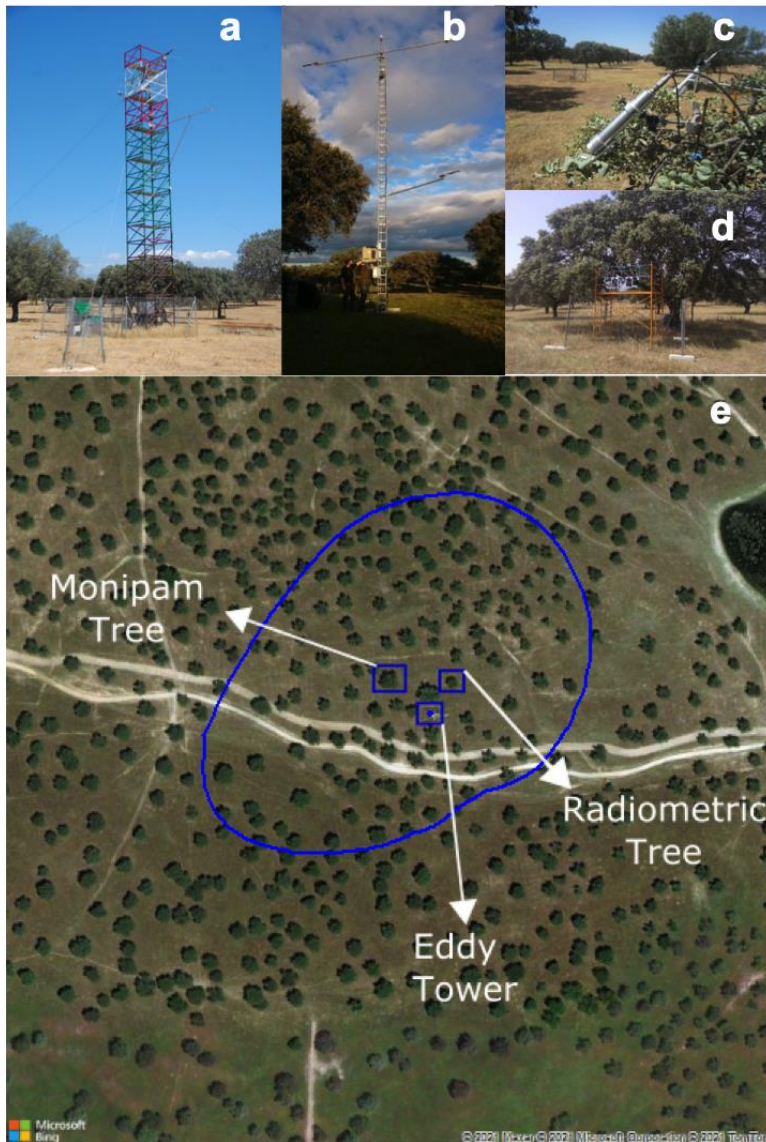


New Phytologist Supporting Information

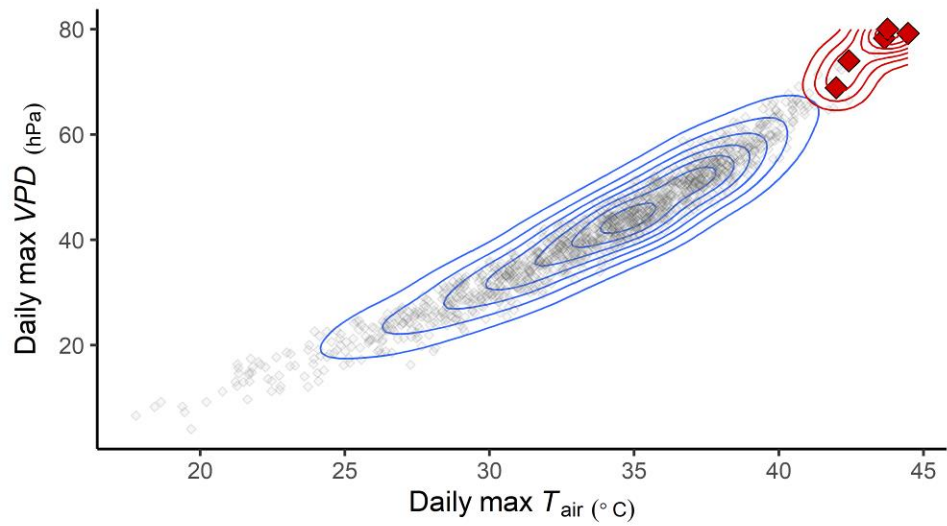
Heatwave breaks down the linearity between sun-induced fluorescence and gross primary production

