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UNTWIST will use the resilient European oilseed crop camelina in a multidisciplinary approach to decipher the diverse heat and drought stress response mechanisms associated with genetic diversity and use this knowledge to establish predictive models for the tangible improvement of cropping systems.

Using metabolomics and predictive metabolomics to study the physiology of an old rustic oilseed plant

Malo Le Boulch¹, Millena Barros-Santos^{1,2,3}, Susana Silvestre⁴, Dominik Grosskinsky⁶, Anaïs Da Costa⁷, Frédérique Tellier⁷, Amélie Flandin^{1,2,3}, Cédric Cassan^{1,2,3}, Paloma Leon⁹, Sophie Colombié^{1,2,3}, Javier Prieto⁹, Federica Zanetti⁸, Jean-Denis Faure⁷, Claudia Jonak⁶, Björn Usadel⁵, Richard Haslam⁴, Yves Gibon^{1,2,3}, Pierre Pétriaccq^{1,2,3*}, Sylvain Prigent^{1,2,3*}

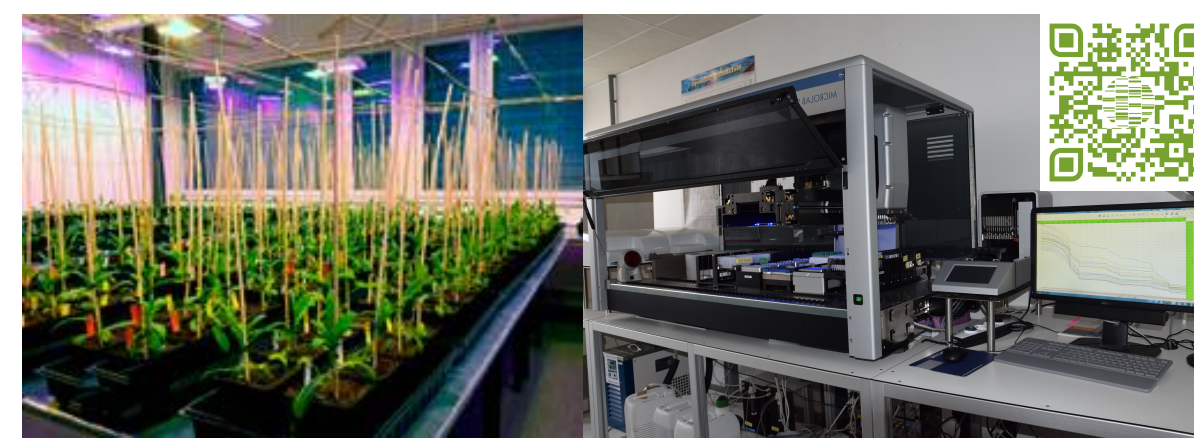
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Introduction

- Targeted and untargeted metabolomics analyses on 54 *Camelina sativa* lines grown under three different conditions (control, heat, and drought stress).
- The same 54 lines were also phenotyped in field trials across Europe (France, England, Italy and Spain) and genotyped.
- We used machine-learning and data analysis to link greenhouse metabolome and field phenotypes of the different *Camelina sativa* lines.

Methodology



Greenhouse data acquisition
- On leaves of plants grown in greenhouses under control and stress conditions
- Targeted and untargeted metabolomics
- Genome sequencing of the 54 lines



Phenotyping data acquisition in fields
- Under agronomical conditions
- In four different locations across Europe

