Supporting information
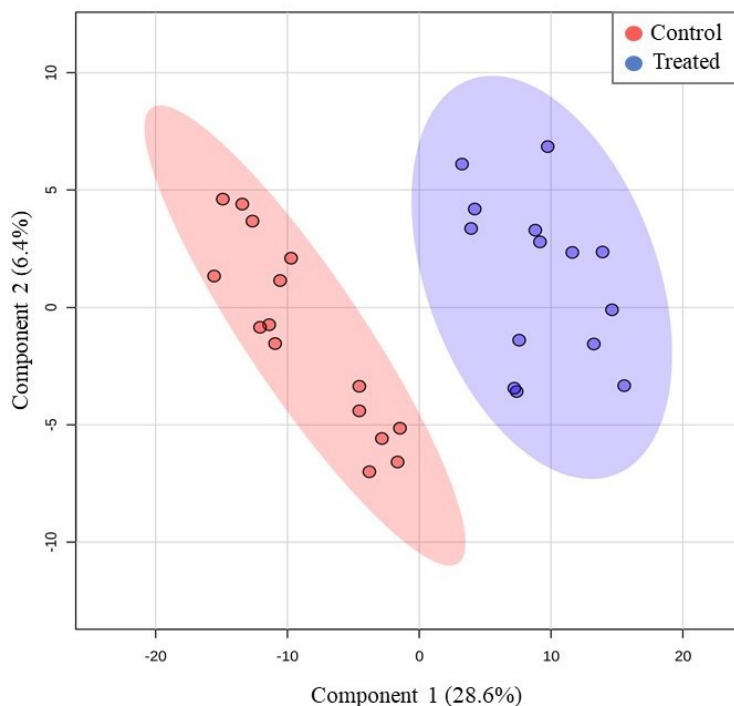
Table A.1. MZmine parameters used in pre-processing MS data analysis.

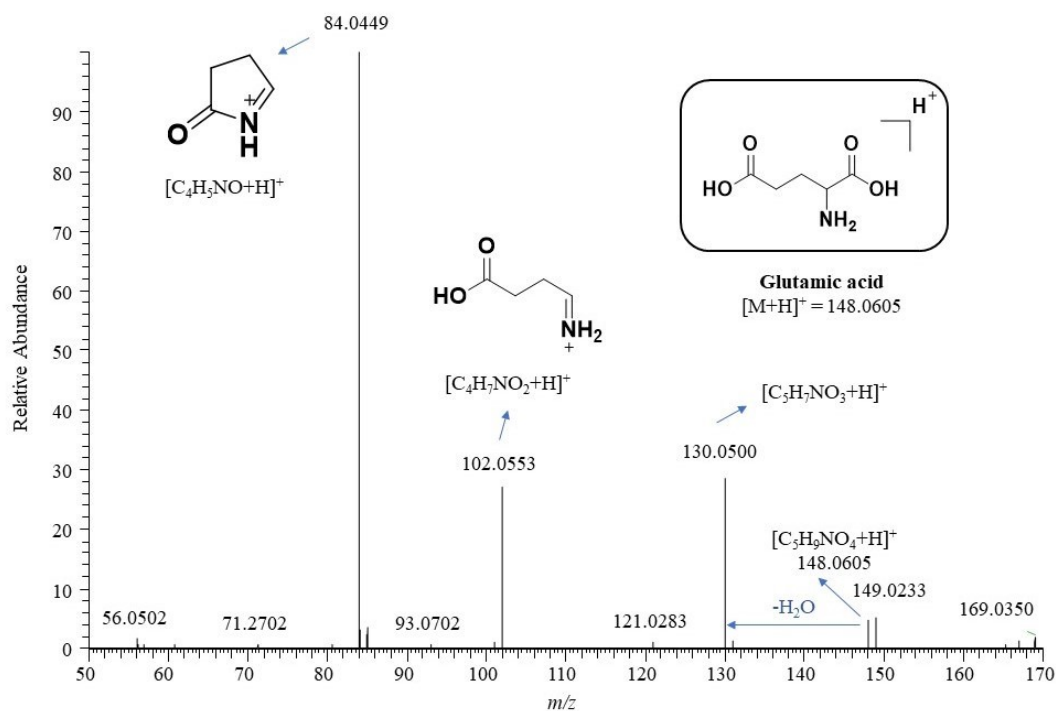| Method	Parameters	Value
Mass detection MS^1	Mass detector	Centroid
	Noise level	$1E^7$
Mass detection MS^2	Noise level	$1E^3$
Chromatogram building (ADAP Chromatogram builder)	Min. group size in # of scans	4
	Group intensity threshold	$3E^7$
	Min. highest intensity	$3E^7$
	m/z tolerance	10 ppm
Chromatogram deconvolution (Local minimum search algorithm)	Chromatographic threshold	10%
	Search min. in RT range	0.01 min
	Min. relative height	10%
	Min. absolute height	$3E^7$
	Min. ratio of peak top/edge	2
	Peak duration range	0.05 - 2.00 min
	m/z range for MS2 scan pairing	0.01 Da
	RT range for MS2 scan pairing	0.02 min
Isotope grouping (Isotopic peaks grouper)	*m/z* tolerance	10 ppm
	Retention time tolerance	0.02 min
	Maximum charge	2
Feature alignment (Join aligner)	*m/z* tolerance	10 ppm
	Weight for *m/z*	75
	Retention time tolerance	0.05 min
	Weight for RT	25
Isotope filter and others (Feature list rows filter)	Min. peaks in a row	2
	Keep only peaks with MS2 scan	Selected
Gap filling (Peak finder)	Intensity tolerance	10%
	m/z tolerance	10 ppm
	Retention time tolerance	0.05 min

Table A.2. Features detected in Vorax™ data using MZmine 2.53 according to parameters shown in Table A.1.

