

SUPPLEMENTARY INFORMATION

NMR-based metabolomics approach to study the influence of different conditions of water irrigation and greenhouse ventilation on zucchini crops

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Table S1. Chemical analysis of desalinated seawater (DW) and groundwater (GW)*

Parameter	DW	GW
pH	8.14	7.43
Conductivity at 20 °C (µS/cm)	397	2360
Total hardness (mg/L CaCO ₃)	80	753
Sodium adsorption ratio (SAR)	4.40	4.02
Chloride (mmol/L)	3.10	10.40
Nitrate (mmol/L)	<0.04	<0.01
Sulfate (mmol/L)	0.07	4.84
Carbonate (mmol/L)	<0.02	<0.16
Bicarbonate (mmol/L)	1.10	6.13
Sodium (mmol/L)	2.78	11.00
Potassium (mmol/L)	0.08	0.30
Calcium (mmol/L)	0.50	3.92
Magnesium (mmol/L)	0.29	3.61
Iron (mg/L)	<0.10	<0.20
Manganese (mg/L)	<0.10	<0.10
Copper (mg/L)	<0.20	<0.10
Zinc (mg/L)	<0.01	<0.05
Boron (mg/L)	0.76	0.37

*analyses performed by a laboratory accredited by the Spanish National Accreditation Body (ENAC)

Table S2. Quantification of 13 discriminating metabolites (biomarkers) identified on zucchini extracts from plants irrigated with desalinated seawater (DW) or groundwater (GW)*

	DW (mg/g extract)	GW (mg/g extract)
1. glucose	150.5 ± 21.3	141.0 ± 14.6
2. fructose	46.9 ± 5.2	44.8 ± 3.3
3. sucrose	1.7 ± 0.7	4.8 ± 1.7
4. uracil	0.2 ± 0.1	0.1 ± 0.0
5. uridine	0.4 ± 0.1	0.5 ± 0.0
6. adenosine	0.5 ± 0.1	0.4 ± 0.1
7. asparagine	6.1 ± 2.0	8.0 ± 1.7
8. aspartate	4.1 ± 1.4	4.7 ± 1.2
9. glutamine	11.8 ± 2.6	14.3 ± 0.9
10. fumarate	1.3 ± 0.4	0.7 ± 0.2
11. trigonelline	0.5 ± 0.1	0.6 ± 0.0
12. niacin	0.0 ± 0.0	0.0 ± 0.0
13. alanine	0.9 ± 0.3	1.2 ± 0.2

*Mean ± SD values are shown for zucchinis collected from 2nd to 6th harvests; zucchini extracts were prepared with CD₃OD:D₂O KH₂PO₄ buffer, 50:50 v/v.