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Table S1: Morpho-physiological parameters and method(s) of measurement/estimate

Morpho-physiological parameter	Abbreviation (units)	Method of measurement
Above ground biomass dry mass	Above Ground Biomass (DW, g)	Freeze-dried dry weight of the above ground part of the individuals, after harvesting
Below ground biomass dry mass	Below Ground Biomass (DW, g)	Freeze-dried dry weight of the below ground part of the individuals, after harvesting
Plant height	PH (cm)	Final plant above ground height, after harvesting
Number of leaves	Number of leaves	Number of leaves after harvesting
Relative Growth Rate	RGR (g DW day ⁻¹)	Based on the mean of natural logarithm transformed dry weights according to Hoffmann and Poorter (2002) . DW _{start} was estimated from the measured fresh weight (FW _{start}) at the beginning of the experiment, based on the proportionality coefficient that was calculated from the FW and DW measurements (below and above ground; 60 °C) of 10 morphologically identical replicates not used in the mesocosms (15 cm height). RGR = [ln (DW _{end}) – (lnDW _{start})] / (t _{days})
Chlorophyll <i>a</i> concentration and <i>b</i>	Chl- <i>a</i> ; Chl- <i>b</i> (mg DWg ⁻¹)	Photosynthetic pigments concentrations were determined spectrophotometrically after extraction overnight in the darkness in 96% ethanol according to Lichtenthaler (1987) .
Ratio Chlorophyll <i>a</i> concentration: <i>b</i>	Chl <i>a</i> : <i>b</i>	
Carotenoids concentration	Carotenoids (mg DWg ⁻¹)	
Specific leaf area	SLA (cm ² g ⁻¹)	Ratio of leaf area used to leaf dry mass; measurements refer to the leaf used for photosynthesis measurements
%N per leaf DW	%LeafN	Tissue content (percentage per dry weight) of carbon and nitrogen were determined for all leaves used for photosynthesis measurements, above ground organs (shoot) and below ground organs (root) for each individual which means triplicate samples of each treatment by catalytic combustion at 900 °C on a C/N analyzer (CE Instruments).
%C per leaf DW	%LeafC	
%N per Root DW	%RootN	
%C per Root DW	%RootC	
%N per Shoot DW	%ShootN	
%C per Shoot DW	%ShootC	
Ratio C:N in root	C:N _{root}	Ratio between %C content per dry weight and %N root (below ground) content per dry weight
Ratio C:N in leaf	C:N _{leaf}	Ratio between %C content per dry weight and %N leaf content per dry weight
Ratio C:N in Shoot	C:N _{shoot}	Ratio between %C content per dry weight and %N shoot (above ground) content per dry weight
N content in the leaf	FoliarN (mgN)	Concentration of N in mgN in the leaf used for photosynthesis
Photosynthetic N use efficiency	PNUE; (μmolCO ₂ /gN/s)	Maximum Photosynthesis rate (P _{max}) per unit leaf area divided by leaf N concentration. (Photosynthetic rate X SLA) / (Foliar N concentration) (Hidaka and Kitayama, 2009)
Maximum Photosynthesis rate	P _{max} ; [μmol (CO ₂) m ⁻² s ⁻¹]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)
Light compensation point	I _c ; [μmol (photons) m ⁻² s ⁻¹]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)
Quantum yield	φ; [mmol (CO ₂) mmol ⁻¹ (photons)]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)
Dark respiration rate	R _d ; [μmol (CO ₂) m ⁻² s ⁻¹]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)
Light saturation point	I _k ; [μmol (photons) m ⁻² s ⁻¹]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)
Maximum gross photosynthesis rate	G _{max} ; [μmol (CO ₂) m ⁻² s ⁻¹]	From light response curve fitted using rectangular hyperbola Michaelis-Menten model (Baly, 1935)