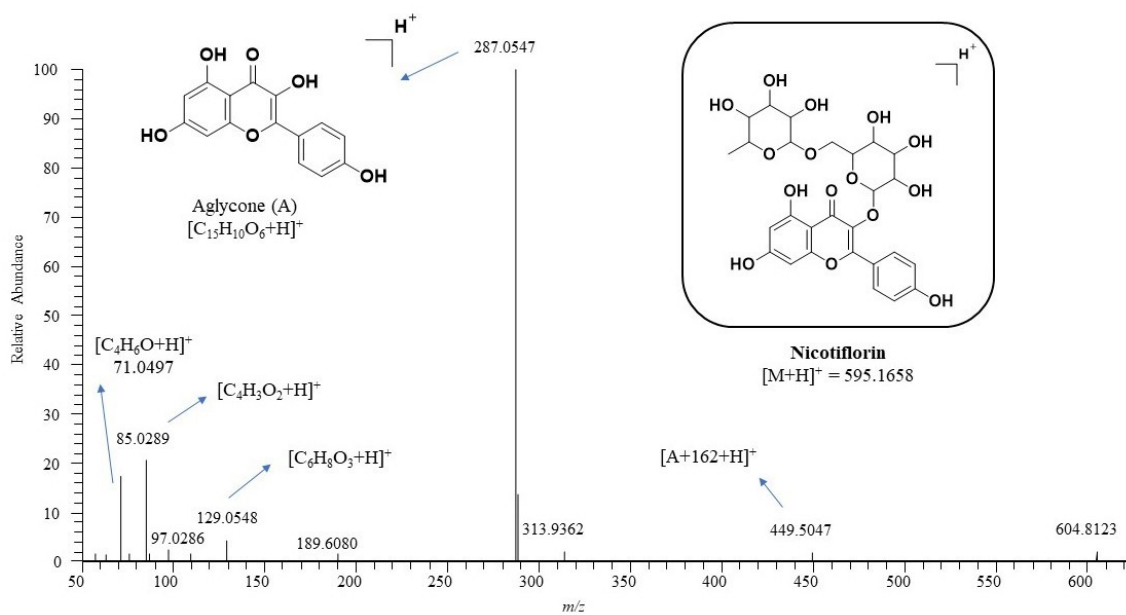| Sample Label	V1_25.mzXML Vorax 25 min	V2_25.mzXML Vorax 25 min	V1_30.mzXML Vorax 30 min	V2_30.mzXML Vorax 30 min
1/111.0204mz/18.81min	4.64E+08	4.53E+08	287630.3998	215932.7659
2/154.9902mz/18.92min	6.82E+08	7.05E+08	8425.767673	6454.069045
3/110.0202mz/18.90min	7.26E+08	7.24E+08	20964.2658	9543.340144
4/113.9637mz/18.92min	5.03E+08	4.84E+08	3402.150537	1822.245117
5/139.9880mz/18.81min	2.12E+08	2.06E+08	112757.5261	66297.10008
6/102.0340mz/18.84min	2.03E+08	2.08E+08	NA	NA
7/112.0181mz/18.80min	1.60E+08	1.63E+08	86959.79605	91130.41563
8/149.0234mz/18.80min	5.76E+08	5.98E+08	2058551.385	1563215.175
9/279.1590mz/18.79min	5.53E+08	5.89E+08	3872478.106	6534015.295
10/111.0204mz/22.35min	51679.53852	30781.27165	7.87E+08	8.39E+08
11/110.0202mz/22.50min	163931.3796	147936.5471	1.13E+09	1.14E+09
12/154.9903mz/22.50min	318126.9205	482037.643	1.16E+09	1.16E+09
13/139.9881mz/22.36min	8169.156328	18785.8942	3.60E+08	3.69E+08
14/113.9637mz/22.50min	1824060.092	574990.6511	7.11E+08	7.25E+08
15/102.0340mz/22.43min	110795.6055	191195.5768	3.40E+08	3.61E+08
16/112.0181mz/22.35min	9182.209292	33141.90933	2.85E+08	2.93E+08
17/123.0405mz/22.36min	144313.1498	225371.2682	2.33E+08	2.41E+08
18/149.0234mz/22.40min	2.69E+07	2.76E+07	4.70E+08	1.83E+08
19/279.1591mz/22.22min	7.97E+07	1.77E+07	3.56E+08	1.28E+09
20/149.0234mz/22.27min	4.63E+07	3.53E+07	2.41E+08	2.96E+08
21/279.1590mz/22.27min	5.73E+07	1.45E+07	2.32E+08	3.92E+08
22/536.1649mz/16.53min	61532.91271	41737.55105	38567.2023	108063.4168
23/148.0606mz/0.80min	4.11E+08	3.86E+08	3.81E+08	3.35E+08
24/118.0863mz/0.84min	1.03E+08	3.61E+08	2.42E+08	2.09E+08
25/104.1071mz/0.77min	2.63E+08	2.84E+08	2.25E+08	2.20E+08
26/199.1078mz/1.45min	1.17E+08	1.23E+08	1.53E+08	1.14E+08
27/247.1289mz/1.50min	1.64E+08	8.94E+07	1.22E+08	9.22E+07
28/213.1232mz/2.16min	1.48E+08	1.19E+08	1.33E+08	1.39E+08
29/149.0234mz/22.37min	2.69E+07	4.19E+07	1.28E+09	1.89E+08
30/279.1590mz/22.36min	1.69E+07	1.45E+07	1.25E+09	2.23E+08
31/132.1020mz/1.15min	3.67E+08	3.26E+08	2.98E+08	4.04E+08
32/130.0500mz/0.98min	1.99E+08	2.13E+08	3.82E+07	1.18E+08
33/118.0863mz/0.89min	1.79E+08	1.39E+08	8.41E+07	1.11E+08
34/116.0707mz/0.80min	2.74E+08	2.07E+08	2.57E+08	2.40E+08
35/148.0605mz/0.89min	1.14E+08	9.49E+07	5.64E+07	4.28E+07
36/130.0501mz/0.90min	2.91E+08	2.84E+08	9.32E+07	3.06E+08
37/149.0234mz/22.25min	5.83E+07	3.18E+07	3.48E+08	1.35E+09
38/279.1591mz/6.14min	2.45E+07	1.65E+07	5.25E+07	5.78E+08
39/156.9907mz/22.36min	8447.341162	14201.04281	1.89E+08	1.62E+08
40/149.0235mz/6.08min	4.27E+07	6.62E+07	2.17E+07	3.46E+08
41/149.0234mz/4.72min	3.10E+07	2.37E+07	2.14E+07	6.83E+07
42/149.0235mz/5.34min	1.07E+07	3.39E+07	4.69E+07	3.30E+08