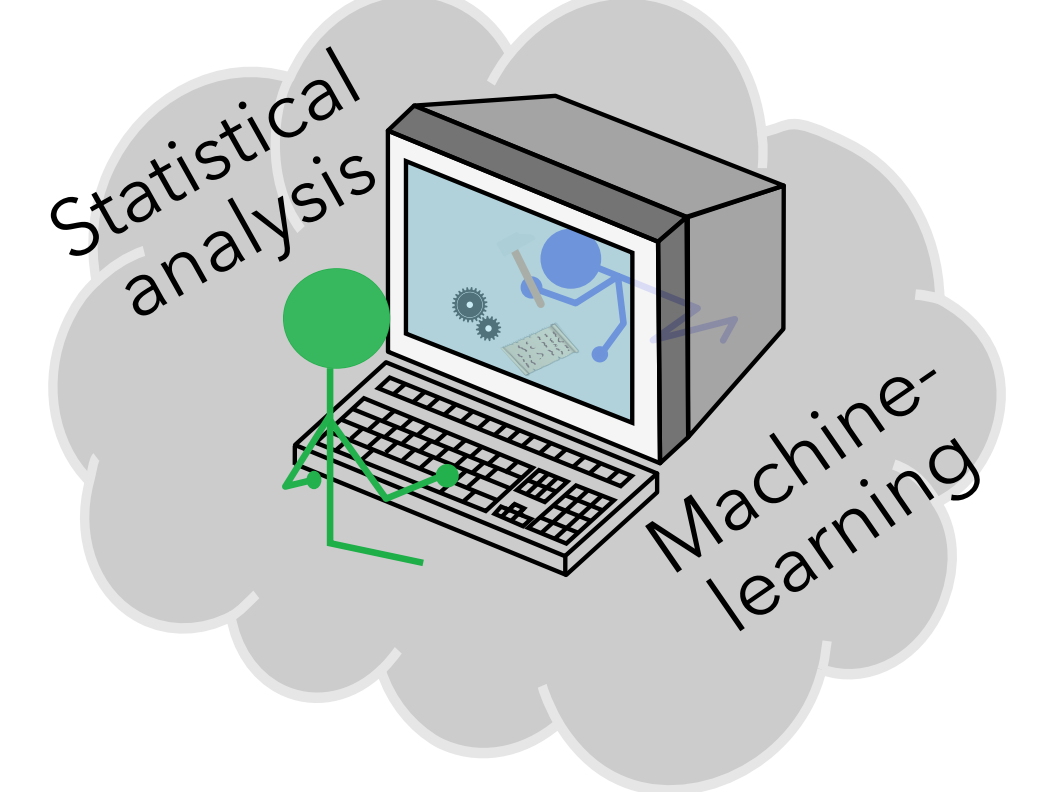
54 lines
3 conditions
950 samples

ESI- Blanks QC

