.5	10653.08	5581.399	2666.819	3072.716	5593.324	9537.648	6143.37	1151.19	1046.89	676.8254	4473.116	1381.045	1922.015	1632.815	2661	3545.951	1491.906	4841.091
Garnem	C	2	11492.51	3769.95	10099.31	10120.43	5972.097	2613.482	2980.535	5145.858	9569.82	5959.069	1059.095	1071.177	744.508	4499.735	1242.941	1753.262	1436.877	2920	3825.018	1447.149	4744.269
Garnem	C	3	11144.25	3506.053	11439.02	12570.64	6535.266	2352.134	2673.263	6767.922	10577.26	6428.048	1016.731	942.2006	879.873	5233.546	1298.182	2171.877	1355.237	2956	3333.194	1745.53	4018.106
Garnem	D	1	5548.63	6847.58	20647.67	22993.18	8630.805	2621.282	6632.028	11800.05	17983.29	13259.61	2484.683	2255.769	1427.876	2100.033	2980.793	4148.401	3444.695	5427	7653.44	3080.899	10431.26
Garnem	D	2	5493.144	6710.628	20234.71	21843.52	9444.69	2359.154	6433.067	10856.04	19520.86	12861.82	2285.908	2308.102	1570.664	2202.224	2682.713	3784.171	3031.332	5708	8255.765	2988.472	10222.64
Garnem	D	3	5326.685	6240.884	22918.91	24312	7767.725	2437.793	5769.865	12509.38	20678.1	13874.04	2194.472	2030.192	1856.239	2457.039	2801.945	4687.693	2859.097	5936	7194.233	3604.652	8657.949
Garnem	H	1	9420.476	4776.758	13699.45	13028.68	17442.52	5583.389	4645.904	7033.885	11751.34	8030.601	1364.126	1940.293	900.2739	3845.928	1832.842	2747.208	2040.399	3036	4713.784	2780.056	6515.542
Garnem	H	2	9043.657	4442.385	14017.27	14331.55	19087.35	5025.05	4237.993	6189.819	13115.8	8662.609	1309.561	1901.487	936.2848	4208.599	1961.14	2692.264	1938.379	3219	5072.032	2446.449	5994.299
Garnem	H	3	8953.221	4060.244	15206.39	15373.84	15698.27	5192.552	4041.936	8511.001	10931.9	6826.011	1200.431	1746.264	1170.356	4115.267	1722.871	3104.345	1693.531	3533	4430.957	2373.056	5407.9
Garnem	D+H	1	4693.94	9653.64	26305.73	29314.53	11774.89	5449.027	10453.28	14215.2	22973.37	18068.85	3069.284	4006.851	1819.418	1882.243	4123.894	6181.218	4123.567	6029	10606.01	5990.281	13455.09
Garnem	D+H	2	4506.182	8977.885	26916.03	32245.98	12599.13	5340.046	9535.485	14278.06	25640.85	19490.87	2946.513	3926.714	1892.195	2059.738	4412.566	6057.594	3917.388	6567	11412.07	5271.448	12378.68
Garnem	D+H	3	4461.12	8205.594	29199.37	34591.14	13787.23	4806.042	9094.356	17200.4	22299.28	15358.52	2700.97	3606.166	2365.243	1932.03	3876.46	6984.776	3422.56	6906	9969.654	5113.304	11167.72
Rootpac 20	C	1	16309.24	7950.25	11839.67	18066.77	13620.09	4051.662	4133.837	10366.93	12547.16	12331.22	1993.463	1277.692	738.7888	6117.572	1730.443	4073.12	2321.12	3045	3314.153	1621.676	5203.234
Rootpac 20	C	2	16146.15	8506.767	12313.25	16621.43	14164.89	4359.588	3927.145	10781.61	13500.75	12207.91	1853.92	1386.935	731.4009	5628.167	1770.59	4480.432	2540.002	3167	3023.171	1556.809	5780.793
Rootpac 20	C	3	15656.87	6757.712	12598.92	18283.57	12258.08	3768.046	3582.342	9487.818	14999.33	10481.54	1754.247	1359.196	760.657	7157.56	1894.531	4390.823	2413.002	3383	3252.932	1897.361	5318.329
Rootpac 20	D	1	11817.05	10015.02	27287.95	26819.25	21972.55	6713.746	7735.598	13059.35	22157.21	15466	2898.134	2631.129	1665.475	4255.743	3476.797	5130.958	4017.893	6687	8926.972	3881.045	12167.03
Rootpac 20	D	2	11344.36	10716.08	25382.42	25478.29	24044.56	6579.471	7503.53	13581.73	24051.66	15002.02	2666.283	2692.171	1832.022	3957.841	3129.117	5644.054	3535.746	7429	9629.525	3764.614	11923.69
Rootpac 20	D	3	11230.92	9512.771	28749.48	31646.71	19775.29	5921.524	6729.97	11951.92	27474.94	16182.68	2559.632	2368.016	2165.117	3641.213	3268.189	5531.172	3334.851	7806	8391.354	4540.823	10098.63
Rootpac 20	H	1	11527.81	9466.094	16633.88	22758.93	13734.23	5541.179	5207.444	13763.58	17159.89	15533.79	2511.189	1609.524	930.6611	4738.568	2179.86	4838.695	2923.943	4165	4174.879	2042.845	6554.576
Rootpac 20	H	2	10605.59	9276.772	17299.24	20938.22	14695.63	5962.308	4947.072	12662.49	18464.04	15378.45	2335.406	1747.139	921.3545	5185.414	2230.433	4413.857	3199.671	4331	3808.324	1961.131	7282.134
Rootpac 20	H	3	11066.7	8627.398	17700.58	23032.04	16081.43	5153.296	4512.719	11667.55	20513.55	13203.72	2209.846	1712.196	958.2087	5544.124	2386.563	5467.725	3039.687	4627	4097.757	2390.129	6699.563
Rootpac 20	D+H	1	8205.27	12160.81	36957.66	36927.86	17157.39	7636.016	13168.13	17907.06	28280.01	22761.55	3866.414	5047.478	2291.943	3111.762	5194.918	7786.555	5194.507	8091	13360.52	6987.064	16949.53
Rootpac 20	D+H	2	7548.848	11309.55	37815.08	40620.65	17843.69	6872.414	12011.96	15758.22	31419.09	24552.88	3711.757	4946.529	2383.62	2893.939	5558.562	7630.824	4934.781	8118	14375.92	6148.617	15593.57
Rootpac 20	D+H	3	7877.059	12250.89	43220.67	43574.88	15441.65	7101.495	11456.27	16653.93	35067.22	19347.32	3402.444	4542.731	2979.526	2662.424	4883.223	8798.807	4311.44	9445	12558.89	5964.158	14068.11
Rootpac 40	C	1	24443.06	11684.71	21534.94	26762.82	18057.97	5690.94	5882.483	19347.19	21643.1	16611.63	2604.196	2011.905	1154.709	7363.288	2563.354	5689.947	3221.752	4990	5991.724	2667.048	9285.649
Rootpac 40	C	2	24198.63	11451.02	22396.33	24621.79	19322.03	6123.452	5588.359	18759.24	23287.98	16113.28	2421.902	2183.923	1143.162	7872.656	2622.824	5190.369	3525.563	5190	5465.651	2560.366	10316.36
Rootpac 40	C	3	23465.34	10649.44	22915.93	27083.97	21144.1	5292.574	5097.701	17706.55	25872.94	14181.77	2291.692	2140.245	1188.889	8249.115	2806.422	5605.599	3349.285	5544	5881.04	3120.446	9491.048
Rootpac 40	D	1	19835.75	14651.61	39567.53	34060.45	26749.85	6895.199	9437.429	22763	32133.77	17940.56	3245.91	3552.024	2633.062	6486.484	4415.532	6944.011	4781.292	8893	13820.15	8409.463	17236.62
Rootpac 40	D	2	19042.32	15677.22	36804.51	32357.42	29272.36	6757.295	9154.306	21616.21	34653.08	17402.35	3005.472	3634.43	2454.909	6061.951	4088.455	6636.989	4207.537	8901	13836.81	8027.361	18243.24
Rootpac 40	D	3	18851.9	14956.43	41686.74	40191.33	24074.86	6750.537	8210.563	22348.72	33672.32	18771.91	2986.237	3365.213	2686.349	6633.593	4150.6	6504.249	4427.123	9694	14925.76	7786.54	18453.54
Rootpac 40	H	1	22216.05	13657.3	33531.81	31537.45	22558.79	6081.565	8738.36	20259.98	27946.04	16684.44	2765.034	3288.911	2066.422	7050.526	3973.978	6033.626	3968.473	8012	13006.6	4691.593	16891.89