	Peak Name	Metabolite Name	RT	Quan Ion	Chem. Cat.*	fold change OPEN_NL4 over OPEN_NL1	fold change OPEN_NL5 over OPEN_NL1	fold change SH_NL1 over OPEN_NL1	fold change SH_NL4 over OPEN_NL4	fold change SH_NL5 over OPEN_NL5	OPEN_NL1_R1	OPEN_NL1_R2	OPEN_NL1_R3	SH_NL1_R1	SH_NL1_R2	SH_NL1_R3	OPEN_NL4_R1	OPEN_NL4_R2	OPEN_NL4_R3	SH_NL4_R1	SH_NL4_R2	SH_NL4_R3	OPEN_NL5_R1	OPEN_NL5_R2	OPEN_NL5_R3	SH_NL5_R1	SH_NL5_R2	SH_NL5_R3
1	3-methylbenzoate 1TMS	3-methylbenzoate	18.302	193	1	0.97	1.59	1.93	1.17	0.68	0.029	0.057	0.028	0.033	0.047	0.032	0.030	0.034	0.031	0.038	0.028	0.031	0.033	0.038	0.038	0.037	0.035	0.041
2	alpha-linolenic acid 1 TMS	alpha-linolenic acid	34.858	79	1	1.19	1.64	0.94	0.91	0.90	0.063	0.059	0.074	0.068	0.103	0.093	0.054	0.077	0.050	0.026	0.052	0.034	0.046	0.057	0.067	0.077	0.064	0.080
3	caffeic acid 3TMS	caffeic acid	33.474	219.1	1	1.601	1.15	0.09	1.69	1.22	1.601	0.147	0.728	1.228	1.839	2.243	0.978	0.840	1.355	0.820	0.339	0.826	0.742	1.003	0.930	0.621	0.601	0.784
4	citrate 4TMS	citrate	26.596	273.3	1	1.25	0.84	0.08	0.23	0.28	4.136	0.332	5.172	1.205	3.465	0.958	0.781	0.619	1.074	0.774	1.116	1.632	0.586	1.591	0.628	1.220	0.918	1.521
5	ethanolamine 3TMS	ethanolamine 3TMS	11.166	174.2	3	0.44	0.26	0.90	1.73	0.13	0.048	0.043	0.021	0.036	0.012	0.002	0.065	0.061	0.009	0.073	0.036	0.025	0.061	0.023	0.019	0.182	0.110	0.146
6	fructose MeOx 1	fructose MeOx 1	25.829	307.1	2	2.77	1.56	0.70	0.38	1.48	0.684	0.480	1.894	0.726	1.064	1.570	4.482	3.775	1.552	1.728	3.550	2.860	3.385	3.970	3.496	1.993	2.939	3.337
7	fumarate 2TMS	fumarate	15.867	245	1	0.47	0.54	0.19	1.52	0.73	0.214	0.041	0.100	0.152	0.115	0.084	0.165	0.206	0.309	0.201	0.111	0.246	0.169	0.299	0.199	0.348	0.255	0.260
8	gluconate 6 TMS	gluconate	27.886	292.2	1	0.97	0.78	0.52	0.41	0.68	0.065	0.034	0.063	0.026	0.050	0.034	0.062	0.057	0.073	0.040	0.062	0.059	0.073	0.087	0.066	0.073	0.059	0.057
9	glucose total	glucose total			2	2.53	1.11	0.75	0.26	1.33	4.501	3.386	11.380	3.014	5.015	6.670	15.103	20.338	32.441	11.462	17.516	19.342	19.466	21.985	21.841	13.437	17.364	21.384
10	glutamate_total	glutamate_total			3	1.25	0.55	0.44	0.18	2.10	0.320	0.141	0.399	0.070	0.176	0.369	1.036	0.713	0.301	0.331	0.871	0.617	0.466	0.679	0.572	1.544	1.339	0.589
11	glycerate 3TMS	glycerate	14.818	292	1	1.01	1.04	0.43	0.84	1.02	0.158	0.068	0.159	0.134	0.163	0.166	0.193	0.397	0.485	0.328	0.248	0.281	0.374	0.490	0.374	0.682	0.680	0.426
12	glycerol 3TMS	glycerol	12.002	204.9	1	1.04	2.31	1.74	0.73	0.66	0.017	0.030	0.018	0.013	0.040	0.026	0.023	0.031	0.029	0.040	0.057	0.032	0.034	0.037	0.035	0.049	0.040	0.030
13	lactate 2 TMS	lactate	6.989	117.2	1	0.52	2.37	0.66	2.87	0.90	0.063	0.042	0.033	0.095	0.151	0.136	0.044	0.049	0.035	0.061	0.141	0.114	0.028	0.040	0.029	0.041	0.070	0.068
14	9,12-(Z,Z)-Octadecadienoic acid (1TMS)	linoleic acid	34.372	337.3</																								

Table S3: Mean values and standard deviation ($\pm$ SD) of all morpho-physiological parameters