Fig S1. PLS-DA scores plot of leaf extracts from non-treated (C) and Vorax^{TM}-treated (T) samples with 35% of the total variance (28.6% for Component 1 and 6.4% for Component 2). The data were acquired by UHPLC-MS/MS, positive mode, with n = 5 (three repetitions).
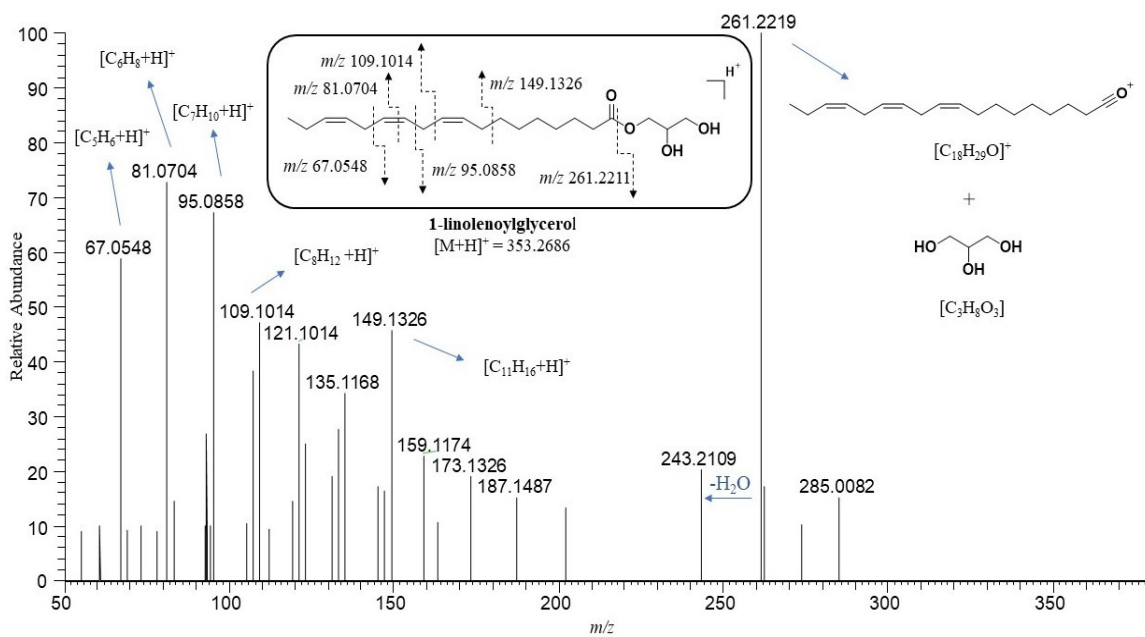

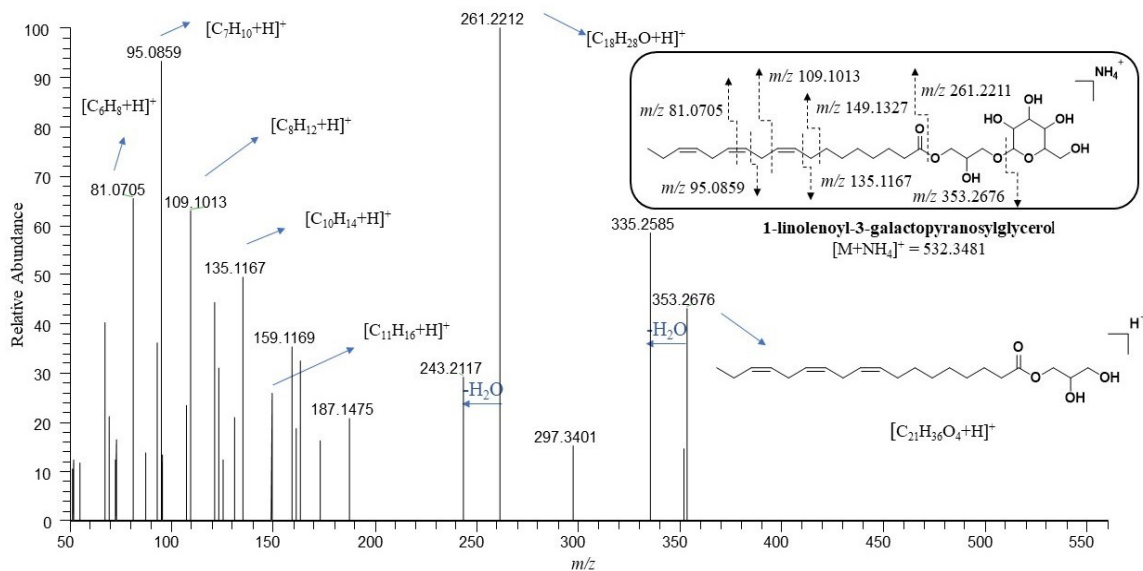**Fig S2.** MS/MS spectra of *m/z* 148.0605 [M+H]$^+$ annotated as Glutamic acid.

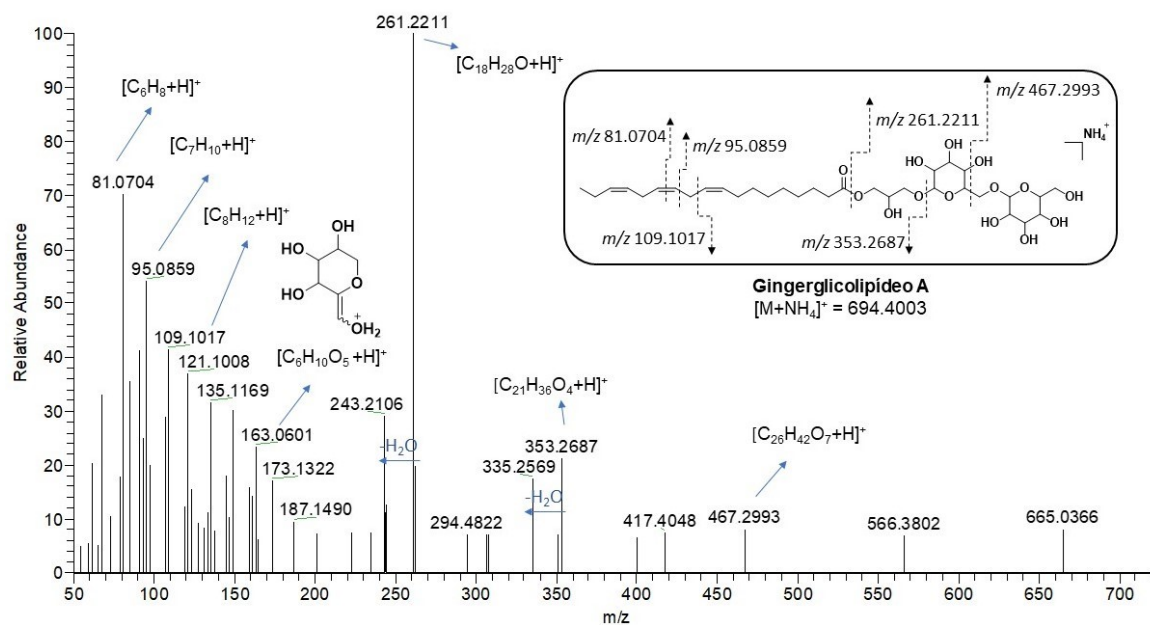**Fig S3.** MS/MS spectra of *m/z* 595.1658 [M+H]$^+$ annotated as Nicotiflorin.