Rootpac 40	H	2	21327.4	13631.29	32861.17	29960.58	23461.14	6358.698	8476.21	20121.08	30335.42	16517.6	2654.433	2960.02	2273.064	6728.766	3679.61	6145.142	3895.868	8426	12811.86	4550.845	14306.39
Rootpac 40	H	3	21114.13	12453.87	35220.31	37214.19	20302.91	6570.655	7602.374	20390.48	31020.1	17381.4	2866.788	3196.821	2231.736	7092.483	3843.148	6429.64	3674.512	8763	12043.15	5489.163	15216
Rootpac 40	D+H	1	19350.26	16472.97	42720.51	40207.81	19502.61	7653.671	13773.25	24672.48	39845.87	22636.66	3712.606	5841.989	3422.98	5444.283	5656.332	8478.159	5299.608	9880	17754.47	9851.761	18615.55
Rootpac 40	D+H	2	17802.24	15319.86	43711.63	44228.59	20867.79	7500.597	12563.96	24563.87	35700.62	24418.16	3564.102	5725.149	2738.384	5063.183	6052.276	8308.596	5034.628	10196	19103.81	8669.549	22233.19
Rootpac 40	D+H	3	18576.25	15002.02	47419.77	47445.21	22835.63	7065.22	11982.72	25722.29	38464.92	19241.16	3267.093	5257.79	2901.257	4658.129	5316.952	9580.319	4398.675	10761	16689.2	9122.001	20454.53
Rootpac R	C	1	21029.43	11585.68	27880.05	13568.66	35171.09	800.3099	719.614	10171.79	11682.99	10285.54	1735.099	1374.3	735.2377	9019.592	1636.681	3459.766	2163.557	3857	3418.636	2027.439	5387.826
Rootpac R	C	2	20619.13	11553.97	28995.25	13283.17	38487.73	861.1334	683.6333	10578.66	12570.9	10182.68	1613.642	1491.803	727.8853	8298.024	1674.652	3155.999	2367.58	4011	3118.48	1946.341	5985.874
Rootpac R	C	3	19388.25	11445.19	29667.94	13611.49	31653.98	744.2882	623.6103	9309.224	13966.27	8742.707	1526.888	1461.967	757.0007	10552.92	1791.877	3545.972	2249.201	4285	3355.485	2372.104	5507.004
Rootpac R	D	1	8127.179	20434.76	55307.81	31471.09	22671.88	5844.749	6645.027	28662.5	27297.61	17920.32	2700.648	2514.882	1437.318	3423.134	3014.315	7095.098	3549.893	6643	8599.234	5941.381	13154.67
Rootpac R	D	2	7802.092	20935.2	56590.95	28953.4	24261.63	6288.95	6312.776	29809	29372.22	17741.12	2511.602	2729.904	1581.05	3745.936	3084.247	7804.607	3884.648	6673	8158.223	5759.001	14614.84
Rootpac R	D	3	7724.071	18219.55	61391.67	31848.74	26551.46	5435.617	5758.514	26231.92	32632.54	15232.28	2376.57	2675.306	1868.514	4005.067	3300.144	7648.515	3690.416	7268	8440.382	5586.231	13445.65
Rootpac R	H	1	15480.79	12820.14	41498.78	14350.93	29660.63	1031.102	1105.988	11710.78	14632.26	10595.2	2071.787	2120.233	1432.695	6964.759	2700.824	3909.536	3247.705	5979	7844.221	3481.979	9438.671
Rootpac R	H	2	16882.33	12947.55	43158.73	14133.38	30847.06	1010.48	1072.809	10773.92	15883.32	10277.35	1906.044	2169.422	1418.368	6477.226	2430.741	3900.569	2857.98	6006	7563.013	3342.7	9249.897
Rootpac R	H	3	15181.56	12547.12	44160.01	15134.1	26694.57	909.4323	962.2098	14170.05	18144	11086.18	1829.802	1908.21	1475.102	5959.048	2538.774	3822.558	2695.595	6218	7109.233	4073.916	7834.097
Rootpac R	D+H	1	7389.278	24099.35	63241.25	47281.4	22593.51	7256.172	15558.67	36390.92	40529.08	24313.45	3850.11	7302.486	3266.947	2891.155	6651.428	9969.687	5839.383	10096	15480.95	6544.32	31497.01
Rootpac R	D+H	2	6798.135	22412.39	61976.42	52009.54	22697.25	6530.555	14192.62	32024.01	45027.81	26226.92	3696.106	7156.436	3397.625	2688.774	7117.028	9770.293	5547.414	10500	17417.5	6125.135	28977.25
Rootpac R	D+H	3	7093.706	22484.44	70197.78	55792.06	22334.16	6748.24	13536.04	44033.02	50256.06	20666.43	3388.097	6572.238	4247.031	2473.672	6252.342	11265.75	4846.688	12216	13952.09	7166.408	26142.52
Marianna 2624	C	1	12304.2	1723.011	29606.2	4162.489	3025.071	986.0618	839.3578	7265.566	10071.54	9183.516	1285.259	1025.597	517.773	4934.643	1288.725	2979.809	1626.735	2488	2424.565	1325.123	4176.609
Marianna 2624	C	2	12181.16	1771.621	29990.45	3829.49	3146.074	1061.003	797.3899	7556.189	10836.98	9091.68	1195.291	1113.286	512.5953	4804.516	1318.623	3277.789	1780.136	2588	2211.688	1272.119	4640.213
Marianna 2624	C	3	11812.03	1804.559	30222.22	4212.439	2722.564	917.0375	727.379	6649.446	12039.89	7805.988	1131.028	1091.02	533.0991	5621.284	1410.927	3212.234	1691.129	2765	2379.776	1550.394	4268.996
Marianna 2624	D	1	9269.11	2892.046	83579.63	6337.004	2645.255	1270.421	1991.476	13659.46	18028.41	12358.25	2416.532	2530.414	1676.488	3562.192	3150.241	4136.022	3788.123	7400	8821.499	4010.247	11009.27
Marianna 2624	D	2	8527.581	2748.206	77743.22	6970.704	2830.423	1245.013	1816.624	12566.7	19569.83	11987.5	2223.21	3100.559	1844.137	3312.838	2835.217	3681.157	3333.548	7950	9515.751	3889.939	10789.08
Marianna 2624	D	3	8898.345	2897.831	88056.1	7477.665	3097.332	1274.962	1732.584	12338.95	21175.21	12930.92	2134.281	3038.548	2179.434	3047.811	2961.226	4560.083	3144.142	8222	8292.209	4691.988	9137.69
Marianna 2624	H	1	10194.73	2364.069	52056.07	5074.923	4003.574	1120.512	1290.025	11864.38	14394.61	11997.05	2023.82	1705.238	857.5812	4217.644	1909.024	4549.624	2523.573	4752	3987.497	2364.805	6284.36
Marianna 2624	H	2	9786.945	2477.584	54138.31	4821.177	4381.111	1147.466	1251.324	14794.95	15488.6	11877.08	1882.153	2473.04	849.0054	4615.367	1953.314	4458.632	2761.546	4942	3637.395	2270.213	6981.924
Marianna 2624	H	3	9689.075	2264.459	55394.32	5988.409	3603.217	1185.715	1122.321	10858.28	17207.84	10197.49	1780.962	2225.736	882.9656	4420.155	2090.046	4035.472	2623.468	5280	3913.837	2766.822	6423.37
Marianna 2624	D+H	1	6056.785	4910.448	103239.2	13217.27	9605.597	2964.111	2665.237	20343.05	23525.66	16494.06	2923.677	4397.387	2182.581	2276.5	4268.645	5889.227	4633.128	8268	11973.16	7633.294	14505.64
Marianna 2624	D+H	2	5572.242	5254.18	105634.4	12159.89	9989.821	3189.383	2531.975	16527.94	26257.26	17792.14	2806.73	4487.129	2269.885	2117.145	4567.451	5771.443	4401.472	8955	12883.12	6717.299	13345.19
Marianna 2624	D+H	3	5814.513	4173.881	114595.6	13375.88	8645.037	2756.623	2309.668	16812.44	22355.22	14019.95	2572.836	4038.416	2837.356	1947.773	4012.527	6654.827	3845.496	9620	11254.77	6515.78	12039.68
Myrobalan 29C	C	1	11085.41	4654.849	12050.02	15416.63	14828.05	3652.081	3108.732	8474.556	12409.15	10711.65	1499.126	1196.256	603.9304	4426.208	1503.169	3391.153	1897.423	3406	2828.012	1545.624	4871.597
Myrobalan 29C	C	2	11984.56	4189.01	12532.02	14183.3	16226.34	3828.716	2953.296	8813.538	13352.24	10604.54	1394.187	1298.536	597.8911	3885.546	1538.042	3093.409	2076.35	3188	2579.713	1483.799	5412.344