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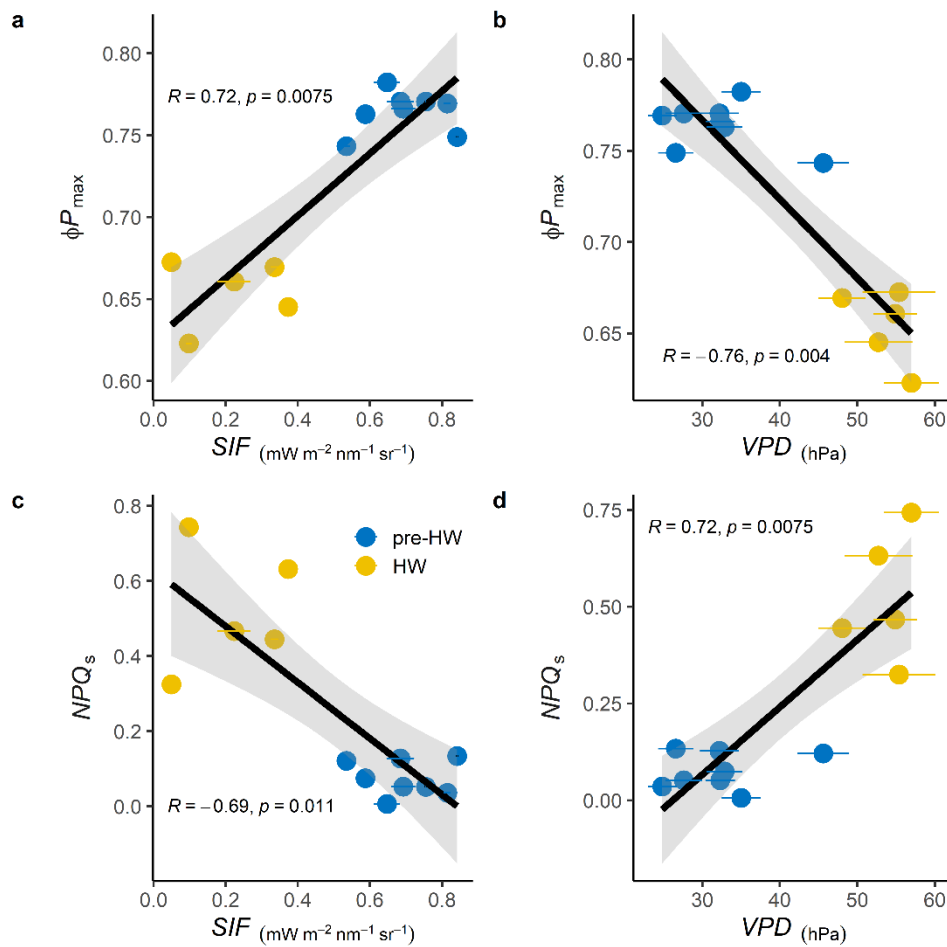
Supplementary Fig. S1. (a) Picture of the eddy covariance tower. (b) Picture of the radiometric tower. (c,d) picture of the MONI-PAM system. (e) Satellite picture of the experimental site at Majadas de Tiétar. The eddy-covariance tower, the tree measured by the radiometric tower and the tree measured by the MONI-PAM are highlighted. The blue circle represents the footprint climatology of the eddy covariance tower, here defined as the isoline corresponding to 80% of the total flux footprint contributions.



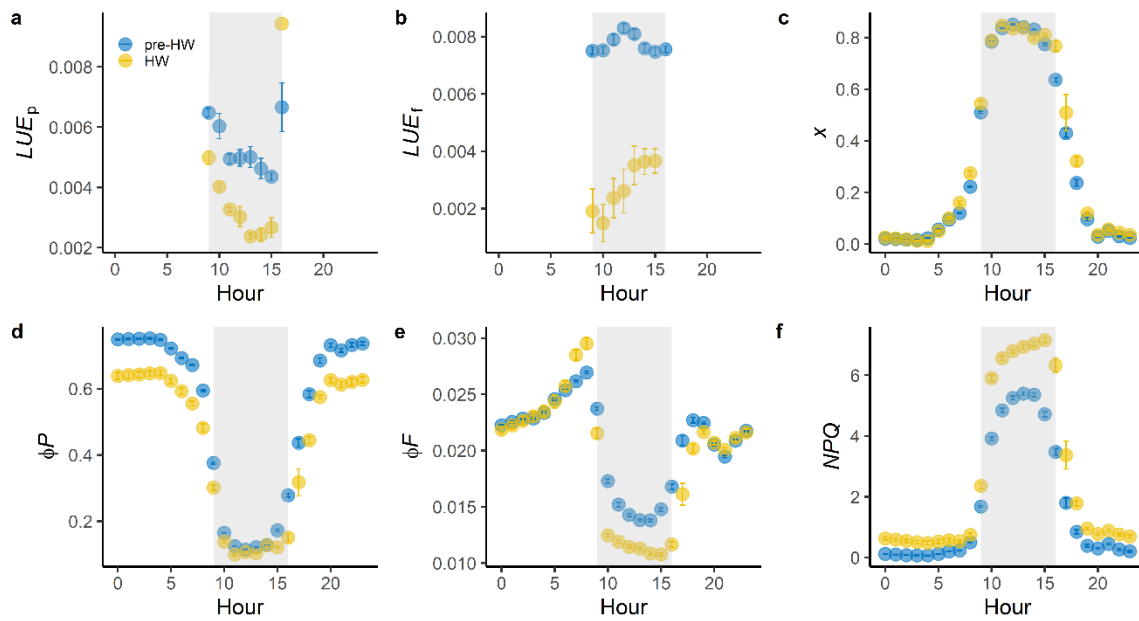
Supplementary Fig. S2. 2D kernel density estimation of daily maximum air temperature (T_{air}) and daily maximum vapor pressure deficit (VPD) from 2004 to 2018 in June, July and August at the Majadas de Tiétar site in blue, and in red for the 2018 heatwave. The red dots correspond to the daily maximum T_{air} and VPD during the 2018 heatwave.