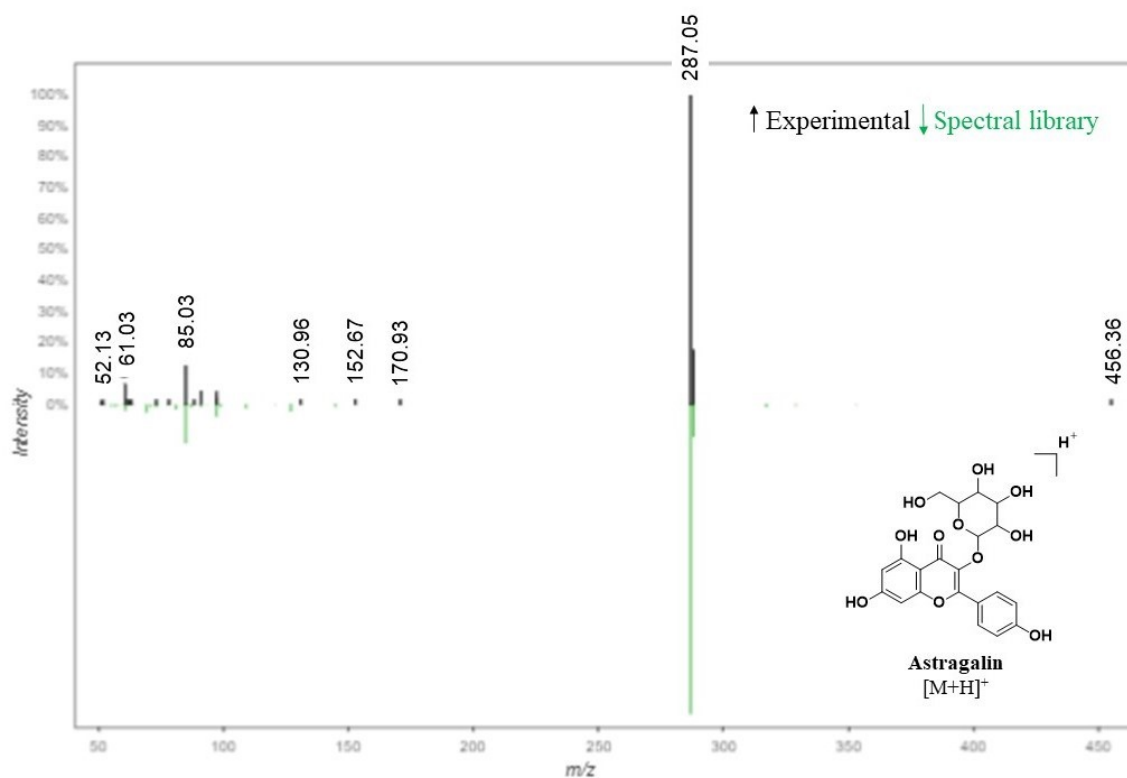**Fig S4.** MS/MS spectra of *m/z* 353.2687 [M+H]$^+$ annotated as 1-linolenoylglycerol.

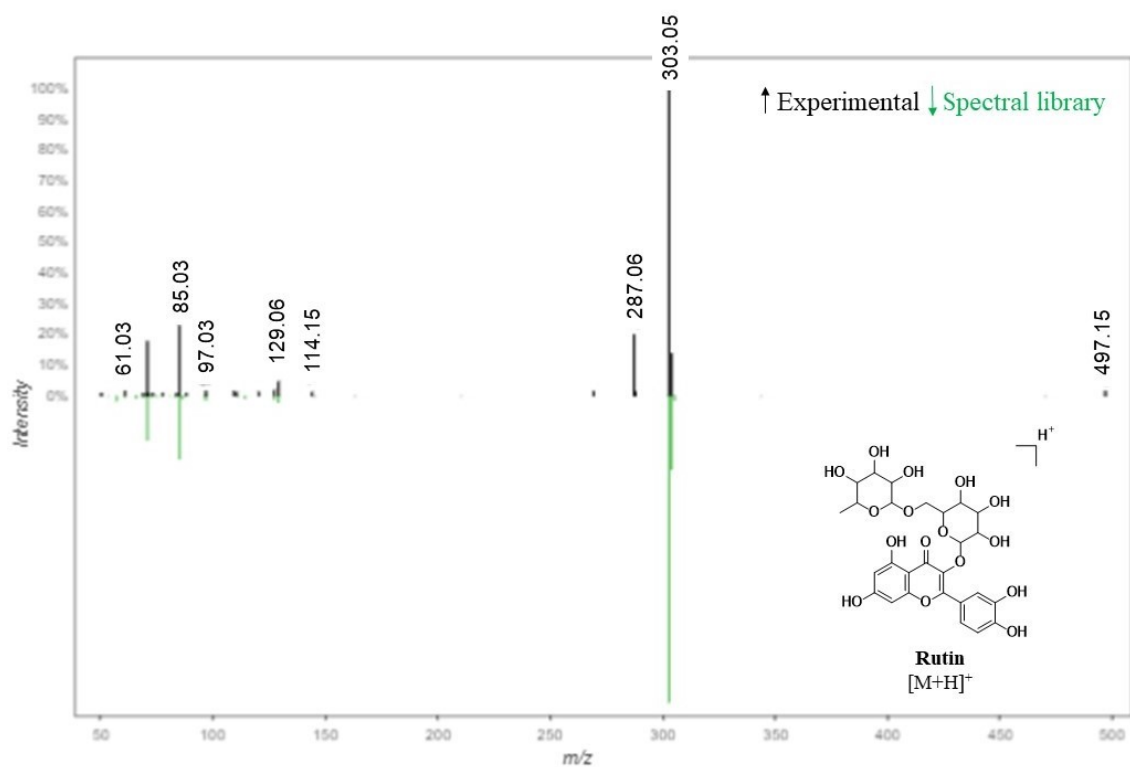**Fig S5.** MS/MS spectra of *m/z* 532.3482 [M+NH₄]⁺ annotated as 1-linolenoyl-3-galactopyranosyl- glycerol.