Myrobalan 29C	C	3	11682	4656.622	12822.76	15601.62	13345.25	3396.435	2693.996	7755.914	14834.34	9104.905	1319.231	1272.566	621.8068	3987.574	1645.705	3475.649	1972.533	3066	2775.771	1808.38	4979.357
Myrobalan 29C	D	1	8356.339	7727.547	21337.48	21731.84	11203.97	4249.875	6829.478	11805.67	18270.93	14019.95	1905.804	3100.559	1534.813	3408.183	3112.165	4582.343	2891.351	5335	7862.592	2621.076	9578.801
Myrobalan 29C	D	2	8022.086	7528.475	21832.51	23905.02	11652.13	4391.537	6229.85	10567.82	19271.74	13635.96	1925.055	3038.548	1537.029	3320.979	3330.017	4490.696	3064.238	5304	7982.104	2839.499	8641.744
Myrobalan 29C	D	3	7941.865	7468.415	23684.6	25643.57	10083.57	4150.043	5941.646	11119.34	18254.49	12517.81	1764.634	2790.503	1480.102	3135.529	2925.435	4849.952	2848.213	5129	7390.837	3066.659	9333.084
Myrobalan 29C	H	1	9004.832	5913.794	19347.14	18796.01	13729.68	4254.129	4777.869	9756.755	15541.73	11590.57	1790.024	1845.552	1180.625	3634.148	2480.504	3832.002	2677.176	4806	6256.382	2426.922	8534.314
Myrobalan 29C	H	2	8914.784	5795.519	19996.12	17856.21	15024.39	3929.639	4634.533	8976.215	16870.55	11034.15	1646.822	1888.369	1298.688	3783.083	2232.454	3823.214	2506.427	4775	6748.759	2354.115	8363.628

Rootstock	Treatment	Block	Aspartate	Glutamate	Asparagine	Serine	Glutamine	Histidine	Glycine	Threonine	Arginine	Alanine	Tyrosine	Cystine	Valine	Methionine	Tryptophan	Phenylalanine	Isoleucine	Leucine	Lysine	Hydroxyproline	Sarcosine
Myrobalan 29C	H	3	8644.639	5889.832	20383.36	22179.29	12356.71	3956.34	4156.746	9785.018	16445.49	11545.46	1580.949	1660.997	1423.175	3480.437	2331.674	3746.749	2364.017	4621	5880.999	2542.444	7083.481
Myrobalan 29C	D+H	1	6597.631	7187.237	23897.97	23470.38	9797.242	4722.083	7375.837	12008.89	20392.4	14726.84	2165.687	3348.604	1850.128	2804.875	3361.138	4948.93	3483.555	6206	8491.6	4989.081	11244.68
Myrobalan 29C	D+H	2	6989.82	7284.131	24452.41	25817.42	10483.05	4705.264	6728.238	13454.4	20280.74	15885.84	2079.059	3281.632	1598.51	2608.534	3596.418	5178.048	3309.377	5777	9136.961	4390.391	10345.11
Myrobalan 29C	D+H	3	6293.726	7109.152	26526.75	27695.05	11471.6	4611.159	6416.978	14530.75	22635.57	14709.11	2005.266	3013.744	1998.138	2399.851	3159.47	5592.291	3225.514	5591	8460.149	4258.68	10411.74

Data S1b. Concentrations of organic acids in the leaf extracts (ng μL^{-1}).

Rootstock	Treatment	Block	Oxalic acid	Propionic acid	Tartaric acid	Butyric acid	Malonic acid	Malic acid	Lactic acid	Citric acid	Maleic acid	Fumaric acid	Succinic acid
GF 677	C	1	4.69102	7.340544	28.30954	45.68627	49.83247	18.16809	53.30383	88.96939	21.4151	19.19321	64.35418
GF 677	C	2	5.347763	6.60649	24.23296	35.27582	55.96698	19.9849	56.18224	80.07245	26.98303	23.03185	52.77042
GF 677	C	3	6.631226	7.340544	20.59802	38.83333	49.85241	17.10707	53.5248	96.08695	18.78768	24.67158	66.49073
GF 677	D	1	3.606768	9.102275	16.2648	51.65986	33.14196	14.76857	69.65514	50.8518	14.91086	16.9776	93.40176
GF 677	D	2	3.967445	9.008431	13.82508	53.88735	40.43319	12.64189	66.09675	52.16219	13.00743	13.92163	84.78737
GF 677	D	3	4.065811	11.10477	13.98773	52.03666	37.78183	14.86997	76.62065	50.1552	11.05632	15.34302	79.04397
GF 677	H	1	4.411518	8.148004	15.8922	47.72904	46.63915	15.38185	59.20687	54.91994	17.54218	20.5429	67.29156
GF 677	H	2	4.522887	8.107588	14.30298	47.2696	40.86263	16.86113	61.01827	61.18934	17.56039	20.55965	70.57498
GF 677	H	3	4.0986	7.38396	12.24335	47.01047	45.89293	18.54724	65.94791	55.07041	15.1956	18.88612	77.63247
GF 677	D+H	1	3.120768	14.55644	16.4119	58.89224	38.14582	10.92269	88.00537	43.46849	11.8422	12.95676	117.6862
GF 677	D+H	2	3.557676	17.75886	14.04858	63.95691	31.27957	12.01496	109.1267	45.76662	10.06587	15.54811	129.4548
GF 677	D+H	3	3.27888	15.98297	11.9413	72.91088	38.16107	10.2848	92.75766	39.12164	12.683	12.74945	93.2661
Garnem	C	1	11.57759	9.044284	19.58078	53.28846	117.4146	33.68895	65.67565	138.6404	33.28526	15.11276	75.06271
Garnem	C	2	9.080079	9.989359	17.6227	45.29519	140.8975	42.44808	81.43781	154.0449	38.25509	17.8961	61.55142
Garnem	C	3	9.988086	9.097777	15.08503	41.14572	115.536	46.69289	69.22214	144.1319	32.74636	14.87096	77.55479
Garnem	D	1	5.572649	17.40583	20.2211	97.5991	54.39991	16.48777	128.3932	75.39139	17.72415	31.209	161.7402
Garnem	D	2	4.383412	18.06299	17.30926	113.8585	65.27989	20.7746	134.5229	67.85225	15.17187	37.4508	132.6269
Garnem	D	3	5.435431	19.1116	14.71287	84.96902	53.52951	22.85206	135.3264	67.66686	14.79345	30.70966	167.11
Garnem	H	1	8.190144	11.21491	43.07138	60.69556	100.1099	28.6655	75.66266	133.4555	27.8344	18.13532	78.48888
Garnem	H	2	9.336764	13.68219	36.8691	55.13527	82.0901	31.53205	75.18061	120.1099	26.41687	23.98077	98.89598
Garnem	H	3	3.845098	11.09929	31.33874	62.8542	100.1499	26.99144	93.22396	126.2663	31.07867	28.77693	108.7856
Garnem	D+H	1	4.443899	21.23511	40.00879	114.8225	44.49328	13.45784	159.2075	61.79622	12.89609	38.56133	162.0854
Garnem	D+H	2	4.888289	22.3981	36.00791	129.7987	36.48449	14.80363	153.3561	62.6545	13.81274	51.67219	204.2277
Garnem	D+H	3	4.386418	27.32569	30.82277	130.7828	44.51108	12.67191	190.1616	56.38905	11.74083	62.00662	224.6504
Rootpac 20	C	1	15.83387	18.4799	37.57819	99.14293	136.9524	56.46507	133.6786	197.1193	62.32735	60.27044	135.4439
Rootpac 20	C	2	14.02921	16.63191	31.94146	90.22007	164.3428	52.30028	113.6268	189.7987	78.53246	72.32452	148.9882
Rootpac 20	C	3	12.95065	20.51269	32.31725	107.0365	134.7611	57.5303	147.0464	182.5178	62.34159	49.66398	151.6971
Rootpac 20	D	1	11.20109	27.5967	58.90575	124.8915	103.4099	39.20383	188.9501	123.6156	39.15017	39.31435	191.0947
Rootpac 20	D	2	11.18756	26.13762	50.42333	143.4289	109.9617	39.94554	182.8229	137.3506	40.57151	39.42487	194.917
Rootpac 20	D	3	10.36052	25.27369	42.85983	133.9289	96.45764	41.28677	185.0766	155.5727	41.92984	38.68532	188.6537
Rootpac 20	H	1	12.30632	22.25541	49.29483	113.8396	126.1096	41.50816	165.7457	164.8208	44.62074	44.97794	187.6823
Rootpac 20	H	2	12.76925	22.74632	44.36535	113.6513	117.6783	46.66535	175.5945	164.266	49.47746	41.04461	154.6961
Rootpac 20	H	3	12.84705	23.80475	37.97674	113.0229	126.1601	43.12421	155.3995	170.8188	51.10842	47.17722	170.6202