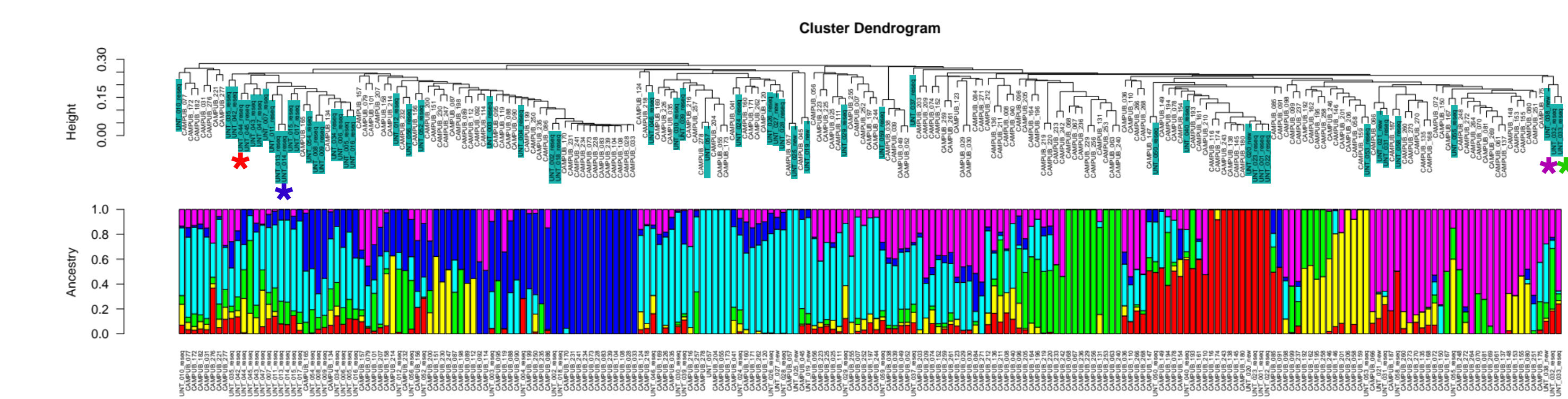
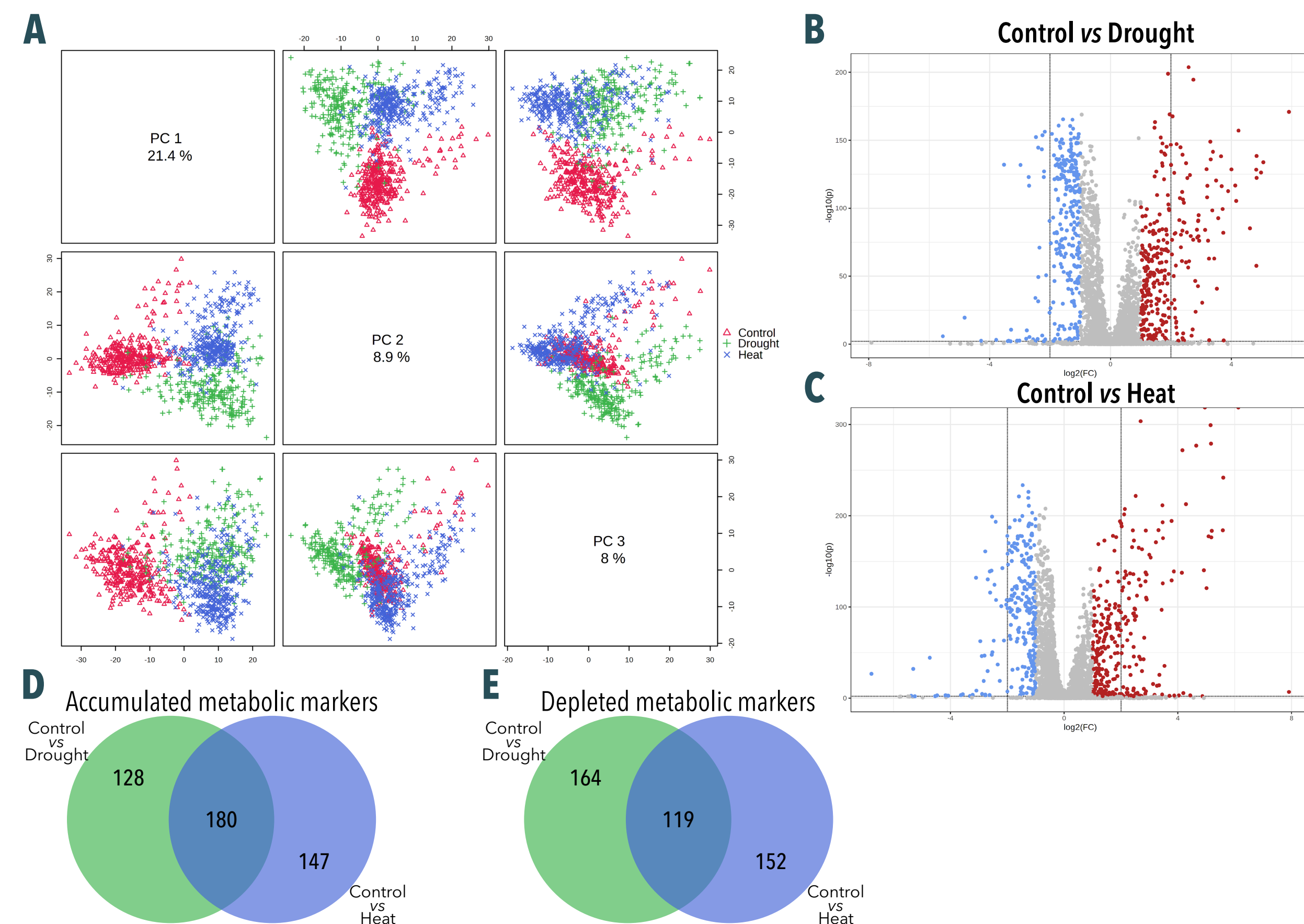