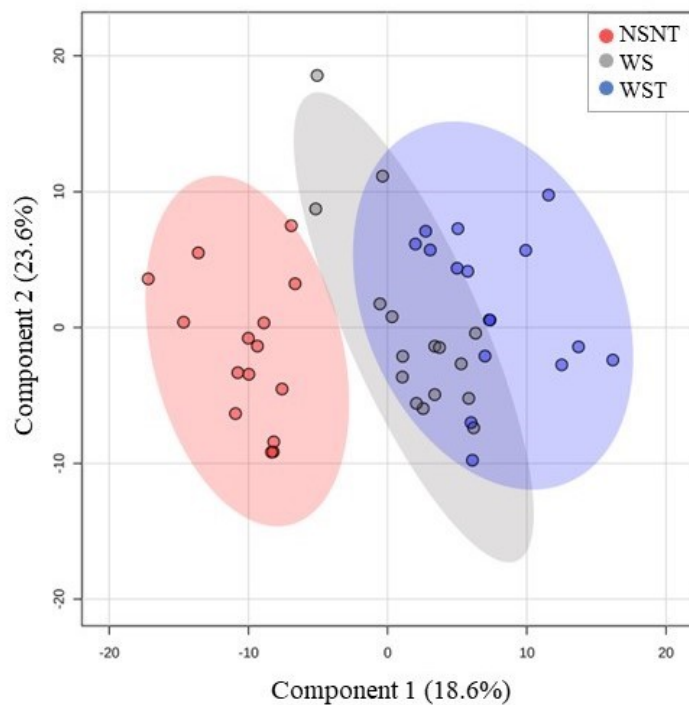**Fig S6.** MS/MS spectra of *m/z* 694.4003 [M+NH₄]⁺ annotated as gingerglycolipid A.

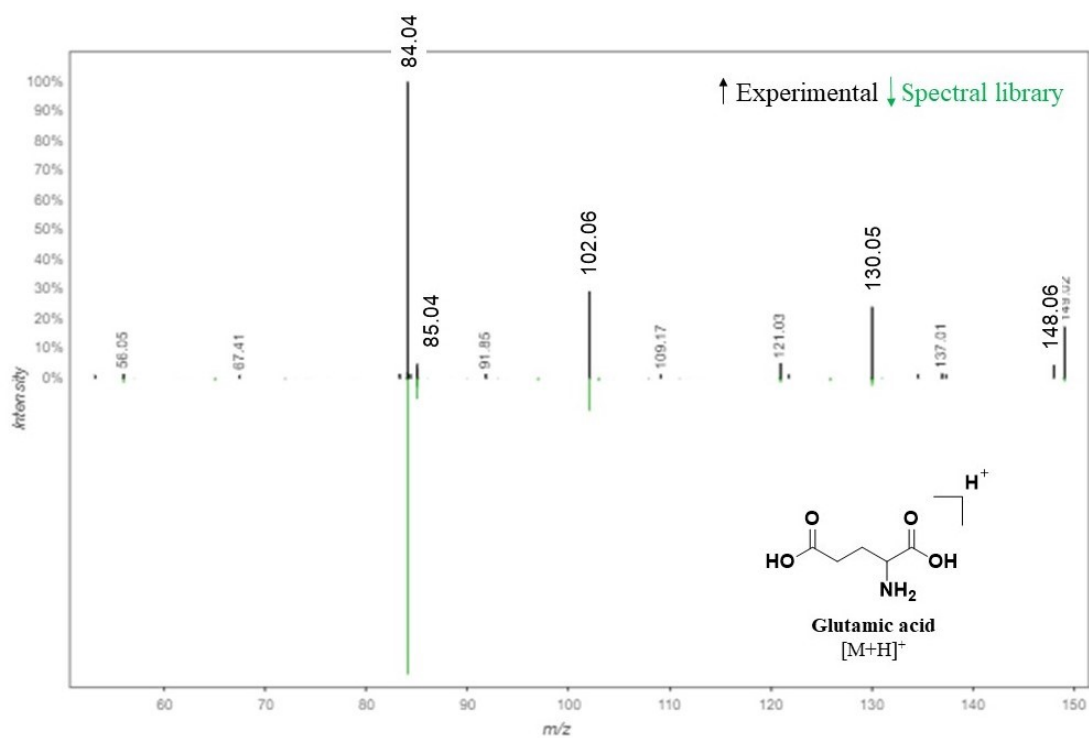**Fig S7.** Mirror match obtained from GNPS for astragalin annotation (*m/z* 449.1078), cos = 0.92.