	TREATMENTS									
Traits	SH-NL1	SH-NL2	SH-NL3	SH-NL4	SH-NL5	OPEN-NL1	OPEN-NL2	OPEN-NL3	OPEN-NL4	OPEN-NL5
Above Ground Biomass (DW, g)	0.34 $\pm$ 0.078	0.97 $\pm$ 0.42	1.04 $\pm$ 0.66	3.29 $\pm$ 0.47	4.00 $\pm$ 1.37	0.26 $\pm$ 0.06	0.96 $\pm$ 0.45	1.43 $\pm$ 0.84	2.72 $\pm$ 1.67	3.17 $\pm$ 1.67
Below Ground Biomass (DW, g)	0.84 $\pm$ 0.52	2.38 $\pm$ 1.02	2.63 $\pm$ 1.30	8.61 $\pm$ 1.34	8.57 $\pm$ 4.09	1.08 $\pm$ 0.26	3.01 $\pm$ 1.52	3.62 $\pm$ 1.99	5.61 $\pm$ 2.60	9.11 $\pm$ 4.24
Plant height (PH, cm)	31.89 $\pm$ 0.69	33.67 $\pm$ 1.53	47.22 $\pm$ 10.18	53.56 $\pm$ 3.36	56.22 $\pm$ 9.79	24.56 $\pm$ 5.01	35.00 $\pm$ 7.17	32.33 $\pm$ 7.37	43.56 $\pm$ 3.59	47.44 $\pm$ 6.54
Number of leaves	4.67 $\pm$ 0.58	10.00 $\pm$ 1.73	9.33 $\pm$ 2.08	17.00 $\pm$ 6.00	20.67 $\pm$ 3.51	5.67 $\pm$ 1.53	10.67 $\pm$ 1.15	15.00 $\pm$ 1.00	20.33 $\pm$ 11.15	20.33 $\pm$ 6.81
RGR [DW(g/days)]	0.02 $\pm$ 0.01	0.03 $\pm$ 0.01	0.03 $\pm$ 0.01	0.05 $\pm$ 0.00	0.05 $\pm$ 0.01	0.02 $\pm$ 0.00	0.03 $\pm$ 0.01	0.04 $\pm$ 0.01	0.04 $\pm$ 0.01	0.05 $\pm$ 0.01
Chl- <i>a</i> (mg DWg ⁻¹)	4.46 $\pm$ 0.73	8.06 $\pm$ 0.63	7.92 $\pm$ 0.32	8.12 $\pm$ 1.12	9.52 $\pm$ 1.71	3.98 $\pm$ 0.98	4.26 $\pm$ 1.40	6.47 $\pm$ 0.55	6.12 $\pm$ 0.71	6.95 $\pm$ 0.96
Chl- <i>b</i> (mg DWg ⁻¹)	1.58 $\pm$ 0.21	2.74 $\pm$ 0.22	2.68 $\pm$ 0.12	2.68 $\pm$ 0.32	3.13 $\pm$ 0.64	1.50 $\pm$ 0.27	1.47 $\pm$ 0.45	2.12 $\pm$ 0.17	2.08 $\pm$ 0.25	2.25 $\pm$ 0.24
Chl- <i>a+b</i> (mg DWg ⁻¹)	6.03 $\pm$ 0.93	10.80 $\pm$ 0.85	10.60 $\pm$ 0.43	10.80 $\pm$ 1.44	12.65 $\pm$ 2.35	5.48 $\pm$ 1.25	5.73 $\pm$ 1.85	8.58 $\pm$ 0.72	8.20 $\pm$ 0.95	9.20 $\pm$ 1.18
Chl <i>a:b</i>	2.82 $\pm$ 0.087	2.94 $\pm$ 0.018	2.96 $\pm$ 0.029	3.03 $\pm$ 0.09	3.05 $\pm$ 0.09	2.64 $\pm$ 0.17	2.89 $\pm$ 0.07	3.05 $\pm$ 0.04	2.94 $\pm$ 0.11	3.08 $\pm$ 0.17
Carotenoids (mg DWg ⁻¹)	0.71 $\pm$ 0.24	1.26 $\pm$ 0.43	1.31 $\pm$ 0.57	1.86 $\pm$ 0.38	2.24 $\pm$ 0.39	0.50 $\pm$ 0.54	0.85 $\pm$ 0.13	1.16 $\pm$ 0.45	1.29 $\pm$ 0.07	1.66 $\pm$ 0.21
Specific Leaf Area, SLA (cm ² g ⁻¹)	187.32 $\pm$ 58.88	191.74 $\pm$ 14.24	197.13 $\pm$ 73.60	185.72 $\pm$ 21.06	142.52 $\pm$ 38.63	171.63 $\pm$ 28.51	183.42 $\pm$ 22.11	163.42 $\pm$ 13.93	125.63 $\pm$ 11.14	132.04 $\pm$ 24.76
%N per leaf DW (%LeafN)	2.19 $\pm$ 0.17	3.08 $\pm$ 0.27	3.05 $\pm$ 0.15	3.16 $\pm$ 0.61	3.54 $\pm$ 0.65	2.59 $\pm$ 0.31	2.67 $\pm$ 0.35	3.07 $\pm$ 0.27	2.88 $\pm$ 0.15	3.08 $\pm$ 0.59