Supplementary Table S1. Spearman's rank correlation coefficient (R) and p value between compared variables. Slope and intercept are obtained with total least square regression. SIF_{ifld} is obtained from the Improved Fraunhofer Line Discrimination Method (ifld) and SIF_{sfm} is obtained with the spectral fitting method (SFM).

Compared variables (Y - X)	R	Slope	Intercept	p value
$SIF_{ifld} - SIF_{sfm}$	0.988	0.723	0.22	< 0.01



Supplementary Fig. S3. (a) Scatterplot between the maximum value at night of quantum yield of photosystem II (ΦP_{\max}) (correspondent to the widely used F_v/F_m) and daily means of SIF . (b) Scatterplot between ΦP_{\max} and daily means of VPD . (c) Scatterplot between daily means of the sustained component of the nonphotochemical quenching (NPQ_s) and sun-induced fluorescence at 760 nm (SIF). (d) Scatterplot between daily means of NPQ_s and vapor pressure deficit (VPD). Yellow points correspond to the pre-heatwave (pre-HW) period and blue points correspond to the heatwave (HW) period. Daily mean values in (a) to (d) are computed between 11 and 13 UTC. In each panel the Spearman's rank correlation coefficient (R) and p value are reported for the overall data. The black line is the overall fit from a linear regression. The shaded area represents the 95% confidence interval of the fit.



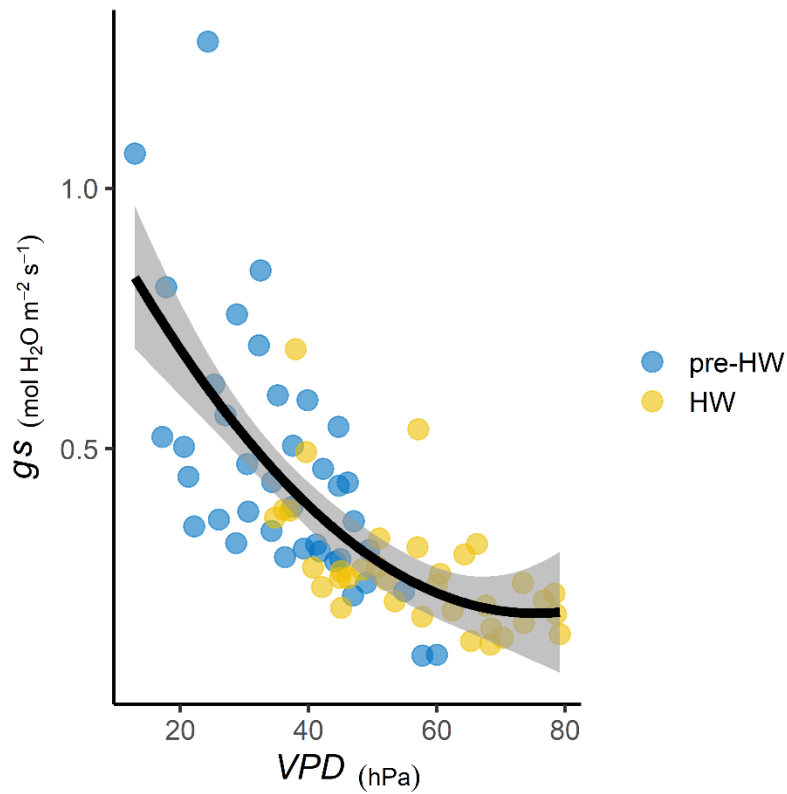
Supplementary Fig. S4. Mean daily cycles for (a) light use efficiency of photosynthesis (LUE_p), (b) light use efficiency of *SIF* emission (LUE_r), (c) relative light saturation of photosynthesis (x), (d) yield of photochemistry (ϕ_P), (e) yield of fluorescence (ϕ_F) and (f) nonphotochemical quenching (NPQ). Blue points correspond to the pre-heatwave (pre-HW) period and yellow points correspond to the heatwave (HW) period. Error bars correspond to 1 standard error. The shaded gray area highlights the hours (UTC + 0) between 9 and 16.