Fig S8. Mirror match obtained from GNPS for rutin annotation (*m/z* 611.1598), cos = 0.90.
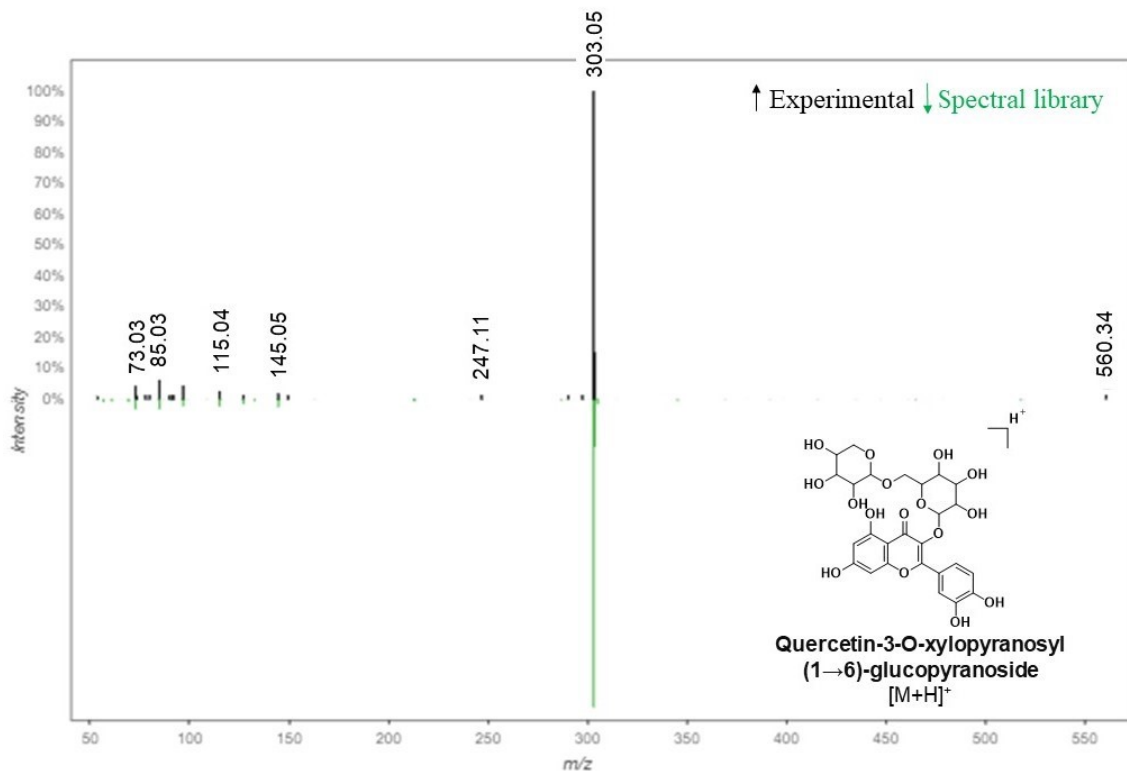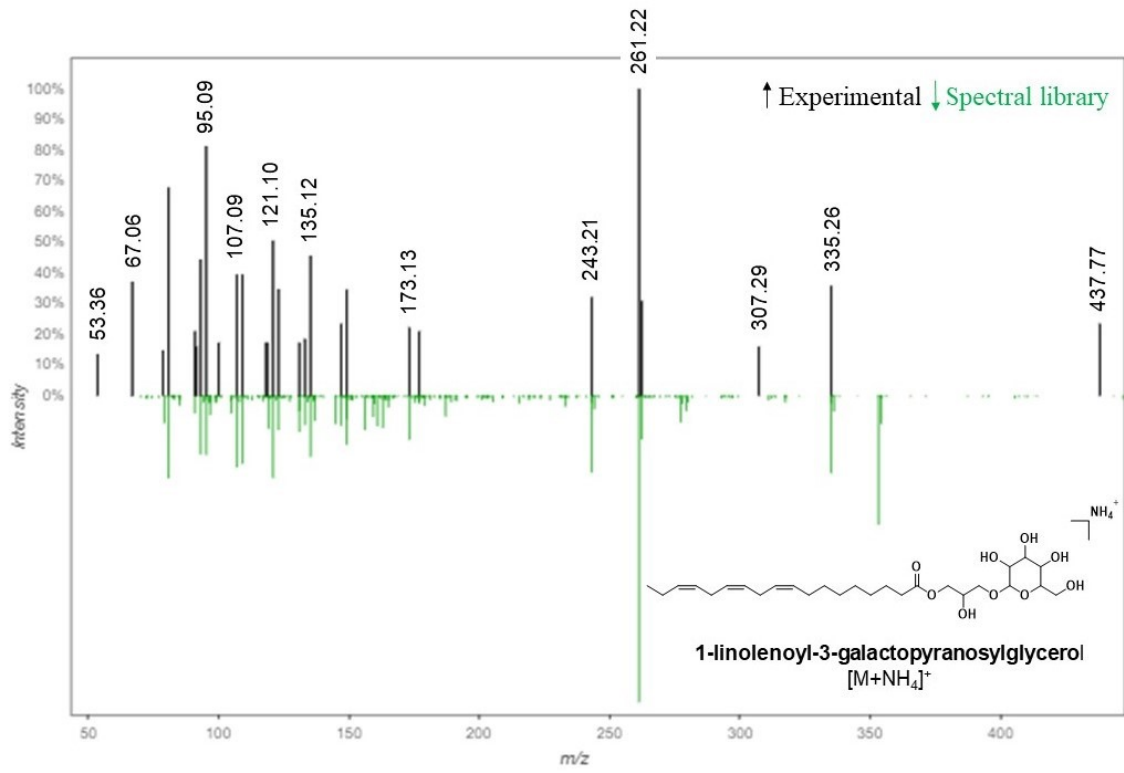
Fig S9. PLS-DA scores plot of leaf extracts from WST, WS and NSNT samples with 