Rootpac 20	D+H	1	7.575524	33.66798	51.3931	152.545	76.57118	36.91433	234.2981	100.4296	38.19535	33.65658	204.181
Rootpac 20	D+H	2	9.39365	29.0418	43.68414	142.3764	93.41684	34.1213	217.7371	120.5155	32.46605	32.58253	257.268
Rootpac 20	D+H	3	9.469405	28.05379	44.19807	163.5089	87.29115	29.20783	201.1052	90.38664	33.27765	26.71768	282.9948
Rootpac 40	C	1	17.11563	32.07987	62.17366	106.4492	184.064	70.60537	200.0894	269.5141	92.34835	42.80626	184.0883
Rootpac 40	C	2	15.67837	32.78748	55.95629	122.2721	170.4296	77.66591	187.5994	242.8055	60.09972	42.12136	187.9982
Rootpac 40	C	3	15.41949	30.91275	47.89859	122.0699	150.9325	69.96929	190.972	242.5627	73.29234	39.57765	170.4522
Rootpac 40	D	1	13.64883	40.4379	66.93292	152.9228	121.0929	50.48289	242.7757	210.3525	44.91491	70.87357	214.7697
Rootpac 40	D	2	13.52587	37.71356	57.29458	143.8496	122.0368	48.58241	236.8053	210.8518	42.6275	58.40116	210.558
Rootpac 40	D	3	12.64385	39.77903	48.7004	155.3576	121.1413	56.75515	228.1019	199.0209	45.65406	57.12198	224.498
Rootpac 40	H	1	15.01371	36.43054	64.82013	142.6419	153.3867	63.60845	220.7052	227.1807	48.5081	48.26542	207.8685
Rootpac 40	H	2	14.23405	33.9422	55.09711	132.0539	142.0247	68.67373	222.0992	220.9132	56.66834	51.36752	206.7981
Rootpac 40	H	3	14.12018	35.60865	55.74531	134.1428	139.7523	56.03601	201.2845	218.5249	52.47068	52.89072	208.3122
Rootpac 40	D+H	1	12.29624	48.53042	69.01276	162.6118	114.0344	47.25078	282.8463	189.3173	38.17767	85.04828	262.4734
Rootpac 40	D+H	2	11.09109	44.15473	62.11149	163.8447	100.0301	40.44667	253.1931	158.1388	36.23338	76.54346	288.7207
Rootpac 40	D+H	3	11.38724	53.86877	53.16743	176.9523	99.29619	42.95526	313.9594	175.7098	41.23188	91.85215	231.9513
Rootpac R	C	1	15.51947	17.35496	84.4199	86.94282	125.5778	83.52211	111.2733	269.0996	86.18636	31.37576	229.5292

Rootstock	Treatment	Block	Oxalic acid	Propionic acid	Tartaric acid	Butyric acid	Malonic acid	Malic acid	Lactic acid	Citric acid	Maleic acid	Fumaric acid	Succinic acid
Rootpac R	C	2	15.64463	15.61946	72.26344	101.0685	126.5567	69.02654	115.1172	269.7383	88.59482	30.33845	289.2068
Rootpac R	C	3	17.23208	17.15807	61.42392	91.97237	125.6281	59.08671	130.9098	290.6276	70.67282	24.87753	318.1275
Rootpac R	D	1	9.352284	44.55892	81.75512	144.0793	103.735	36.03842	242.9921	144.1345	41.55377	49.5316	121.7665
Rootpac R	D	2	9.450073	47.26124	69.49185	131.1121	102.9738	39.64226	226.4713	175.8441	42.60777	50.337	133.9432
Rootpac R	D	3	10.77308	48.92569	70.3094	117.8863	102.8348	36.58986	230.5427	158.2597	50.12679	50.45222	136.3785
Rootpac R	H	1	12.19021	19.264	39.73993	116.5034	125.4082	52.24288	162.7297	224.7819	50.67533	42.04351	207.1462
Rootpac R	H	2	13.89684	21.27601	33.77894	115.2181	118.2579	57.46717	131.2336	242.1896	63.85092	46.54038	227.8608
Rootpac R	H	3	12.51571	25.95673	34.17634	114.3343	104.5069	49.19189	144.0008	202.3037	53.68579	36.70952	232.0038
Rootpac R	D+H	1	9.277466	58.28886	40.5326	153.208	71.14269	28.60192	293.0806	119.6698	37.535	56.75656	127.0633
Rootpac R	D+H	2	8.590975	52.51249	36.47934	164.2504	86.79408	30.23955	266.4369	143.6037	32.12996	60.40439	104.1919
Rootpac R	D+H	3	8.51	54.36188	31.22632	174.6571	81.10267	25.88506	285.873	107.7028	27.31046	68.67544	131.2818
Marianna 2624	C	1	13.27352	12.95146	48.96357	79.58153	121.8968	44.40294	107.3031	216.6576	59.10771	26.15383	151.7129
Marianna 2624	C	2	13.21866	11.65631	41.61903	90.72294	146.2762	48.84323	91.20763	194.9918	74.47571	21.44614	191.1583
Marianna 2624	C	3	11.64343	14.37612	42.10867	72.41919	119.9465	45.08237	118.0334	198.5443	48.46832	29.01715	210.2741
Marianna 2624	D	1	9.351064	23.73518	49.94022	119.306	82.98083	29.36864	145.7476	147.4451	37.30931	36.59668	148.2066
Marianna 2624	D	2	7.481827	22.85335	44.9462	120.8453	83.47027	31.89298	161.6929	132.7006	36.19667	35.38677	121.5294
Marianna 2624	D	3	9.218359	21.38304	38.47395	107.2766	94.59815	30.74778	161.2939	165.4536	34.83596	36.30611	153.1271
Marianna 2624	H	1	11.43077	19.24474	52.6568	90.18305	101.8337	32.30551	138.2804	183.8373	37.47638	30.25509	142.0284
Marianna 2624	H	2	11.52295	21.14046	45.07422	101.4101	101.2366	35.24042	137.0998	177.5882	43.78082	29.77101	156.2313
Marianna 2624	H	3	10.66021	20.81362	38.31309	99.23	101.793	37.25815	141.8359	176.9342	45.6078	31.64614	159.0719
Marianna 2624	D+H	1	5.542094	25.39261	27.98587	135.8895	56.01787	25.41139	200.4993	74.79362	31.85492	58.84747	108.7201
Marianna 2624	D+H	2	6.872197	31.98129	23.78799	137.7636	68.3418	21.75215	177.4233	89.75234	29.61056	42.81799	119.5921
Marianna 2624	D+H	3	6.927618	26.21417	24.06784	134.3904	63.86037	27.65351	171.4677	67.31426	29.68127	49.03956	121.7665
Myrobalan 29C	C	1	9.832234	13.99329	33.40744	65.75025	95.98175	37.31339	102.1123	135.411	42.21979	42.27548	132.3274
Myrobalan 29C	C	2	9.791603	14.36174	28.59677	71.01027	115.1781	41.04473	112.3769	121.8699	53.19694	50.73058	108.5084
Myrobalan 29C	C	3	8.821264	15.36463	24.30725	79.85047	94.44604	37.88434	107.6263	124.0902	34.62023	36.91206	136.7206
Myrobalan 29C	D	1	7.896454	17.07181	34.48138	95.15377	74.24448	24.67953	132.2081	103.512	24.67547	28.97997	126.8111
Myrobalan 29C	D	2	7.840697	17.71282	29.30918	93.94173	74.48673	26.80082	126.6192	110.5839	24.88283	26.08197	139.4922
Myrobalan 29C	D	3	7.113922	17.05474	29.65399	100.4401	74.21479	24.45719	132.5352	103.4085	23.03965	25.66466	142.0284
Myrobalan 29C	H	1	8.535518	15.95749	35.16917	92.82389	79.71387	29.6138	116.2589	110.9926	31.27201	31.54887	125.4241
Myrobalan 29C	H	2	8.624766	15.77646	31.65225	84.46974	80.15197	31.30937	113.3446	111.793	26.76884	31.29837	158.0343
Myrobalan 29C	H	3	8.467234	15.53255	27.09433	88.10534	80.18403	27.14749	119.4652	114.8983	26.64951	30.50583	135.458
Myrobalan 29C	D+H	1	6.926714	23.86663	37.08226	105.8192	60.85613	22.23381	145.429	92.15322	22.75352	23.76357	173.8377
Myrobalan 29C	D+H	2	6.240283	18.94971	31.74241	106.9996	65.72462	20.93536	140.5473	93.16081	21.1504	24.14997	170.6771
Myrobalan 29C	D+H	3	6.828414	19.56281	26.98105	108.4753	65.33924	23.23825	164.3436	82.9379	19.58371	25.01478	187.7448

Data S1c. Concentrations of phenolic compounds in the leaf extracts (μg L^{-1}).