Supplementary Table S2. Spearman's rank correlation coefficient (R) and p value between compared variables. Gross primary production from day time partitioning (GPP_{DT}) is obtained according to Lasslop *et al.* (2010) and GPP from night time partitioning (GPP_{NT}) is obtained according to Reichstein *et al.* (2005). HW refers to the heatwave period and pre-HW refers to the days before the HW.

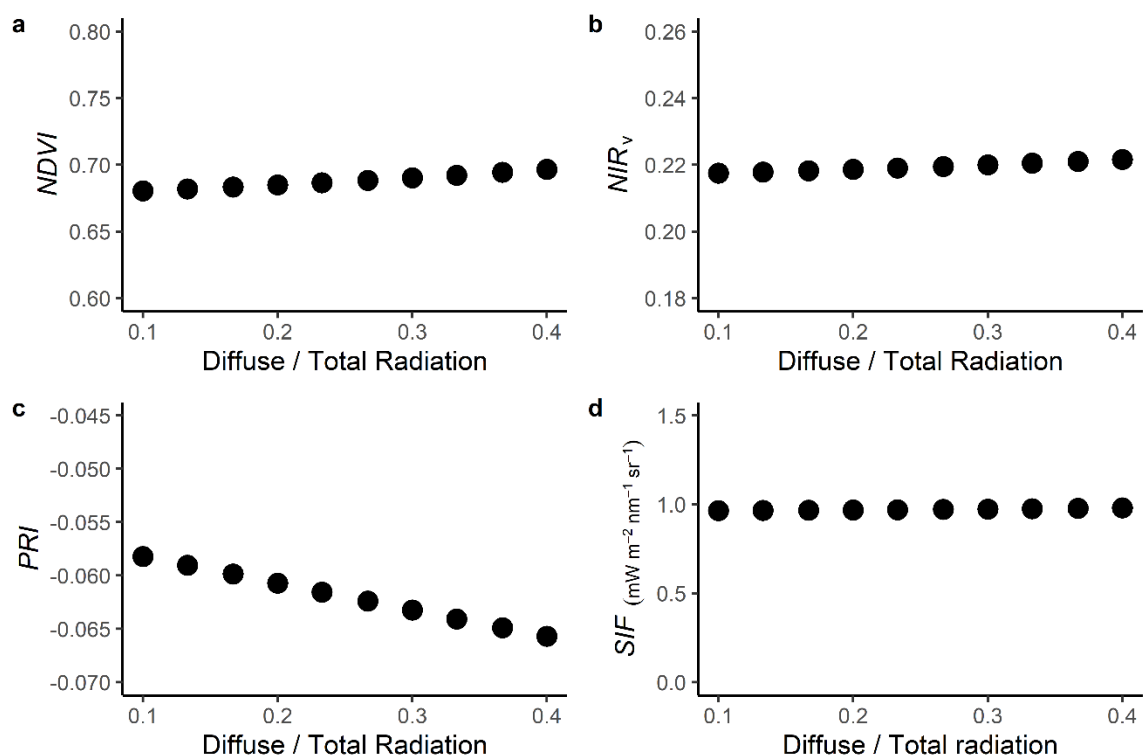
Compared variables (Y - X)	Period	R	p value
$GPP_{DT} - SIF_{tot}$	HW	-0.36	0.0342
$GPP_{DT} - SIF_{tot}$	pre-HW	0.522	< 0.01
$GPP_{NT} - SIF_{tot}$	HW	0.075	0.672
$GPP_{NT} - SIF_{tot}$	pre-HW	0.314	0.0176

Supplementary Table S3. Spearman's rank correlation coefficient (R) and p value between compared variables. Slope and intercept are obtained with total least square regression. Gross primary production from day time partitioning (GPP_{DT}) is obtained according to Lasslop *et al.* (2010) and GPP from night time partitioning (GPP_{NT}) is obtained according to Reichstein *et al.* (2005).