42.2% of the overall variance (18.6% for Component 1 and 23.6% for Component 2). The data were acquired by UHPLC-MS/MS, positive mode, with n = 8 (two repetitions).
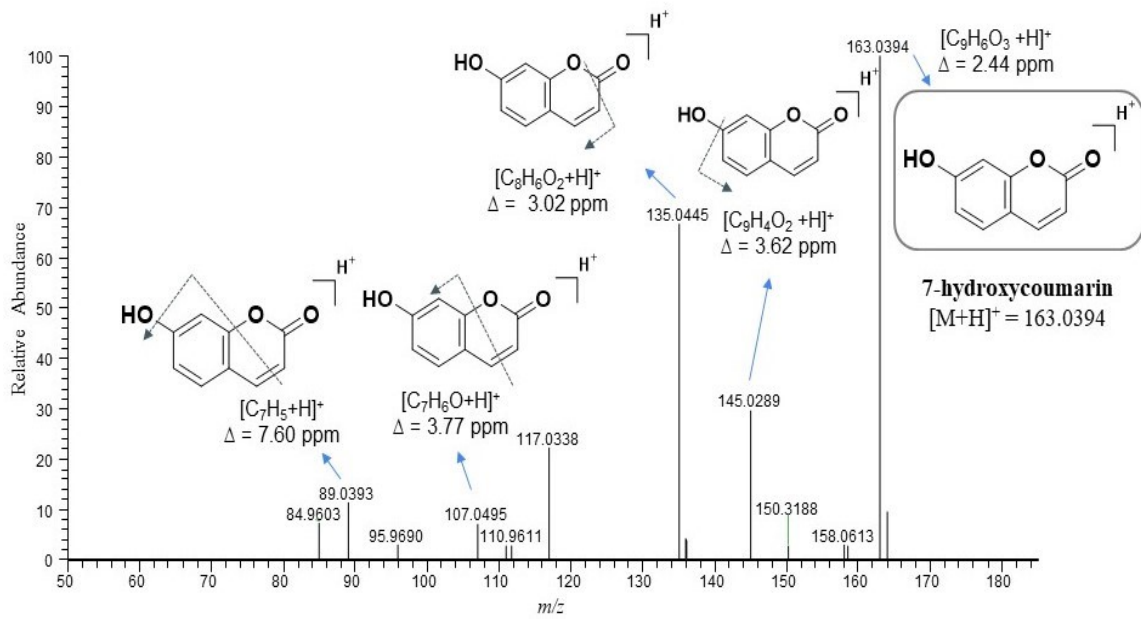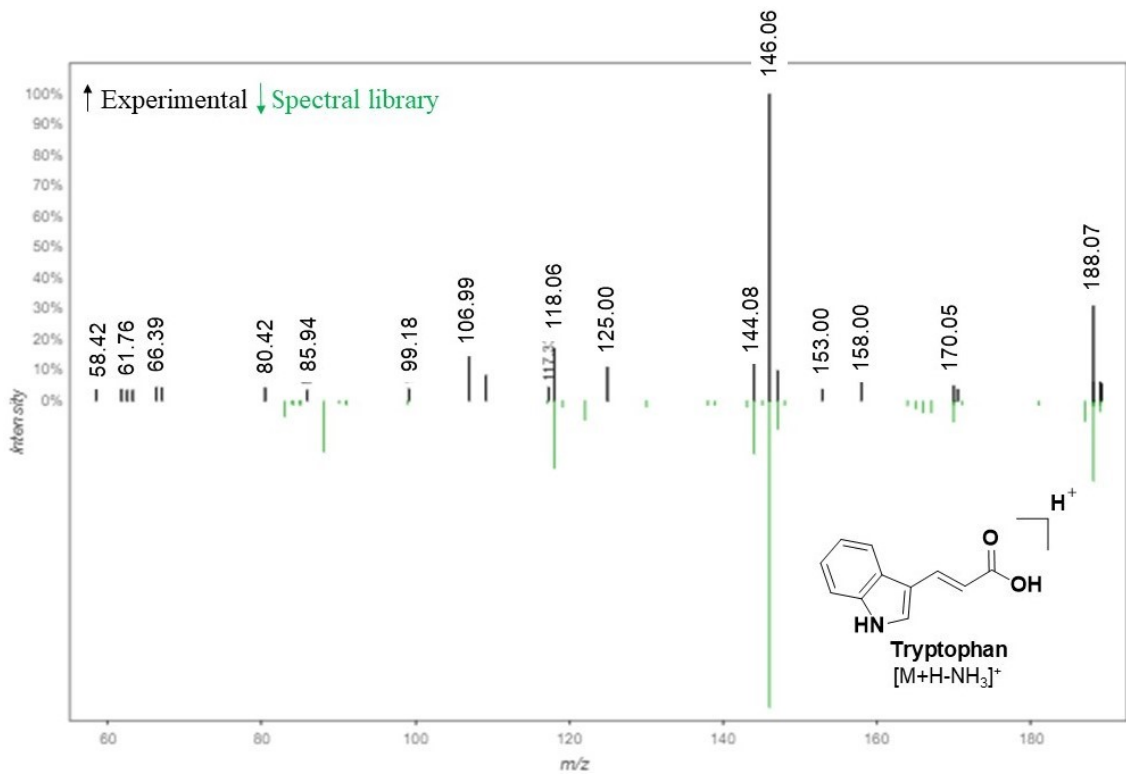