%C per leaf DW (%LeafC)	38.02 $\pm$ 1.81	41.22 $\pm$ 1.16	40.50 $\pm$ 1.17	40.64 $\pm$ 1.48	40.75 $\pm$ 2.31	38.50 $\pm$ 1.88	39.78 $\pm$ 0.45	40.78 $\pm$ 2.68	39.95 $\pm$ 1.16	42.09 $\pm$ 1.50
%N per Root DW (%RootN)	0.77 $\pm$ 0.26	1.36 $\pm$ 0.15	1.47 $\pm$ 0.13	1.30 $\pm$ 0.025	1.95 $\pm$ 0.36	0.78 $\pm$ 0.051	1.15 $\pm$ 0.30	1.23 $\pm$ 0.25	1.09 $\pm$ 0.14	1.48 $\pm$ 0.44
%C per Root DW (%RootC)	38.36 $\pm$ 2.68	39.41 $\pm$ 1.87	39.55 $\pm$ 0.53	35.39 $\pm$ 1.67	38.26 $\pm$ 2.84	36.55 $\pm$ 1.81	37.10 $\pm$ 4.01	37.35 $\pm$ 2.94	37.87 $\pm$ 1.96	37.87 $\pm$ 3.45
%N per Shoot DW (%ShootN)	0.77 $\pm$ 0.25	1.56 $\pm$ 0.27	1.62 $\pm$ 0.25	1.78 $\pm$ 0.22	2.01 $\pm$ 0.41	0.84 $\pm$ 0.12	1.35 $\pm$ 0.20	1.51 $\pm$ 0.18	1.34 $\pm$ 0.21	1.75 $\pm$ 0.34
%C per Shoot DW (%ShootC)	31.95 $\pm$ 4.72	36.25 $\pm$ 1.22	36.40 $\pm$ 0.77	36.42 $\pm$ 0.33	36.73 $\pm$ 0.46	31.93 $\pm$ 3.89	37.22 $\pm$ 0.29	37.34 $\pm$ 0.73	35.52 $\pm$ 2.44	36.90 $\pm$ 0.75
C:N root	53.00 $\pm$ 13.90	29.37 $\pm$ 4.34	27.11 $\pm$ 2.43	27.31 $\pm$ 1.81	20.05 $\pm$ 3.73	46.88 $\pm$ 5.09	33.09 $\pm$ 5.37	31.06 $\pm$ 5.71	35.02 $\pm$ 3.36	26.49 $\pm$ 5.09
C:N_Leaf	17.41 $\pm$ 1.74	13.41 $\pm$ 0.80	13.30 $\pm$ 0.32	13.12 $\pm$ 1.94	11.67 $\pm$ 1.40	14.97 $\pm$ 1.03	15.10 $\pm$ 2.30	13.35 $\pm$ 1.46	13.87 $\pm$ 0.56	14.00 $\pm$ 2.53
C:N_shoot	42.86 $\pm$ 7.30	23.66 $\pm$ 3.74	22.80 $\pm$ 3.26	20.67 $\pm$ 2.65	18.81 $\pm$ 3.95	38.49 $\pm$ 5.22	27.98 $\pm$ 4.15	24.94 $\pm$ 3.41	26.76 $\pm$ 3.58	21.60 $\pm$ 4.09
FoliarN (mgN)	0.10 $\pm$ 0.01	0.11 $\pm$ 0.01	0.13 $\pm$ 0.01	0.16 $\pm$ 0.02	0.21 $\pm$ 0.02	0.10 $\pm$ 0.03	0.13 $\pm$ 0.03	0.12 $\pm$ 0.02	0.16 $\pm$ 0.14	0.20 $\pm$ 0.04
PNUE (μ molCO ₂ /gN/s)	4035.59 $\pm$ 700.15	5258.29 $\pm$ 120.51	4394.53 $\pm$ 1474.91	3532.65 $\pm$ 295.72	2285.03 $\pm$ 480.86	5292.05 $\pm$ 2879.05	4095.06 $\pm$ 769.32	5043.99 $\pm$ 678.52	3112.33 $\pm$ 439.51	2320.56 $\pm$ 237.08
P _{max} [μ mol(CO ₂)m ⁻² s ⁻¹]	10.84 $\pm$ 4.36	17.29 $\pm$ 4.86	18.26 $\pm$ 8.18	22.46 $\pm$ 2.43	22.01 $\pm$ 4.26	12.39 $\pm$ 7.02	16.51 $\pm$ 3.99	20.09 $\pm$ 6.73	23.58 $\pm$ 3.56	22.27 $\pm$ 8.28
G _{max} [μ mol (CO ₂) m ⁻² s ⁻¹]	22.06 $\pm$ 4.54	30.70 $\pm$ 3.93	31.00 $\pm$ 11.00	30.91 $\pm$ 2.82	33.57 $\pm$ 3.46	27.94 $\pm$ 9.82	27.75 $\pm$ 6.99	36.69 $\pm$ 5.23	40.21 $\pm$ 4.12	36.08 $\pm$ 10.61
Ic [μ mol (photons) m ⁻² s ⁻¹]	54.82 $\pm$ 43.31	50.45 $\pm$ 30.46	49.91 $\pm$ 35.58	10.52 $\pm$ 4.57	22.25 $\pm$ 9.26	86.87 $\pm$ 39.76	30.82 $\pm$ 13.92	62.32 $\pm$ 60.09	31.48 $\pm$ 16.47	36.37 $\pm$ 21.67