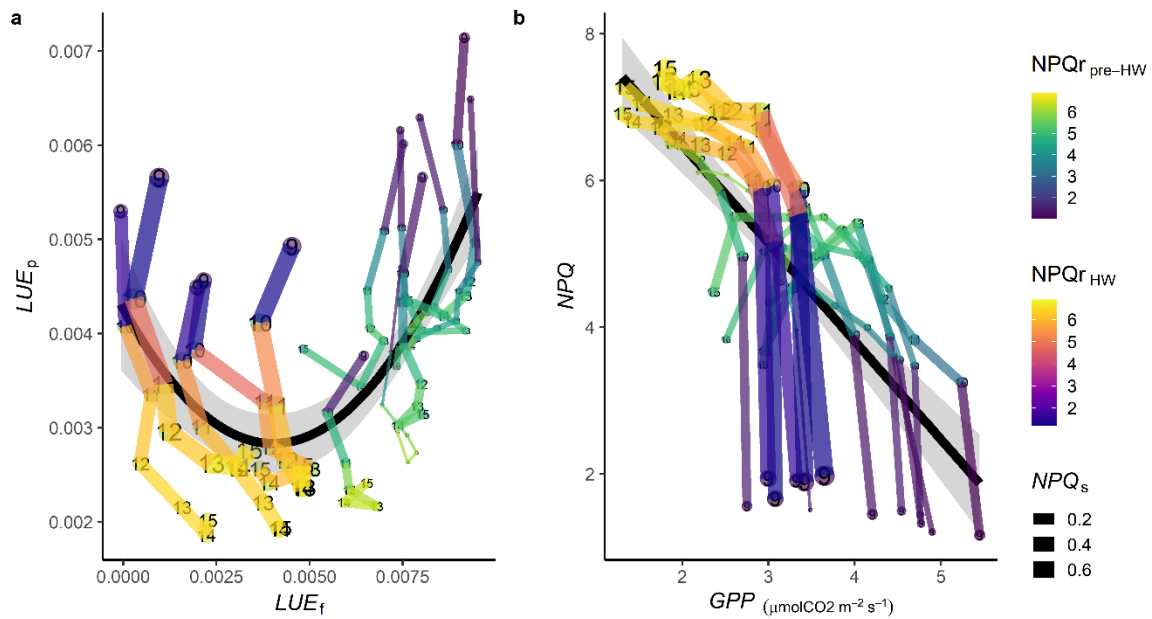
Compared variables (Y - X)	R	Slope	Intercept	p value
$GPP_{DT} - VPD$	-0.928	-0.0549	5.45	< 0.01
$GPP_{NT} - VPD$	-0.766	-0.0546	6.28	< 0.01



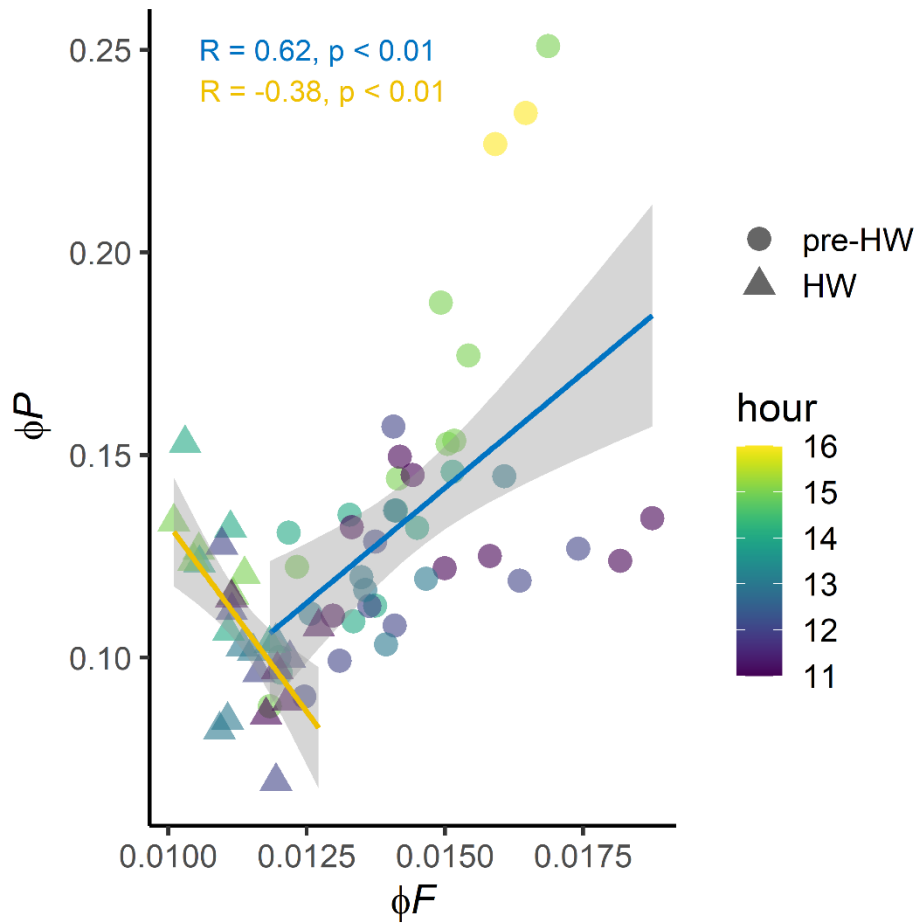
Supplementary Fig. S5. Scatterplot between surface conductance (g_s) and vapor pressure deficit (VPD). Blue points correspond to the pre-heatwave (pre-HW) period and yellow points correspond to the heatwave (HW) period. Hourly mean values are computed from 9 to 16 UTC. The black line is the overall fit from a second-degree polynomial. The shaded area represents the 95% confidence interval of the fit.