Fig S10. Annotation level 2 of differential metabolites obtained by the analysis of the VIP scores in the water stress assay.

↑ Experimental ↓ Spectral library

1-linolenoyl-3-galactopyranosylglycerol
[M+NH₄]⁺

↑ Experimental ↓ Spectral library

Quercetin-3-O-xylopyranosyl
(1→6)-glucopyranoside
[M+H]⁺

↑ Experimental ↓ Spectral library

Tryptophan
[M+H-NH₃]⁺

58.42 61.76 66.39 80.42 85.94 99.18 106.99 118.06 125.00 144.08 146.06 153.00 158.00 170.05 188.07

Intensity

m/z

$[C_9H_6O_3 +H]^+$
Δ = 2.44 ppm

7-hydroxycoumarin
$[M+H]^+ = 163.0394$

$[C_8H_6O_2+H]^+$
Δ = 3.02 ppm

$[C_9H_4O_2 +H]^+$
Δ = 3.62 ppm

$[C_7H_5+H]^+$
Δ = 7.60 ppm

$[C_7H_6O+H]^+$
Δ = 3.77 ppm

163.0394
135.0445
145.0289
117.0338
89.0393
84.9603
95.9690
107.0495
110.9611
150.3188
158.0613
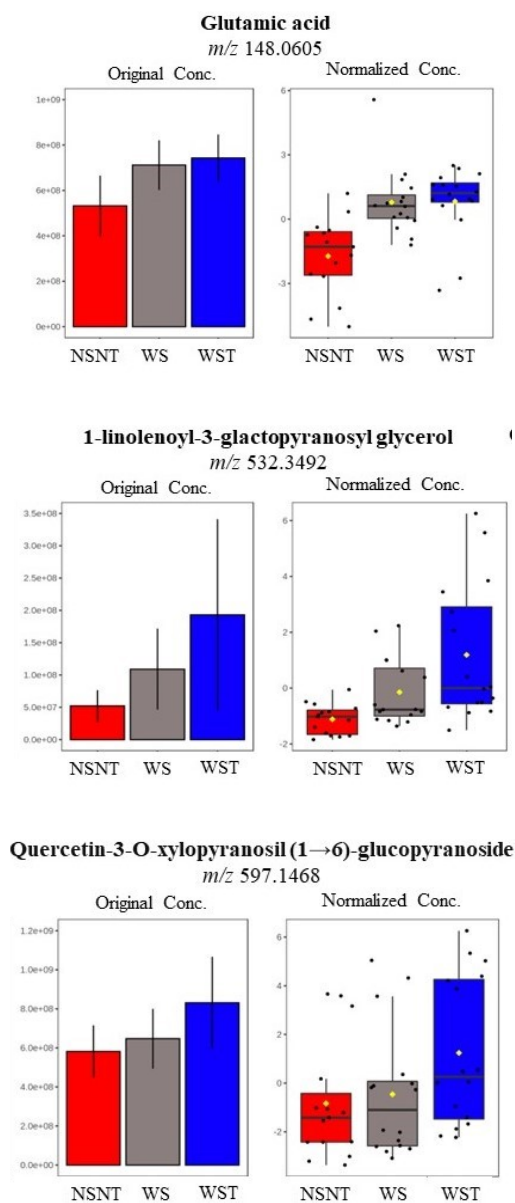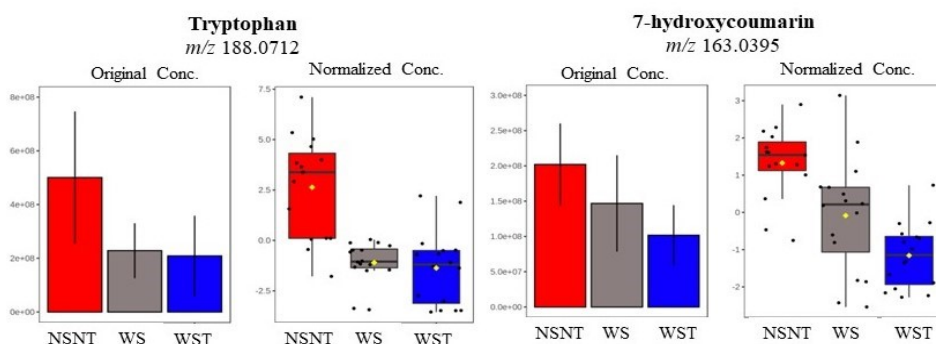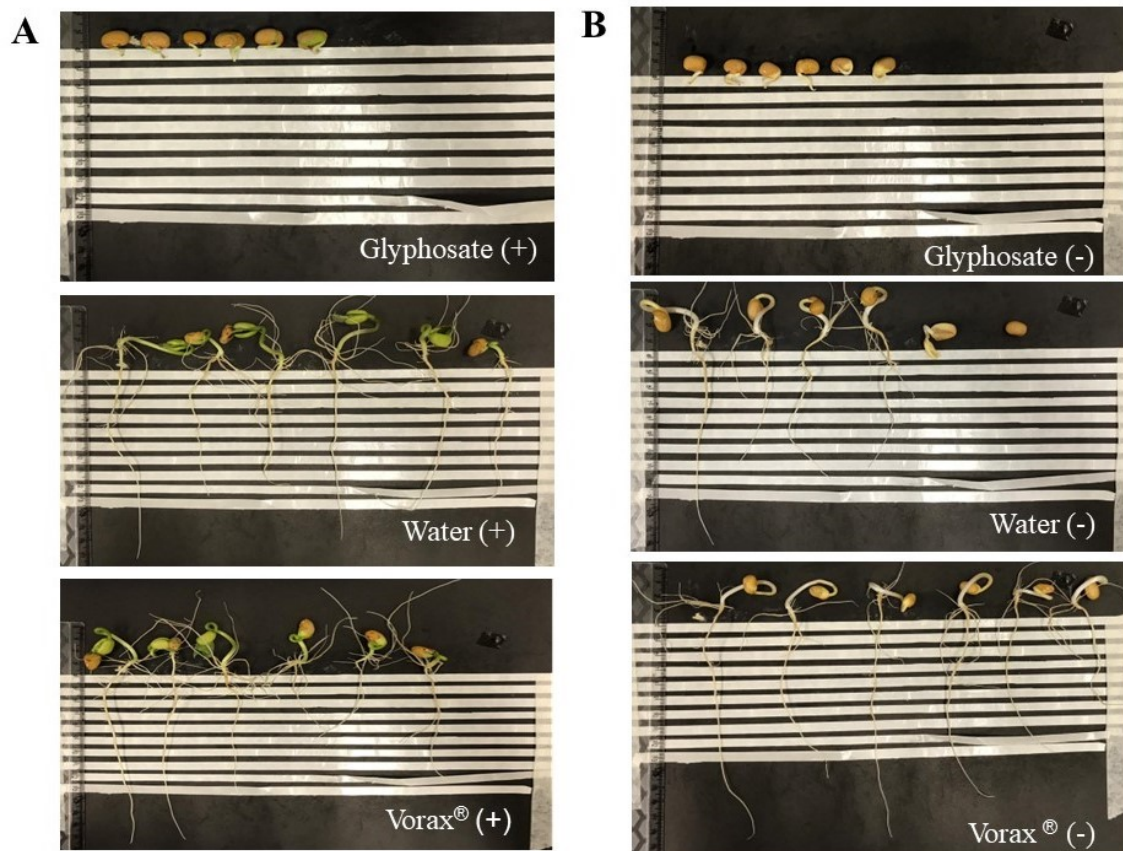
Relative Abundance

m/z

Fig S11. Boxplot chart of the metabolites that exhibited an increase in the concentration in the two trials subjected to water stress but more expressive in WST.

Glutamic acid
m/z 148.0605

1-linolenoyl-3-glactopyranosyl glycerol
m/z 532.3492

Quercetin-3-O-xylopyranosil (1→6)-glucopyranoside
m/z 597.1468

Fig S12. Boxplot chart of the metabolites that exhibited a decrease in the concentration in the two trials subjected to water stress (WS and WST).

Tryptophan
m/z 188.0712

7-hydroxycoumarin
m/z 163.0395

Fig S13. Radicles length for *P. vulgaris* seed germination assays with **A)** Exposure of photoperiod 12h/12h light/dark (+) and **B)** Complete absence of sunlight (-).

Fig S14. A) PLS-DA component 1 (29.7%) x component 2 (15.8%) with data of the two assays (+) and (-), **B)** PLS-DA comp. 1 (15.3%) x comp. 2 (20%) of the (+) data and **C)** PLS-DA comp 1 (21.2%) x comp 2 (21%) of the (-) data. The data were acquired by UHPLC-MS/MS, positive mode, with n = 5 (two repetitions).