ϕ [mmol (CO ₂) mmol ⁻¹ (photons)]	0.09±0.04	0.08±0.01	0.08±0.03	0.10±0.02	0.08±0.01	0.06±0.03	0.08±0.00	0.06±0.02	0.07±0.01	0.07±0.00
Rd [μmol(CO ₂)m ⁻² s ⁻¹]	3.37±1.31	3.23±1.43	3.00±0.69	1.00±0.26	1.53±0.45	4.00±0.10	2.30±0.95	2.90±2.97	1.97±0.83	2.17±1.07
Ik [μmol (photons) m ⁻² s ⁻¹]	462.00±66.16	816.67±190.14	840.67±153.58	955.67±169.15	1071.33±224.63	619.67±140.23	711.33±153.68	950.33±84.13	1015.00±95.41	1150.67±332.54

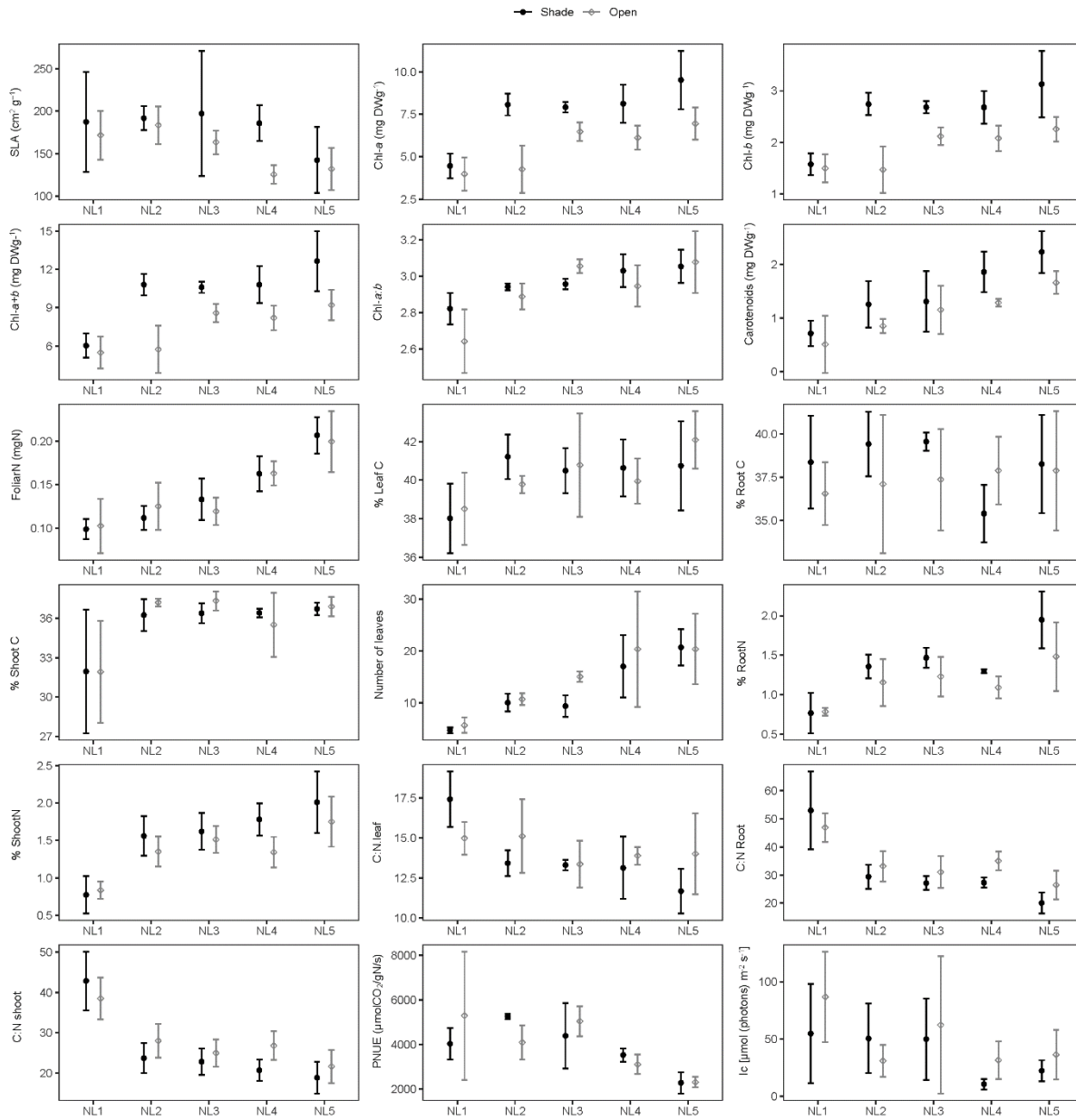


Figure S1: Scatter (XY) plots with standard deviation ($\pm$ SD) of morpho-physiological parameters. Filled black circles: shaded treatments; gray open circles: open treatments. SD estimated over n=3 mesocosms per treatment.