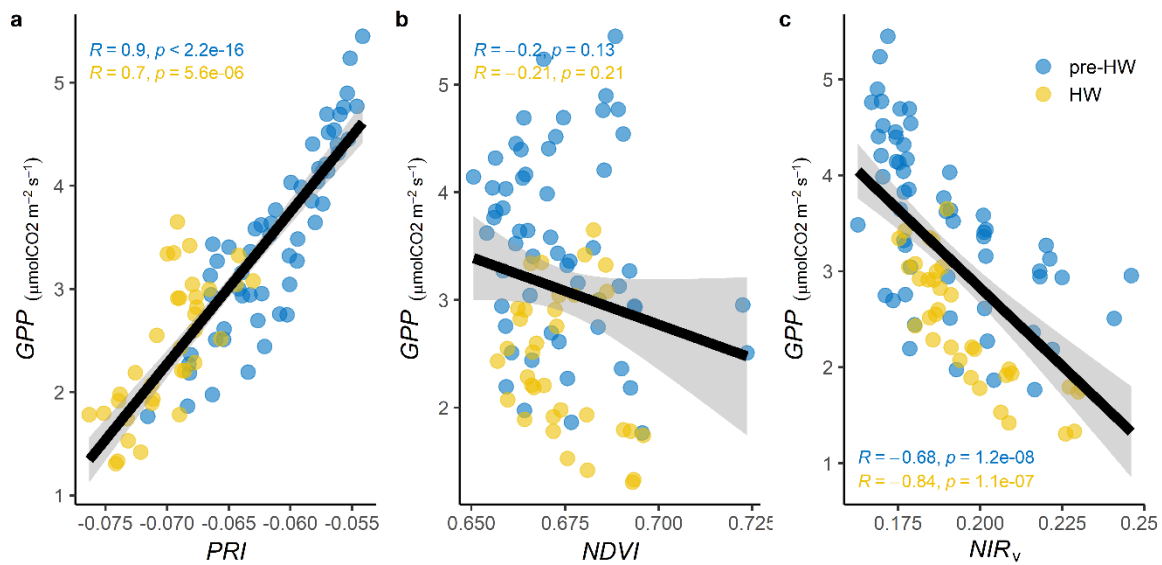
Supplementary Fig. S6: Simulations with the Soil Canopy Observation, Photochemistry and Energy fluxes (SCOPE) model on the effect of diffuse to total radiation on normalized difference vegetation index ($NDVI$) in (a), near-infrared reflectance of vegetation (NIR_v) in (b), photochemical reflectance index (PRI) in (c) and sun-induced fluorescence at 760 nm (SIF) in (d). The range of diffuse to global radiation is consistent with what was observed at the Majadas de Tiétar site during the 2018 heatwave (HW). Simulations were performed with an air temperature (T_{air}) of 43°C.



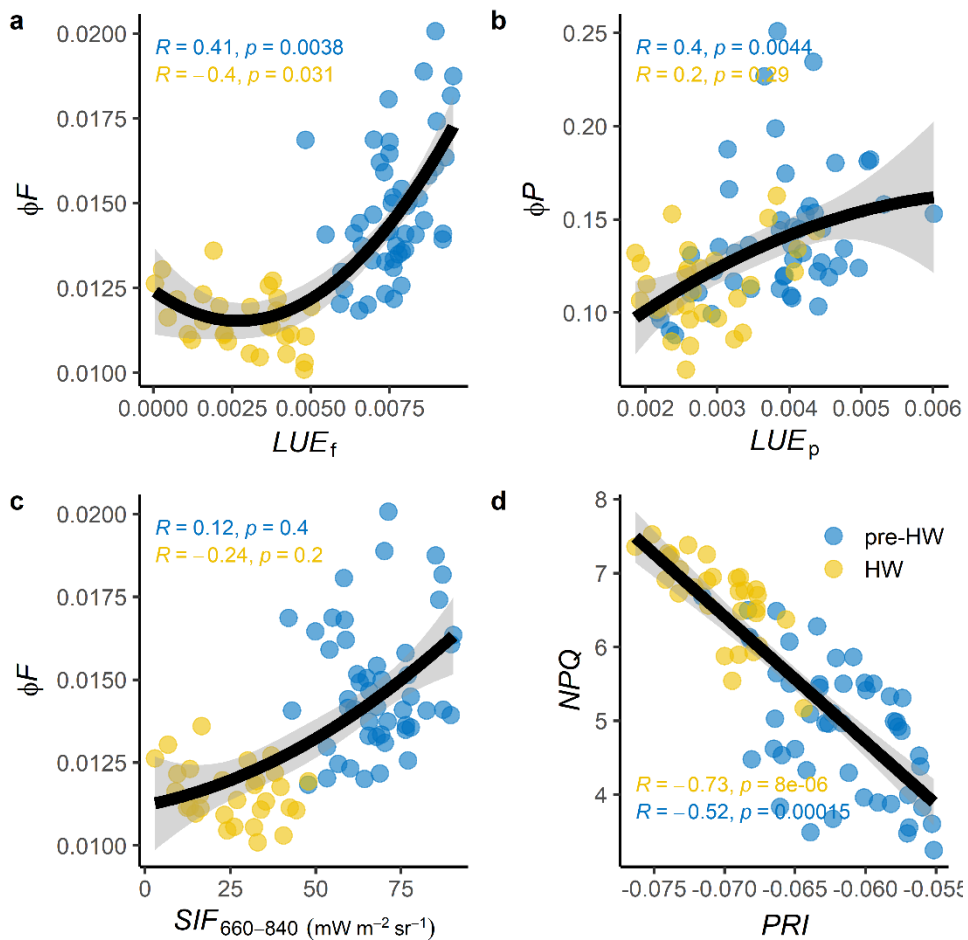
Supplementary Fig. S7. (a) Scatterplot between light use efficiency of photosynthesis (LUE_p) and light use efficiency of *SIF* emission (LUE_f). (b) Scatterplot between nonphotochemical quenching (NPQ) and gross primary production (GPP). The days before the heatwave (pre-HW) and the days during the heatwave (HW) are differentiated by different color gradients. Paths connect consecutive observation in a given day. The color of the points and paths refers to the reversible component of the nonphotochemical quenching (NPQ_r). The size of the paths is proportional to the sustained component of the nonphotochemical quenching (NPQ_s). The hour (UTC) of the observations is also displayed. Hourly mean values are computed from 9 to 16 UTC. The black line is the overall fit from a second degree polynomial in (a) and a linear regression in (b). The shaded area represents the 95% confidence interval of the fit.