Rootstock	Treatment	Block	Gallic acid	Vanillic acid	trans-Caffeic acid	trans-p-Coumaric acid	Ferulic acid	Caftaric acid	Catechin	Epicatechin	Quercetin	Rutin	Myricetin
GF 677	C	1	1.616011	1.913156	1.646536	1.740173	0.9987929	2.433668	2.512763	1.180186	0.6710855	0.2277584	5.35704
GF 677	C	2	1.282181	2.308609	2.330826	2.156693	1.107357	2.754758	2.544618	1.699164	0.688902	0.3006411	3.787871
GF 677	C	3	1.678538	2.341125	2.353025	2.171757	1.12907	2.972238	2.699778	2.390843	0.7601677	0.3461928	3.342237
GF 677	D	1	2.851606	4.314316	4.462118	3.52933	2.420349	3.044732	4.947051	2.978378	8.463243	9.732988	2.046411
GF 677	D	2	3.385712	4.533512	4.56058	3.716583	2.937587	3.45017	5.687299	3.534573	7.947267	8.621527	2.18157
GF 677	D	3	4.329924	6.956813	6.803309	5.897274	3.038212	4.472732	7.202029	1.870609	7.652632	6.978517	2.77831
GF 677	H	1	2.19	2.471187	2.391377	2.271798	1.778048	5.560995	2.969323	1.921625	1.171535	0.6012822	6.033094
GF 677	H	2	1.78914	2.594731	2.441818	2.302088	1.851317	5.766375	3.208827	1.99815	3.961229	0.5010685	6.115626
GF 677	H	3	1.873717	3.225691	3.516528	2.557006	1.990571	8.428603	3.355378	5.17653	5.164234	0.4008548	6.444045
GF 677	D+H	1	5.151333	7.128483	7.394293	6.030835	3.165139	8.811299	8.275208	5.463687	10.48495	10.54381	1.526505
GF 677	D+H	2	6.074741	7.657067	8.564654	6.933602	3.464862	9.115196	8.782576	6.514144	10.6887	10.1	1.828993
GF 677	D+H	3	5.184968	9.229244	9.205658	7.911515	3.519022	11.34436	9.857893	7.054176	10.11271	10.4	1.928155
Garnem	C	1	0.3817046	0.5707447	0.3636348	0.5566335	0.1485371	0.7548362	0.7734147	0.4201794	0.2144157	0.3246951	1.231462
Garnem	C	2	0.4242595	0.5821759	0.4274459	0.5761918	0.1535659	0.7664561	0.8724077	0.4639828	0.2215759	0.334074	2.011743
Garnem	C	3	0.4243218	0.6282131	0.4387462	0.5898894	0.159336	0.8029101	0.875504	0.4851012	0.2314981	0.3616973	2.039407
Garnem	D	1	1.996099	3.165466	2.062845	3.272935	1.276257	1.108711	3.58816	2.316824	1.958579	2.663729	0.3835724
Garnem	D	2	2.89824	4.606532	3.30086	4.710004	1.306531	3.144727	5.847829	3.787328	1.986538	2.650979	1.12207
Garnem	D	3	3.228048	4.746709	3.57937	5.175746	1.348992	3.180655	6.100926	4.227375	2.05486	1.600988	1.161249
Garnem	H	1	1.532054	0.8753637	0.9304112	0.7420439	0.398264	3.802919	2.906219	1.69	1.913886	1.566629	2.093846
Garnem	H	2	1.742023	2.56934	1.784219	2.627052	1.219382	5.522828	3.261686	1.932289	1.854735	1.509481	3.073149
Garnem	H	3	0.5448269	2.702801	1.975157	2.952002	1.245314	5.70255	3.479436	2.201831	0.2615475	0.7857987	3.810743
Garnem	D+H	1	3.581077	5.382223	3.619237	5.18436	1.366952	6.466079	6.110649	4.306507	2.609688	3.363171	0.3305065
Garnem	D+H	2	3.902777	5.413247	4.054074	5.564951	1.681111	7.4657	7.191443	4.430924	2.337787	3.318983	0.3180276
Garnem	D+H	3	4.170577	6.241218	4.220056	5.860477	1.731154	7.614644	8.698021	4.528168	2.117316	2.870388	0.2701531
Rootpac 20	C	1	0.1700004	0.1200608	0.32	5.75104	0.11	6.962966	7.140356	4.306173	0.11	0.13	2.456392
Rootpac 20	C	2	0.2100006	0.1800786	0.28	3.458912	0.18	5.988886	7.004459	3.678148	0.16	0.17	2.436964
Rootpac 20	C	3	0.2300009	0.1601187	0.35	4.285169	0.16	5.366592	5.303877	3.289521	0.14	0.11	1.7962
Rootpac 20	D	1	2.201658	2.884293	3.031636	1.134391	1.551337	4.532067	1.381139	0.9247364	1.067513	2.902855	0.3932919
Rootpac 20	D	2	2.587243	3.464354	3.159947	0.7079514	1.562909	4.249558	1.163825	0.763699	1.014472	2.606747	0.3222795
Rootpac 20	D	3	2.546557	3.53596	3.247142	0.8891099	1.58179	3.426498	1.947173	0.5996617	0.976619	2.44907	0.2786271
Rootpac 20	H	1	0.5427038	0.7684924	0.7675669	2.838303	0.4186902	1.493716	5.292998	2.630835	0.37523	0.7280385	1.318854
Rootpac 20	H	2	0.6896784	0.9035166	0.9496723	3.227295	0.4895876	1.073365	3.92928	2.559452	0.3059299	0.7671812	1.118898
Rootpac 20	H	3	0.9094139	1.217718	1.141368	3.216245	0.555998	0.9713523	3.715273	2.437954	0.2831413	0.9162693	1.028812
Rootpac 20	D+H	1	3.15098	4.015204	3.93053	0.28	1.852564	0.28	0.75	0.29	3.964434	3.886937	0.32
Rootpac 20	D+H	2	3.684143	5.065095	4.244395	0.2500677	2.087282	0.24	0.69	0.25	1.42543	3.599838	0.28
Rootpac 20	D+H	3	3.390107	5.624699	4.834045	0.22	2.520686	0.35	0.72	0.34	1.167062	3.504821	0.24
Rootpac 40	C	1	6.62401	10.01145	6.338629	10.107	1.935779	12.20177	12.72457	7.240162	3.118974	5.555683	4.367091
Rootpac 40	C	2	6.836145	10.48706	7.643901	10.87364	1.975285	13.16506	13.50046	9.060874	3.100317	5.695487	4.505729
Rootpac 40	C	3	7.286589	10.63477	7.7167	11.45398	2.14619	13.24061	13.50046	9.307988	3.03831	5.856895	4.644366
Rootpac 40	D	1	10.22772	12.48285	8.960836	12.90665	2.693258	13.48616	15.30293	10.95624	3.93636	8.534332	7.798376
Rootpac 40	D	2	9.989251	13.73657	9.938381	13.1339	2.726924	13.56837	18.2489	11.07898	3.97938	7.697633	7.245766
Rootpac 40	D	3	8.577296	14.4751	9.973471	13.59206	2.748223	14.63955	20.1731	11.86151	4.060043	7.368844	5.164535
Rootpac 40	H	1	7.631046	11.22559	8.007896	11.6067	2.188272	14.99661	14.14972	9.67866	3.511863	6.626658	5.01037
Rootpac 40	H	2	7.683827	11.66161	8.553525	12.09149	2.18999	17.66045	15.01251	10.25691	3.441626	6.512867	4.856205
Rootpac 40	H	3	8.190126	11.82586	8.634987	12.73683	2.232931	18.94485	15.01251	10.53664	3.182626	6.17792	4.738765
Rootpac 40	D+H	1	10.57271	15.27507	10.48306	14.60489	2.861587	19.63842	20.29277	11.88869	4.267667	9.490178	8.671794