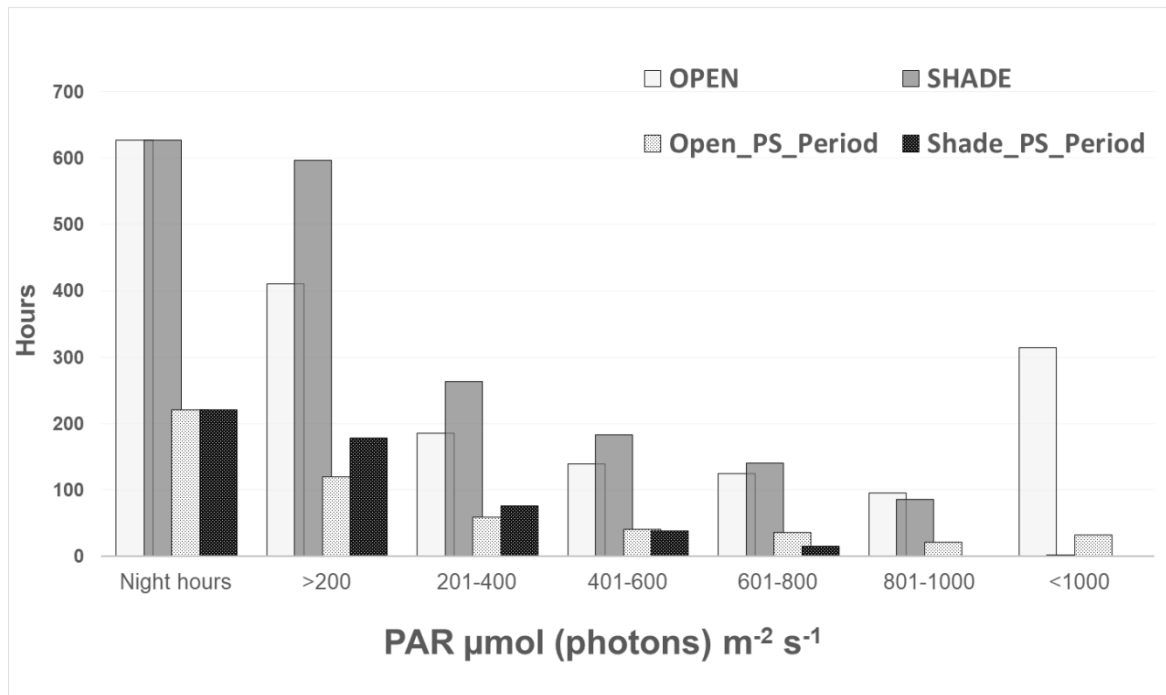


Figure S2: Number of hours per different Photosynthetic Active Radiation (PAR) range for open and shade treatments. Data were collected from the Påskehøjgård weather station and for conversion of KW m^{-2} to $\mu\text{mol photons m}^{-2} \text{ s}^{-1}$, Langhans and Tibbitts (1997) was used for conversion.

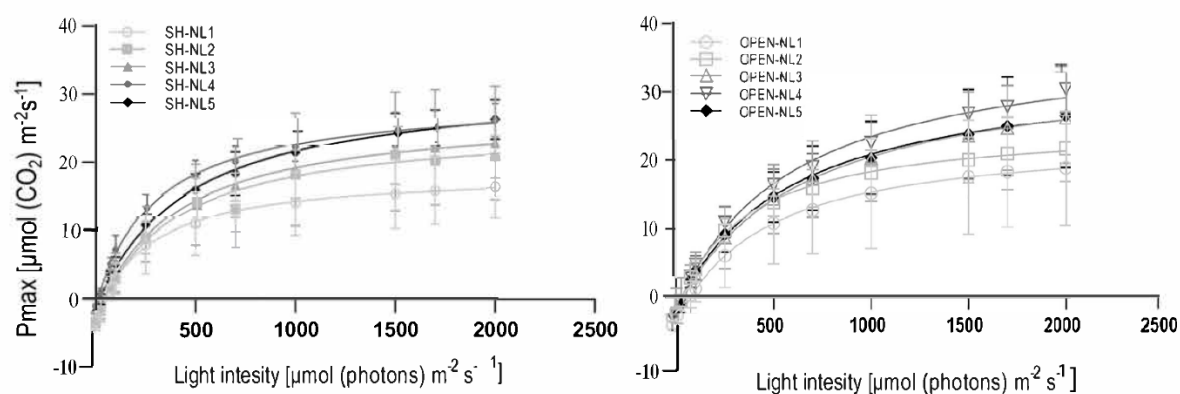


Figure S3: Light response-curves for open and shade treatments. Photosynthetic capacity was characterized from light response curves determined from measurements at eleven irradiances (2000, 1700, 1500, 1000, 700, 500, 250, 100, 75, 25 and 0 $\mu\text{mol m}^{-2}\text{s}^{-1}$). The light response curve of each leaf was fitted using rectangular hyperbola Michaelis-Menten based model of Baly (1935). Graphical representation of P/I curves was performed by GraphPad Prism 8.0.2 software (GraphPad Software, San Diego, CA, USA).