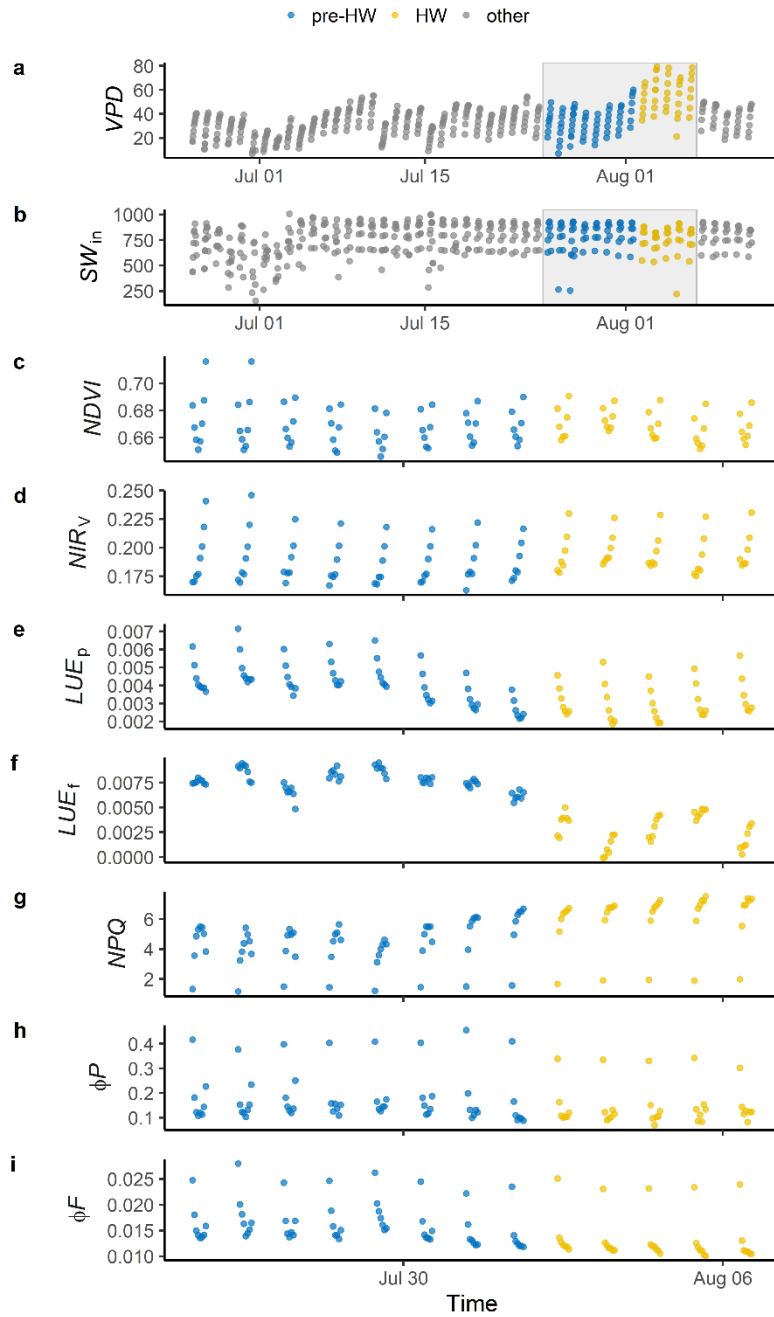
Supplementary Fig. S8. Relationship between yield of photochemistry (ϕP) and yield of fluorescence (ϕF) for the pre-heatwave (pre-HW) period (circles) and for the heatwave (HW) period (triangles) between 11 to 16 UTC. Points are colored by the hour of the day (UTC). Linear regressions for the HW (yellow line) and pre-HW (blue line) is displayed. Spearman's rank correlation coefficient (R) and p value are reported for the pre-HW and HW period. The shaded area represents the 95% confidence interval of the fit.