Rootpac 40	D+H	2	11.49596	15.30792	11.16031	15.11437	2.919986	20.24543	22.43249	12.5414	4.142901	8.708634	8.83816
Rootpac 40	D+H	3	11.22792	16.09631	11.73055	15.45401	2.956437	21.06667	23.39881	13.42723	4.060592	8.559768	9.828034
Rootpac R	C	1	3.214845	4.98793	3.479401	5.447822	2.015597	5.80349	6.05215	3.907787	3.163589	2.642433	2.077106

Rootstock	Treatment	Block	Gallic acid	Vanillic acid	trans-Caffeic acid	trans-p-Coumaric acid	Ferulic acid	Caftaric acid	Catechin	Epicatechin	Quercetin	Rutin	Myricetin
Rootpac R	C	2	3.36682	5.339192	3.645086	5.520459	2.234683	6.414383	6.421183	4.063406	3.247578	2.785697	2.143046
Rootpac R	C	3	4.664682	7.265236	4.523817	6.946481	2.275345	9.629272	9.651791	4.991246	3.571277	4.071257	3.446282
Rootpac R	D	1	8.368616	9.563639	6.896068	10.30034	2.804309	10.01988	12.1407	9.277717	4.098667	6.922332	5.859691
Rootpac R	D	2	6.482731	10.09495	7.156297	10.43768	2.839363	9.340564	12.28	8.550053	4.143461	5.959225	4.674478
Rootpac R	D	3	6.789187	12.35303	7.936984	11.81106	2.979578	10.97281	16.41088	8.222604	4.22745	5.266992	4.176588
Rootpac R	H	1	4.953761	7.28086	5.080024	7.1888	2.278501	12.12785	10.6695	8.004305	3.583534	4.996118	4.124539
Rootpac R	H	2	5.072021	7.65584	5.339588	7.350346	2.522665	15.8817	11.12911	5.637172	3.66609	4.513785	4.051914
Rootpac R	H	3	6.08198	9.430811	6.831011	9.778457	2.782575	11.83909	11.44296	5.265276	4.016694	4.142061	3.92724
Rootpac R	D+H	1	8.887234	12.3796	8.881485	12.22307	3.102383	16.37259	18.14128	9.787082	4.676793	7.831505	6.515977
Rootpac R	D+H	2	9.099396	13.01718	8.912842	12.49775	3.141163	17.03673	18.92275	10.47836	4.583876	7.674759	7.012928
Rootpac R	D+H	3	9.406324	13.76611	9.368243	13.8975	3.296282	18.20632	21.0421	10.50238	4.534321	7.04272	7.947985
Marianna 2624	C	1	2.019895	3.174415	2.054885	3.576908	2.073255	3.492594	4.149467	2.240286	3.630208	1.870045	1.250022
Marianna 2624	C	2	2.152988	3.219125	2.074455	3.76781	2.115566	3.768325	4.402483	2.301385	3.608493	1.772871	1.289705
Marianna 2624	C	3	2.254766	3.397965	2.152736	3.818048	2.298609	3.860236	4.402483	2.393033	3.536323	1.681695	1.329388
Marianna 2624	D	1	2.951551	4.158036	2.671702	4.320423	2.862174	3.883765	5.950943	2.939459	4.631644	2.33006	2.074004
Marianna 2624	D	2	3.022013	4.381586	2.681135	4.471135	2.884529	4.190378	6.578423	2.932739	4.581572	2.583327	2.232182
Marianna 2624	D	3	3.123947	4.623736	2.818127	4.80431	2.920586	4.292582	6.617448	2.739259	4.489941	2.591026	2.306293
Marianna 2624	H	1	2.270361	3.529949	2.299416	3.977522	2.34368	5.05507	4.614207	2.708914	3.704293	2.230536	1.390024
Marianna 2624	H	2	2.419959	3.579667	2.321315	4.189805	2.345519	5.422712	4.895561	2.605168	4.005746	2.005877	1.434152
Marianna 2624	H	3	2.534357	3.778537	2.408912	4.245669	2.39151	5.621238	4.895561	2.536004	4.087496	1.971433	1.47828
Marianna 2624	D+H	1	3.317544	4.63368	2.989635	4.971902	2.943397	5.794986	7.315206	3.100842	4.821968	2.931329	2.813144
Marianna 2624	D+H	2	3.396742	4.872324	3.00019	5.08363	3.064812	6.030056	7.630323	3.31986	4.726167	2.872659	2.529806
Marianna 2624	D+H	3	3.511316	5.152652	3.153485	5.652997	3.127359	6.444024	8.484919	3.327468	4.725529	2.636088	2.482186
Myrobalan 29C	C	1	3.223992	4.85381	3.221868	5.469239	1.951331	5.34032	6.344705	3.929474	3.606577	3.067069	3.300877
Myrobalan 29C	C	2	3.436425	4.922174	3.252553	5.761137	2.163432	5.761924	6.731577	3.778984	3.416722	2.710793	3.202343
Myrobalan 29C	C	3	4.006814	5.195628	3.375291	5.837952	2.205853	5.902459	6.731577	3.678657	3.328359	2.571381	3.103809
Myrobalan 29C	D	1	4.270829	6.699625	4.749828	6.606104	2.768561	7.72941	7.938204	5.178208	3.777884	3.733841	2.791195
Myrobalan 29C	D	2	4.472723	6.784575	4.929066	6.724665	2.822846	7.798674	8.42224	5.38442	4.085326	3.936278	2.879805
Myrobalan 29C	D	3	3.564781	7.048102	5.264915	6.836549	2.825062	8.291549	8.42224	5.706111	4.1687	3.950013	2.968414
Myrobalan 29C	H	1	3.598875	6.338222	4.203771	6.047361	2.497133	8.414359	7.138672	5.040734	3.68018	3.357771	3.413098
Myrobalan 29C	H	2	3.79967	6.357808	4.418562	6.370113	2.548095	8.619587	7.573957	4.815696	3.702327	3.539819	3.868177
Myrobalan 29C	H	3	3.979291	6.427492	4.705018	6.455048	2.714896	8.672125	7.573957	4.497994	3.770176	3.562757	4.631081
Myrobalan 29C	D+H	1	4.711027	7.147372	5.315057	7.083566	2.880455	9.356767	9.099236	6.613901	4.672591	5.263366	1.911335
Myrobalan 29C	D+H	2	4.823492	7.544448	5.515625	7.178014	2.884576	9.584981	10.05868	6.095164	4.44763	4.453618	1.972012
Myrobalan 29C	D+H	3	5.513252	9.251875	6.11733	8.594727	3.517701	12.93972	13.12708	5.861732	4.359266	4.005052	2.032689

Code S1. Python script that reproduces all analyses in the article from Data S1 (analysis of variance and its factorial partition, additivity contrasts with Benjamini–Hochberg adjustment and the logarithmic-scale sensitivity analysis, mean separation, residual diagnostics, principal component analysis, pooled and residual correlations, and the recovery sensitivity analysis). To run it, save the listing as Code_S1_analysis.py, save Data S1a–S1c as DataS1a.csv, DataS1b.csv and DataS1c.csv, and run: python Code_S1_analysis.py DataS1a.csv DataS1b.csv DataS1c.csv. Requires Python 3 with numpy, pandas, scipy, statsmodels and openpyxl.

