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Bandwagon status for metabolomics in
plant phenotyping?

PHENOME
EMPHASIS | FRANCE




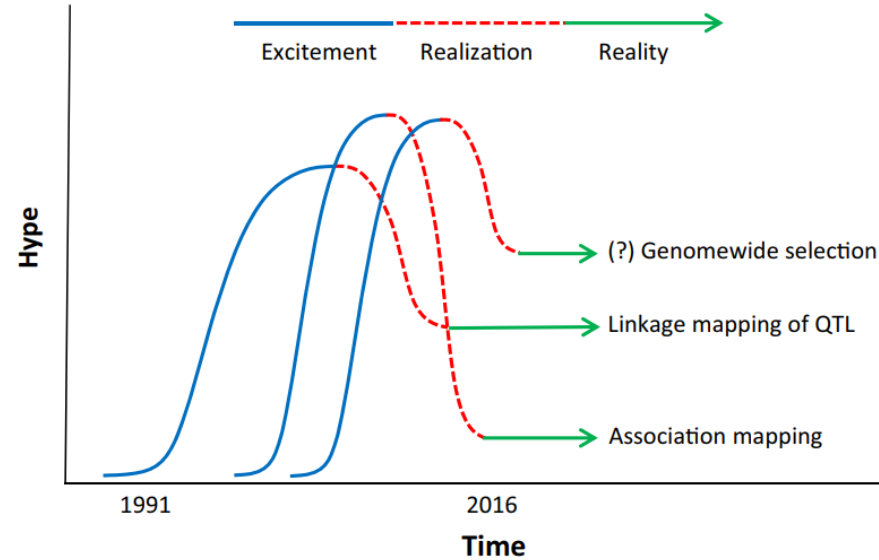
➤ Bandwagons in plant breeding

Theor Appl Genet (2016) 129:2323–2332
DOI 10.1007/s00122-016-2772-5

OPINION PAPER

Bandwagons I, too, have known

Rex Bernardo¹ 



Other advances, such as metabolomics, never achieved bandwagon status in plant breeding. This was likely due to the high level of technical knowledge and skills, as well as equipment and infrastructure, needed for metabolomics investigations.



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Modelling Metabolism
Yves Gibon / UMR1332 BFP

➤ The purpose of non-targeted metabolomics

Quick and reliable information about metabolism

Metabolism provides **energy** and bricks for **biomass construction**, **defence**, **attraction**, **signalling**...

The metabolome contains information about the **past** (slow turnover metabolites), the **present** (high turnover metabolites) and the **future** (precursors of biomass components or volatiles)



➤ Equipment and infrastructure

Combining **robotics** and **high resolution mass spectrometry**

Equipment: 800 k€, 80-160k€/year

Maintenance: 10 k€/year

Running costs: 10 k€/year

Human resource: 50k€/year

20,000 samples per year

Up to 20,000 m/z per sample

8-12€ per sample (from sample to raw data) – instead of 50-500€

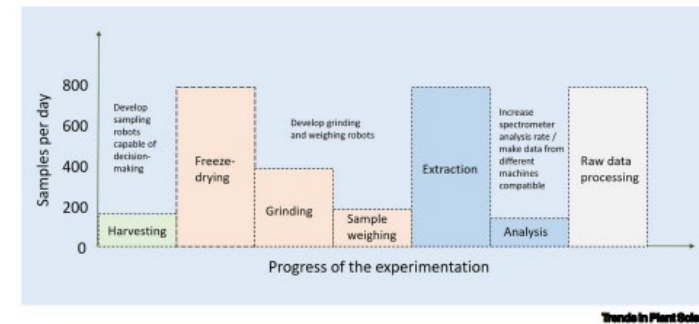


Figure 3. Current sample harvesting and LC-MS-based analysis capacities with indications of where additional developments are required to meet the needs for integration into an *in vivo* HTP (molecular) phenotyping facility. Abbreviations: HTP, high throughput; LC-MS, liquid chromatography-mass spectrometry.