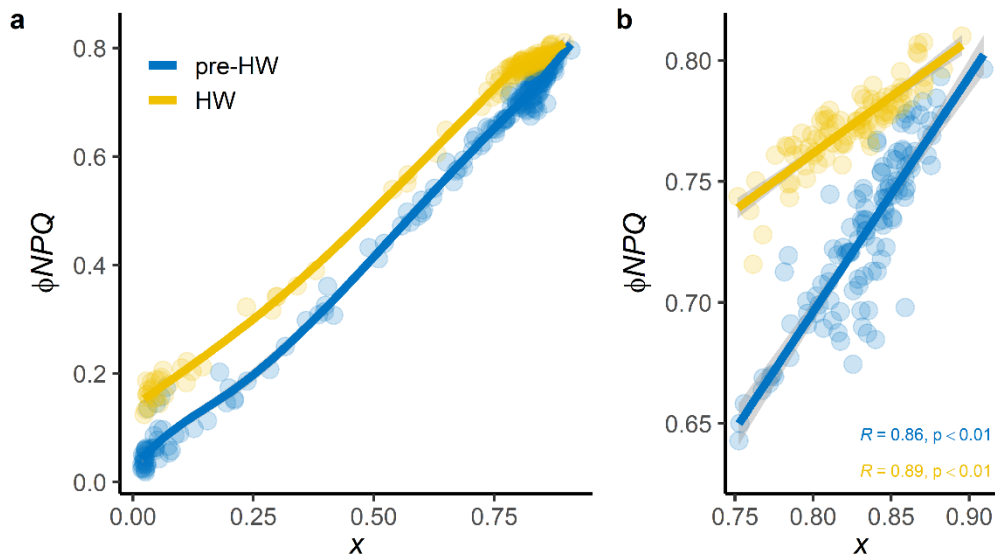
Supplementary Fig. S9. (a) Scatterplot between gross primary production (*GPP*) and photochemical reflectance index (*PRI*). (b) Scatterplot between *GPP* and normalized vegetation index (*NDVI*). (c) Scatterplot between *GPP* and near-infrared reflectance of vegetation (*NIR_v*). Blue points correspond to the pre-heatwave (pre-HW) period and yellow points correspond to the heatwave (HW) period. Hourly mean values are computed from 9 to 16 UTC. In each panel the Spearman's rank correlation coefficient (*R*) and *p* value are reported for the pre-HW and HW period. The black line is the overall fit from a linear regression. The shaded area represents the 95% confidence interval of the fit.



Supplementary Fig. S10. (a) Scatterplot between yield of fluorescence (ΦF) and light use efficiency of *SIF* emission (LUE_f). (b) Scatterplot between yield of photochemistry (ΦP) and light use efficiency of photosynthesis (LUE_p). (c) Scatterplot between ΦF and sun-induced fluorescence integrated between 660 and 840 nm ($SIF_{660-840}$). (d) Scatterplot between nonphotochemical quenching (NPQ) and the photochemical reflectance index (PRI). Blue points correspond to the pre-heatwave (pre-HW) period and yellow points correspond to the heatwave (HW) period. Hourly mean values are computed from 10 to 16 UTC. In each panel the Spearman's rank correlation coefficient (R) and p value are reported for the pre-HW and HW period. The black line is the overall fit from a second degree polynomial in (a) and a linear regression in (b,c,d). The shaded area represents the 95% confidence interval of the fit.



Supplementary Fig. S11. Hourly means of (a) vapor pressure deficit (VPD), (b) shortwave incoming radiation (SW_{in}), (c) normalized difference vegetation index ($NDVI$), (d) near-infrared reflectance of vegetation (NIR_v) (e) light use efficiency of photosynthesis (LUE_p), (f) light use efficiency of SIF emission (LUE_f), (g) nonphotochemical quenching (NPQ), (h) yield of photochemistry (ϕ_P) and (i) yield of fluorescence (ϕ_F).



Supplementary Fig. S12. (a,b) Scatterplot between yield of nonphotochemical quenching (Φ_{NPQ}) and relative light saturation of photosynthesis (x). Blue points correspond to the pre-heatwave (pre-HW) period and yellow points correspond to the heatwave (HW) period. Hourly mean values with $x > 0.75$ are shown in (B). In (a) the lines are a local polynomial regression. In (b) the lines represent linear regression and the Spearman's rank correlation coefficient (R) and p value are reported for the pre-HW and HW period. The shaded area represents the 95% confidence interval of the fit.

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- Reichstein M, Falge E, Baldocchi D, Papale D, Aubinet M, Berbigier P, Bernhofer C, Buchmann N, Gilmanov T, Granier A, et al. 2005.** On the separation of net ecosystem exchange into assimilation and ecosystem respiration: review and improved algorithm. *Global Change Biology* **11**(9): 1424-1439.