

S1. Materials and methods

S1.1 Contribution analysis of biomass and concentration to yield

To evaluate the relative contribution of biomass (DW) and metabolites concentration (C) to yield (Y) variation in time, from T1 to T2, we applied a contribution analysis based on the multiplicative relationship. Yield is defined as follows:

$$Y = DW \times C,$$

using mean values reported in Table 2, the change in yield from T1 to T2 for each metabolite was calculated as:

$$\Delta Y = Y_{T2} - Y_{T1}.$$

Because of the multiplicative nature of the relationship, this variation can be exactly decomposed into three terms:

$$\Delta Y = C_{T1}\Delta DW + DW_{T1}\Delta C + \Delta DW\Delta C,$$

with $\Delta DW = DW_{T2} - DW_{T1}$ and $\Delta C = C_{T2} - C_{T1}$. To consistently allocate the interaction term ($\Delta DW\Delta C$), we adopted a midpoint (Shapley-value) approach [1], by splitting it equally between the two factors. Thus, the contributions were defined as:

$$\Delta Y_{DW} = C_{T1}\Delta DW + \frac{1}{2}\Delta DW\Delta C, \quad \Delta Y_C = DW_{T1}\Delta C + \frac{1}{2}\Delta DW\Delta C.$$

Finally, the relative contributions were expressed as percentages:

$$\% \Delta Y_{DW} = \frac{\Delta Y_{DW}}{\Delta Y} \times 100, \quad \% \Delta Y_C = \frac{\Delta Y_C}{\Delta Y} \times 100.$$

This approach allowed us to quantify whether yield increments from T1 to T2 were predominantly driven by biomass accumulation or by metabolite concentration increases, while accounting for the interaction between the two components.

S2. Results

S2.1 Contribution analysis of biomass and concentration to yield

Table S1. Contribution of biomass accumulation (DW) and metabolite concentration (C) to yield increase (ΔY) from T1 to T2, computed with mean values reported in Table 2.

Plant organ	Compound	% ΔY_{DW}	% ΔY_C
Leaves	RA	69.3%	30.7%
Leaves	QU	43.8%	56.2%
Roots	RA	46.3%	53.7%
Roots	QU	46.1%	53.9%
Total plant	RA	55.9%	44.1%
Total plant	QU	45.9%	54.1%

Contributions (%) are computed on the absolute yield increment, using a Shapley-value (midpoint) decomposition that equally allocates the DW×C interaction between factors.

S2.2 Additional results of Light and Salt stress as main factors

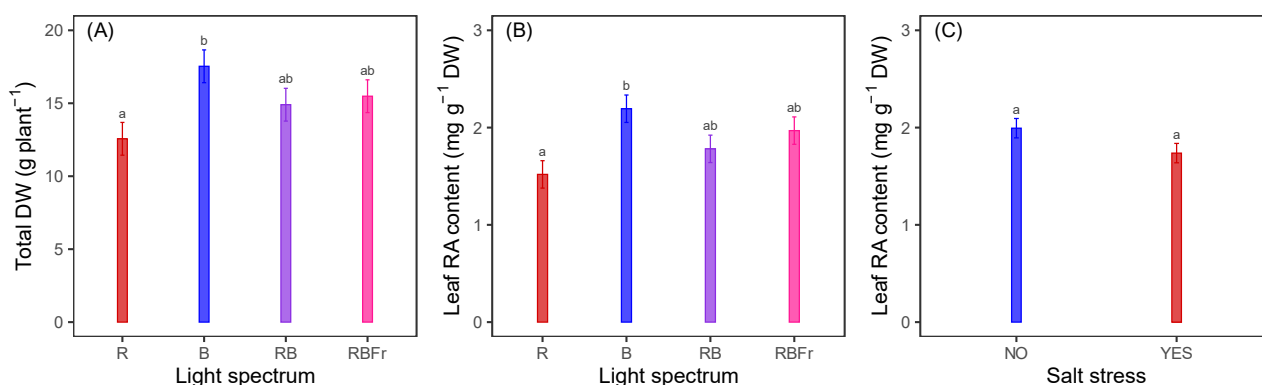


Figure S1. Additional main factors (light and salt stress) effects on *Coleus blumei* total dry weight and rosmarinic acid content. **(A)** Light effect on total plant DW (g plant⁻¹). **(B)** Light effect on leaves RA concentration (mg g⁻¹ DW); colors represent different light spectra. **(C)** Salt stress effect on leaves RA conc. (mg g⁻¹ DW); colors represent the two salinity levels (0 mM-120mM NaCl). Bars indicate SE (n = 4). Means with different letters are significantly different at the 5% level by Tukey's test.

Supplementary references

1. Shorrocks, A.F. Decomposition Procedures for Distributional Analysis: A Unified Framework Based on the Shapley Value. *J Econ Inequal* **2013**, 11, 99–126. <https://doi.org/10.1007/s10888-011-9214-z>.