Hall et al. (2022)

➤ LC-HRMS Metabolomics pipeline

Up to thousands of samples

Data acquisition ↓ *Robotised extraction*
Automated injection (20 min/sample)

Raw data (**#Gb/sample**) -> public data repository in open source version (MetaboLights)

Data pre-processing ↓ *Noise filtering, baseline correction, peak detection, alignment, missing values...*
Quality control (QC) sample or extract for interoperability
Spectral annotation

Pre-processed data: m/z and identified metabolites (**#Mb/sample**) -> public data repository

Data analysis ↓ *Unsupervised* ↓ *Supervised* ↓ *Pathway reconstruction*

Exploration Top-down modelling Bottom-up modelling



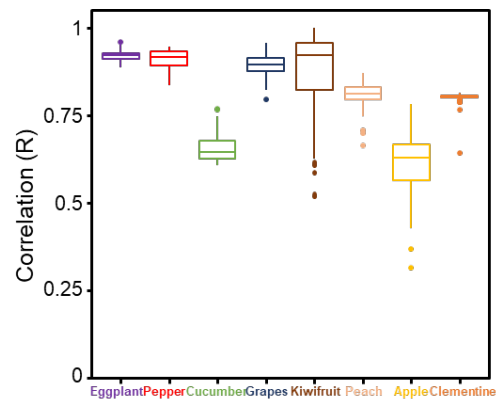
➤ Predictive metabolomics

Diversity: genotypes, species, conditions...

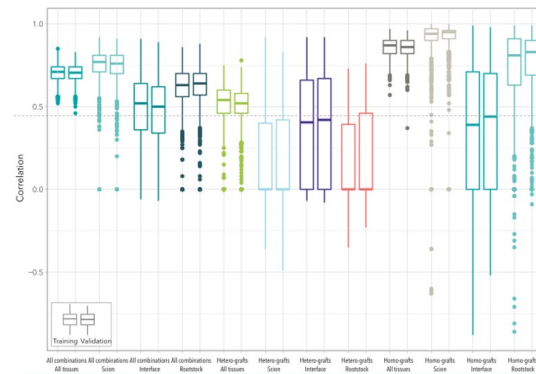
Predictors: metabolic features

Traits to predict: yield, robustness...

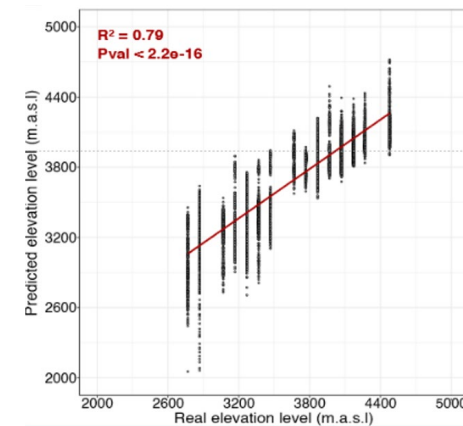
Modelling: Trait = C + a₁*met₁ + a₂*met₂ + a₃*met₃ + + a_n*met_n



**Relative growth rate
in fruit**



Grafting success in grapevine



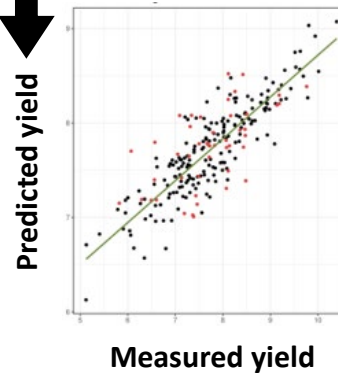
**Elevation at which 24
species grow in the
Atacama desert**

➤ Can we predict yield?