UHPLC-LTQ-Orbitrap mass spectrometry (thermoScientific)
Full Scan
DDA

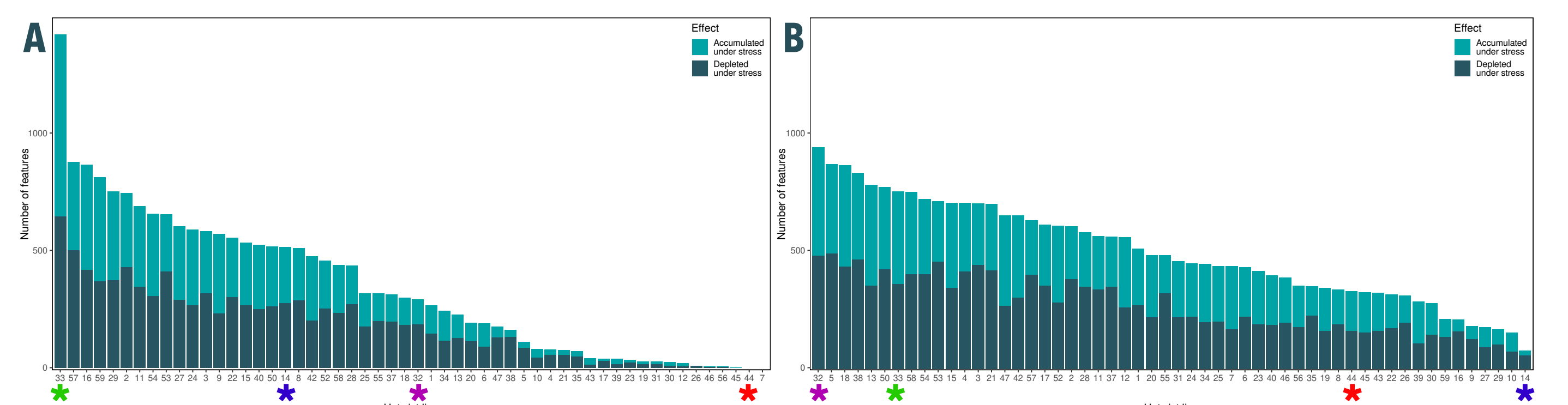
Untargeted LC-MS: (Luna et al. 2020)
- Raw features : 11680
- After SN > 10 : 10869
- After CV QC < 30% : 3016 final features
Targeted measurements:
- 9 major biomass components
- Starch, citrate, glucose, sucrose, malate, chlorophyll A&B, protein and amino-acid