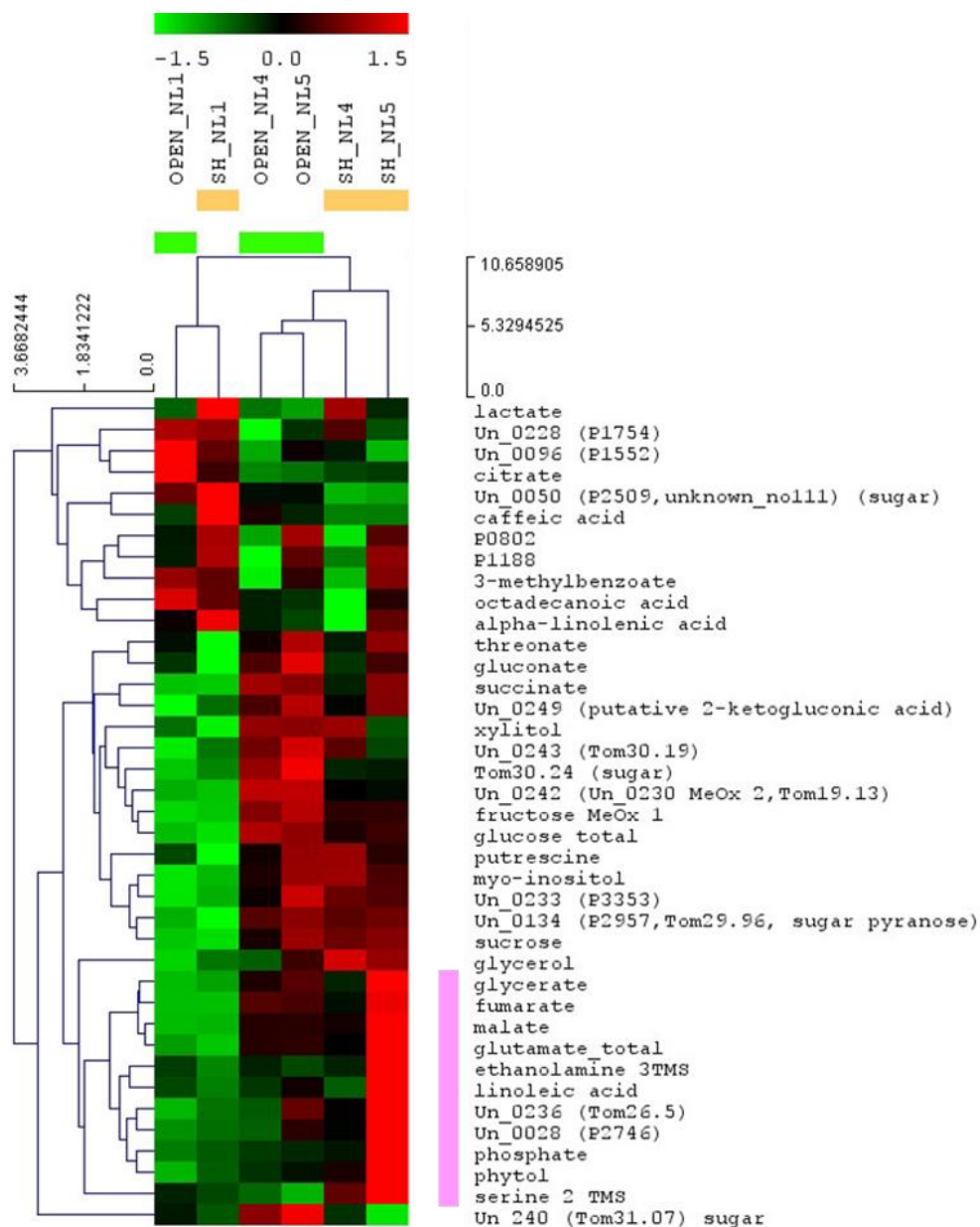


Figure S4: Hierarchical clustering analysis (HCL) of the standardized leaf metabolic profiles (Euclidean distance metric). Highlighted in pink is the cluster that comprises the metabolites that exhibiting a largely different abundance in SH-NL5.

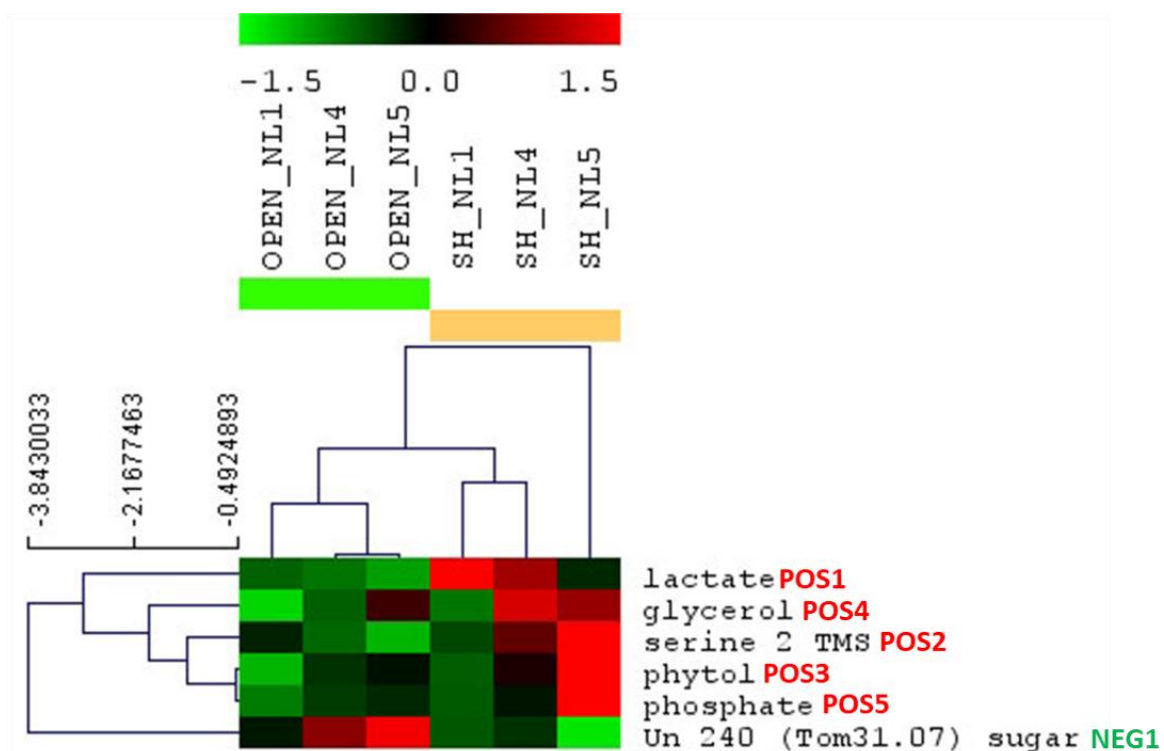


Figure S5: The set of metabolites identified as positively (POS) and negatively (NEG) significant in the shade versus the open treatments, based on SAM. The indication POS or NEG next to the name of each metabolite differentiates, respectively, the positively from the negatively significant in the shade compared to the open treatments; the number depicts the significance hierarchy of each metabolite in its respective group.