```
"""
Code S1. Analysis script for
"Non-Additivity of the Combined Drought and Heat-Shock Response in the Leaf Metabolite
Profile of Seven Prunus Rootstocks".

Input : the replicate-level concentrations of Data S1 (Supplementary Materials).
        Copy Data S1a (amino acids), Data S1b (organic acids) and Data S1c (phenolic
        compounds) into three comma-separated files with the column headers exactly as
        printed (Rootstock, Treatment, Block, compound names) and give them as arguments:
            python Code_S1_analysis.py DataS1a.csv DataS1b.csv DataS1c.csv
        A single file (CSV, or an .xlsx workbook with a sheet "Replicate_data") holding
        all 46 columns is also accepted.
Output: Code_S1_results.xlsx (ANOVA, factorial partition, additivity contrasts, mean separation,
        diagnostics, PCA, correlations, and the sensitivity of the additivity results to
        hypothetical treatment-dependent differences in extraction recovery)
Requires: Python 3, numpy, pandas, scipy, statsmodels, openpyxl
"""
import sys, itertools
from functools import lru_cache
import numpy as np, pandas as pd
from scipy import stats
import statsmodels.api as sm, statsmodels.formula.api as smf
from statsmodels.stats.multitest import multipletests

meta = ["Rootstock", "Treatment", "Block"]
def read_one(path):
    if path.lower().endswith((".xlsx", ".xls")):
        return pd.read_excel(path, sheet_name="Replicate_data")
    return pd.read_csv(path)
files = sys.argv[1:] or ["DataS1a.csv", "DataS1b.csv", "DataS1c.csv"]
df = read_one(files[0])
for f in files[1:]:
    df = df.merge(read_one(f), on=meta, how="inner")
df["Rootstock"] = df["Rootstock"].astype(str).str.strip(); df["Treatment"] = df["Treatment"].astype(str).str.strip()
assert len(df) == 84, "Data S1 should give 84 samples (7 rootstocks x 4 treatments x 3 blocks)"
compounds = [c for c in df.columns if c not in meta]
ROOT = list(dict.fromkeys(df.Rootstock)); TRT = ["C", "D", "H", "D+H"]
df["drought"] = df.Treatment.isin(["D", "D+H"]).astype(int)
df["heat"] = df.Treatment.isin(["H", "D+H"]).astype(int)
DFE, NREP = 54, 3

@lru_cache(maxsize=None)
def qcrit(prob, k, dfe):
    return float(stats.studentized_range.ppf(prob, k, dfe))

def letters(means, differ):
    """compact letter display for a range test; means sorted in descending order"""
    n, groups = len(means), []
    for i in range(n):
        j = i
        while j + 1 < n and not differ(i, j + 1):
            j += 1
        if not any(a <= i and j <= b for a, b in groups):
            groups.append((i, j))
    lab = [""] * n
```

```
    for k, (a, b) in enumerate(groups):
        for i in range(a, b + 1):
            lab[i] += chr(97 + k)
    return pd.Series(lab, index=means.index)

def duncan(means, mse, r, alpha=0.05):
    m = means.sort_values(ascending=False); v = m.values; se = np.sqrt(mse / r)
    def differ(i, j):
        p = j - i + 1
        return v[i] - v[j] > qcrit(round((1 - alpha) ** (p - 1), 12), p, DFE) * se
    return letters(m, differ)

def tukey(means, mse, r, alpha=0.05):
    m = means.sort_values(ascending=False); v = m.values; se = np.sqrt(mse / r)
    q = qcrit(1 - alpha, len(m), DFE)
    return letters(m, lambda i, j: v[i] - v[j] > q * se)

def fit(data, y, formula):
    d = data.rename(columns={y: "y"})
    f = smf.ols(formula, d).fit()
    return f, sm.stats.anova_lm(f, typ=2)

F1 = "y ~ C(Block) + C(Rootstock) * C(Treatment)"          # omnibus model (Table 1)
F2 = "y ~ C(Block) + C(Rootstock) * drought * heat"         # 2 x 2 factorial partition (Table 2)
cell = df.groupby(["Rootstock", "Treatment"])[compounds].mean()
anova_rows, contrast_rows, diag_rows, sep_rows, resid = [], [], [], [], {}
tcrit = stats.t.ppf(0.975, DFE)
for c in compounds:
    f, a = fit(df, c, F1); mse = f.mse_resid; resid[c] = f.resid.values
    _, b = fit(df, c, F2)
    g = lambda t, tab=b: (tab.loc[t, "F"], tab.loc[t, "PR(>F)"])
    anova_rows.append(dict(Compound=c,
        F_R=a.loc["C(Rootstock)", "F"], p_R=a.loc["C(Rootstock)", "PR(>F)"],
        F_T=a.loc["C(Treatment)", "F"], p_T=a.loc["C(Treatment)", "PR(>F)"],
        F_RxT=a.loc["C(Rootstock):C(Treatment)", "F"], p_RxT=a.loc["C(Rootstock):C(Treatment)", "PR(>F)"],
        CV_pct=100 * np.sqrt(mse) / df[c].mean(), MSE=mse,
        F_D=g("drought")[0], p_D=g("drought")[1], F_H=g("heat")[0], p_H=g("heat")[1],
        F_DxH=g("drought:heat")[0], p_DxH=g("drought:heat")[1],
        F_RxD=g("C(Rootstock):drought")[0], p_RxD=g("C(Rootstock):drought")[1],
        F_RxH=g("C(Rootstock):heat")[0], p_RxH=g("C(Rootstock):heat")[1],
        F_RxDxH=g("C(Rootstock):drought:heat")[0], p_RxDxH=g("C(Rootstock):drought:heat")[1]))
    # additivity contrast within each rootstock, arithmetic and ln scale
    dl = df.copy(); dl[c] = np.log(dl[c]); fl, _ = fit(dl, c, F1); cl = dl.groupby(["Rootstock", "Treatment"])[c].mean()
    se, sel = np.sqrt(4 * mse / NREP), np.sqrt(4 * fl.mse_resid / NREP)
    for r in ROOT:
        C_, D_, H_, DH_ = [cell.loc[(r, t), c] for t in TRT]
        I = DH_ - D_ - H_ + C_; t = I / se
        Il = cl[(r, "D+H")] - cl[(r, "D")] - cl[(r, "H")] + cl[(r, "C")]
        contrast_rows.append(dict(Compound=c, Rootstock=r, C=C_, D=D_, H=H_, DH=DH_, I=I, SE=se,
            CI_low=I - tcrit * se, CI_high=I + tcrit * se, I_over_C=I / C_, t=t, p=2 * stats.t.sf(abs(t), DFE),
            I_ln=Il, SE_ln=sel, p_ln=2 * stats.t.sf(abs(Il / sel), DFE)))
    # diagnostics
    sw = stats.shapiro(f.resid); lev = stats.levene(*[d[c].values for _, d in df.groupby(["Rootstock", "Treatment"])], center="median")
    sp = stats.spearmanr(np.abs(f.resid), f.fittedvalues)
    diag_rows.append(dict(Compound=c, Shapiro_W=sw.statistic, Shapiro_p=sw.pvalue, Levene_p=lev.pvalue,
        Spearman_absres_fitted=sp.correlation, Spearman_p=sp.pvalue, Shapiro_p_ln=stats.shapiro(fl.resid).pvalue,
        n_std_resid_gt3=int((np.abs(f.resid) / np.sqrt(mse) > 3).sum())))
    # mean separation of main-effect means
    mr, mt = df.groupby("Rootstock")[c].mean(), df.groupby("Treatment")[c].mean()