Results

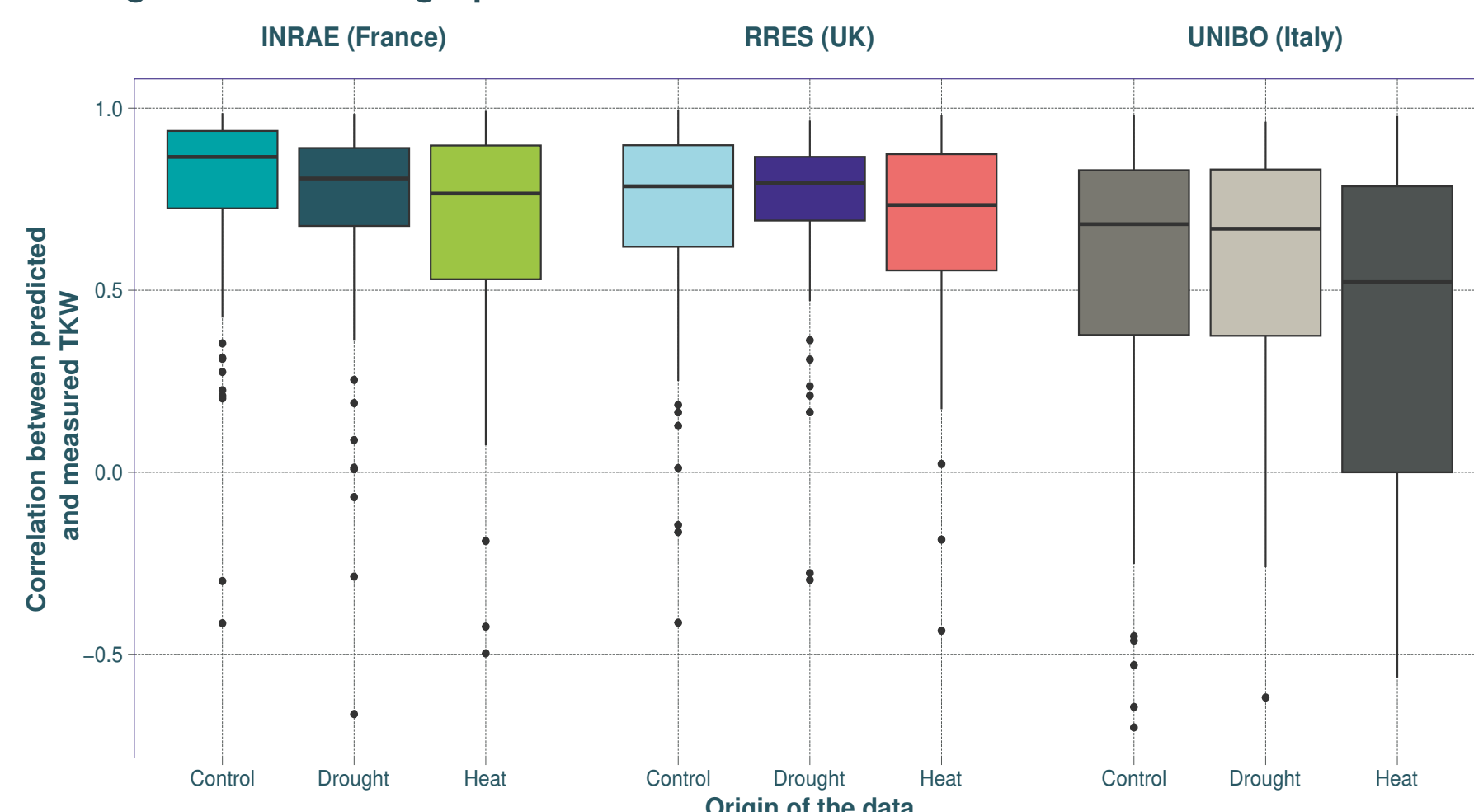


Hierarchical clustering and ADMIXTURE analysis of the Untwist lines and publicly available accessions. IBG distances were hierarchically clustered and 9 sub-populations were assumed.



Metabolomic responses of individual camelina lines to drought and heat stress. Volcano plots for each individual *Camelina* line were constructed. The resulting accumulated and depleted markers were stacked for drought (A) and heat stress (B). Colored stars correspond to highlighted lines in the genetic clustering.

Global metabolic responses of *Camelina* lines to drought and heat stress
(A) PCA score plots of normalised untargeted features (B-C) Volcano plots of metabolic markers that were accumulated (red) or depleted (blue) in response to drought (B) or heat stress (C). (D-E) Venn diagrams showing specific and common metabolic markers identified by volcano plots.



Predictive metabolomics for Thousand Kernel Weight in three locations using three datasets. Machine-learning models were built using Ridge, elastic-net and LASSO regression models splitting randomly the dataset into 80/20% one hundred time, using a 3 time 10-fold CV for training. Best models were chosen based on RMSE and correlation between measured and predicted values is displayed.

Conclusion & Perspectives

- Camelina sativa* lines have very diverse metabolic responses to different stresses
- Stress response from metabolic point of view seems not entirely linked to the genetic background of the lines
- Predictive metabolomics enabled the prediction of an agronomic trait of interest using data coming from greenhouses
- More predictions are ongoing using other machine-learning models and to predict other physiological variables
- Annotation of the different metabolic markers in progress