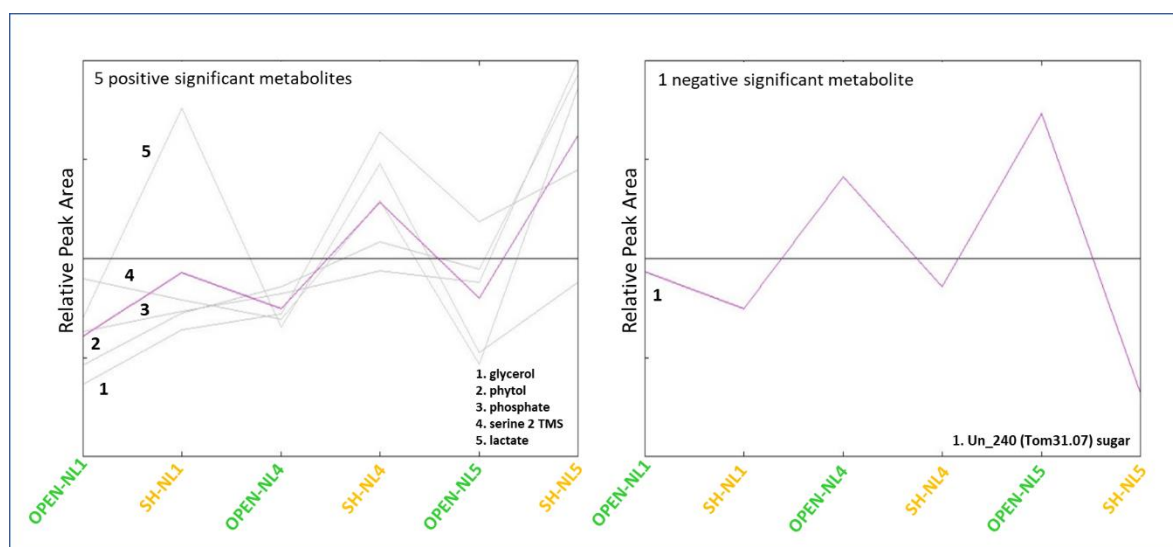


Figure S6: The abundance profiles of the 6 significant metabolites (5 positive, 1 negative) shown in Figure S5.

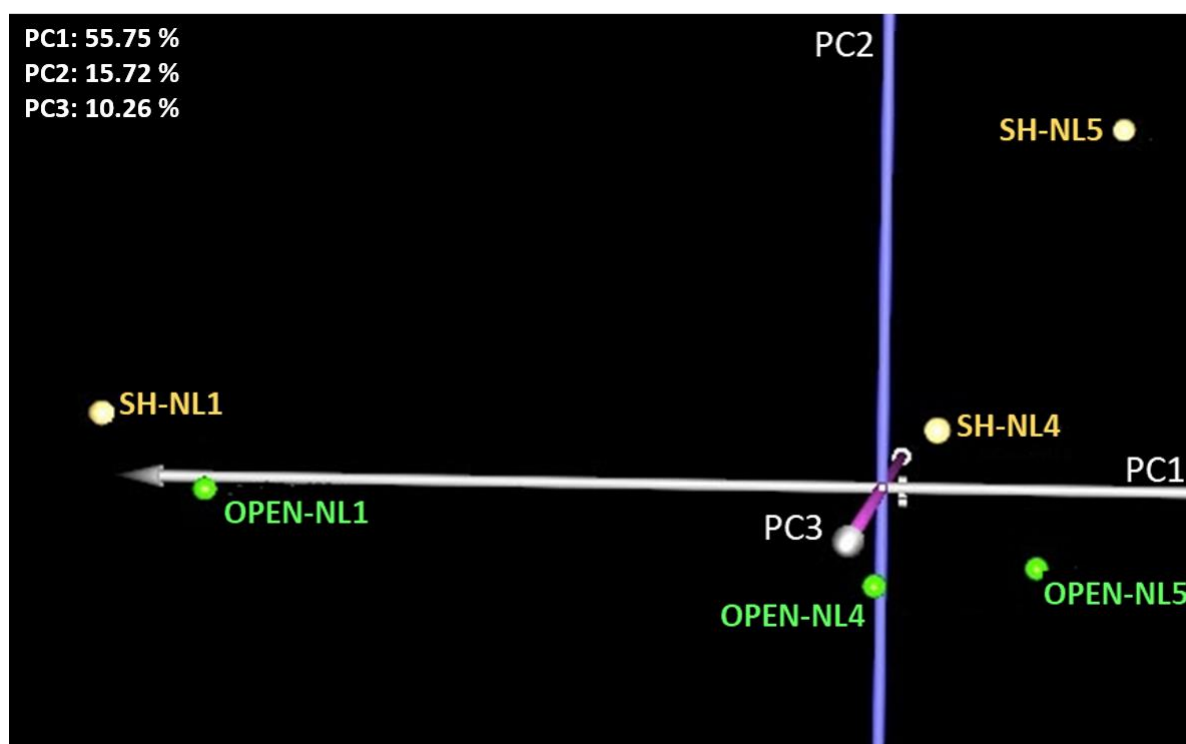


Figure S7: PCA graph of the standardized combined profiles.