    row = dict(Compound=c)
    for nm, fun in (("Duncan", duncan), ("Tukey", tukey)):
        Lr, Lt = fun(mr, mse, 12), fun(mt, mse, 21)
        row.update({f"{nm}_{r}": Lr[r] for r in ROOT}); row.update({f"{nm}_{t}": Lt[t] for t in TRT})
```

```
    sep_rows.append(row)

A = pd.DataFrame(anova_rows)
for k in ("DxH", "RxDxH"):
    A[f"padj_{k}"] = multipletests(A[f"p_{k}"], method="fdr_bh")[1]
K = pd.DataFrame(contrast_rows)
K["p_adj"] = multipletests(K.p, method="fdr_bh")[1]          # Benjamini-Hochberg across the 301 contrasts
K["p_adj_ln"] = multipletests(K.p_ln, method="fdr_bh")[1]
K["Direction"] = np.where(K.p_adj < 0.05, np.where(K.I > 0, "synergistic", "antagonistic"), "additive (ns)")

# PCA of the 28 standardized rootstock x treatment means
X = cell[compounds].values; Z = (X - X.mean(0)) / X.std(0)
U, S, Vt = np.linalg.svd(Z, full_matrices=False)
expl = S ** 2 / (S ** 2).sum(); scores = U * S; load = Vt.T * (S / np.sqrt(len(Z) - 1))
for k in range(3):                                           # fix signs for reproducibility
    if load[:, k].sum() < 0:
        scores[:, k] *= -1; load[:, k] *= -1
PCs = pd.DataFrame(scores[:, :3], index=cell.index, columns=["PC1", "PC2", "PC3"]).reset_index()
PCl = pd.DataFrame(load[:, :3], index=compounds, columns=["PC1", "PC2", "PC3"]).reset_index(names="Compound")
# correlations: pooled and among model residuals
Cpool = df[compounds].corr(); Cres = pd.DataFrame(resid)[compounds].corr()

sig = K[K.p_adj < 0.05]
print("Significant contrasts (BH):", len(sig), "| synergistic", (sig.I > 0).sum(), "| antagonistic", (sig.I < 0).sum())
print("Unadjusted:", (K.p < 0.05).sum(), "| ln scale (BH):", (K.p_adj_ln < 0.05).sum(),
      "positive", ((K.p_adj_ln < 0.05) & (K.I_ln > 0)).sum(), "negative", ((K.p_adj_ln < 0.05) & (K.I_ln < 0)).sum())
print("D x H significant:", (A.p_DxH < 0.05).sum(), "| R x D x H significant:", (A.p_RxDxH < 0.05).sum())
print("PCA variance explained (%):", np.round(100 * expl[:3], 1))
with pd.ExcelWriter("Code_S1_results.xlsx") as w:
    A.to_excel(w, "ANOVA_partition", index=False); K.to_excel(w, "Contrasts", index=False)
    pd.DataFrame(sep_rows).to_excel(w, "Mean_separation", index=False); pd.DataFrame(diag_rows).to_excel(w, "Diagnostics", index=False)
    PCs.to_excel(w, "PCA_scores", index=False); PCl.to_excel(w, "PCA_loadings", index=False)
    Cpool.to_excel(w, "Corr_pooled"); Cres.to_excel(w, "Corr_residual")

# ---------------------------------------------------------------------------
# Sensitivity of the additivity results to treatment-dependent extraction
# recovery (added in revision). Observed concentrations are divided by a
# hypothetical recovery ratio applied to (i) the drought-exposed treatments
# (D, D+H), (ii) the heat-exposed treatments (H, D+H) or (iii) D+H alone,
# over 601 ratios between 0.5 and 2 (log-spaced). For each ratio the 301
# contrasts, the Benjamini-Hochberg adjustment and the R x D x H and D x H
# tests are recomputed with the same balanced RCBD error term as above.
# ---------------------------------------------------------------------------
TI = {t: i for i, t in enumerate(TRT)}
Y = np.zeros((len(compounds), len(ROOT), 4, NREP))
for _, row in df.iterrows():
    Y[:, ROOT.index(row.Rootstock), TI[row.Treatment], int(row.Block) - 1] = row[compounds].values.astype(float)

def contrasts_fast(Yc):
    X = Yc.reshape(len(compounds), len(ROOT) * 4, NREP)
    cm, bm, g = X.mean(2), X.mean(1), X.mean((1, 2))
    res = X - cm[:, :, None] - bm[:, None, :] + g[:, None, None]
    mse = (res ** 2).sum((1, 2)) / DFE
    Mc = cm.reshape(len(compounds), len(ROOT), 4)
    I = Mc[:, :, 3] - Mc[:, :, 1] - Mc[:, :, 2] + Mc[:, :, 0]
    p = 2 * stats.t.sf(np.abs(I / np.sqrt(4 * mse / NREP)[:, None]), DFE)
    q = multipletests(p.ravel(), method="fdr_bh")[1].reshape(p.shape)
    Ibar = I.mean(1)
    p_rdh = stats.f.sf((NREP * ((I - Ibar[:, None]) ** 2).sum(1) / 4 / (len(ROOT) - 1)) / mse, len(ROOT) - 1, DFE)
    p_dh = stats.f.sf((len(ROOT) * NREP * Ibar ** 2 / 4) / mse, 1, DFE)
    return I, q, p_rdh, p_dh
```

```
I0, q0, _, _ = contrasts_fast(Y)
sig0, sgn0 = q0 < 0.05, np.sign(I0)
grid = np.exp(np.linspace(np.log(0.5), np.log(2.0), 601)); grid[300] = 1.0
scen = {"drought_exposed": (1, 1, 0, 1), "heat_exposed": (0, 0, 1, 1), "combined_only": (0, 0, 0, 1)}
srows, keep = [], {}
for name, use in scen.items():
    keep[name] = []
    for r in grid:
        fac = np.array([1.0, r if use[1] else 1.0, r if use[2] else 1.0, r if use[3] else 1.0])
        I, q, p_rdh, p_dh = contrasts_fast(Y / fac[None, None, :, None])
        s = q < 0.05
        kept = s & sig0 & (np.sign(I) == sgn0)
        keep[name].append(kept[sig0])
        srows.append(dict(Scenario=name, Recovery_ratio=r, Significant=int(s.sum()), Synergistic=int((s & (I > 0)).sum()),
                          Antagonistic=int((s & (I < 0)).sum()), Original_retained=int(kept.sum()),
                          Original_reversed=int((s & sig0 & (np.sign(I) != sgn0)).sum()),
                          RxDxH_significant=int((p_rdh < 0.05).sum()), DxH_significant=int((p_dh < 0.05).sum())))
SENS = pd.DataFrame(srows)
ci, ri = np.where(sig0)
TIP = pd.DataFrame({"Compound": [compounds[c] for c in ci], "Rootstock": [ROOT[r] for r in ri]})
for name in scen:
    kp = np.array(keep[name])
    lo, hi = [], []
    for j in range(kp.shape[1]):
        bad = np.where(~kp[:, j])[0]
        lo.append(grid[bad[bad < 300].max()] if (bad < 300).any() else 0.5)
        hi.append(grid[bad[bad > 300].min()] if (bad > 300).any() else 2.0)
    TIP[name + "_lower"], TIP[name + "_upper"] = lo, hi
print("Recovery sensitivity at ratio 1.25 (drought-exposed):",
      SENS[(SENS.Scenario == "drought_exposed") & (np.isclose(SENS.Recovery_ratio, 1.25, atol=0.003))].iloc[0].to_dict())
with pd.ExcelWriter("Code_S1_results.xlsx", mode="a", engine="openpyxl") as w:
    SENS.to_excel(w, "Recovery_sensitivity", index=False); TIP.to_excel(w, "Recovery_tipping", index=False)
```