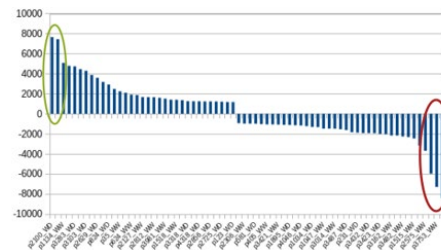
Genotypes grown under (semi)-controlled conditions
-> Leaf samples -> Metabolomics



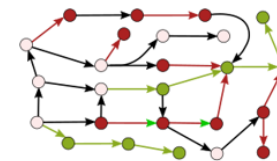
Modelling



Same genotypes evaluated in the field for yield



Identification of the most predictive variables



Elucidation of the mechanisms



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➤ Was metabolism involved in maize selection?

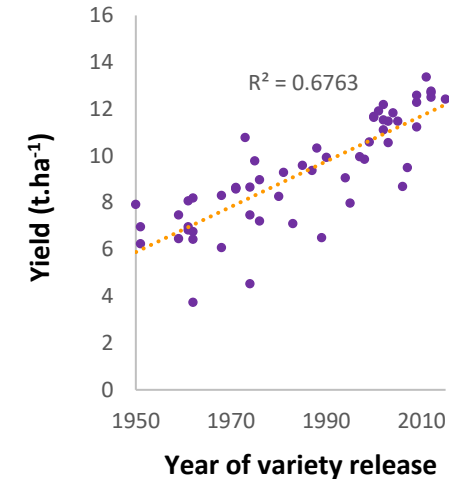
Received: 30 November 2018 | Revised: 14 February 2019 | Accepted: 14 February 2019
DOI: 10.1111/pce.13539

ORIGINAL ARTICLE

WILEY Plant Cell & Environment

Changes in the vertical distribution of leaf area enhanced light interception efficiency in maize over generations of selection

Raphaël P.A. Perez^{1,2}  | Christian Fournier¹ | Llorenç Cabrera-Bosquet¹  |
Simon Artzet¹ | Christophe Pradal² | Nicolas Brichet¹ | Tsu-Wei Chen^{1,3}  |
Romain Chapuis⁴ | Claude Welcker¹ | François Tardieu¹ 

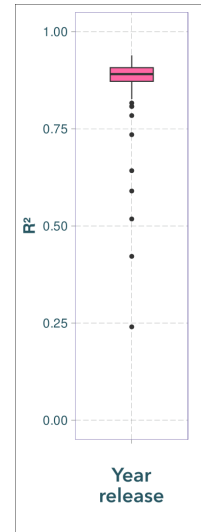
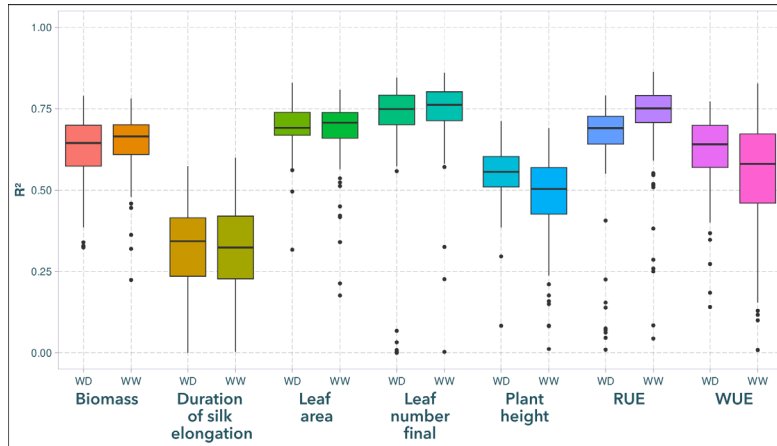


60 maize hybrids released from 1950 to 2015

Authors concluded that a developmental trait (vertical distribution of leaf area) was the main indirect target of selection

To check the involvement of metabolism, leaf samples were taken from plants of this “genetic progress” panel grown under well watered (WW) or water deficit (WD) conditions at PhenoArch and the metabolome was analysed using a non-targeted approach (#3000 m/z)

➤ Modelling the year of release

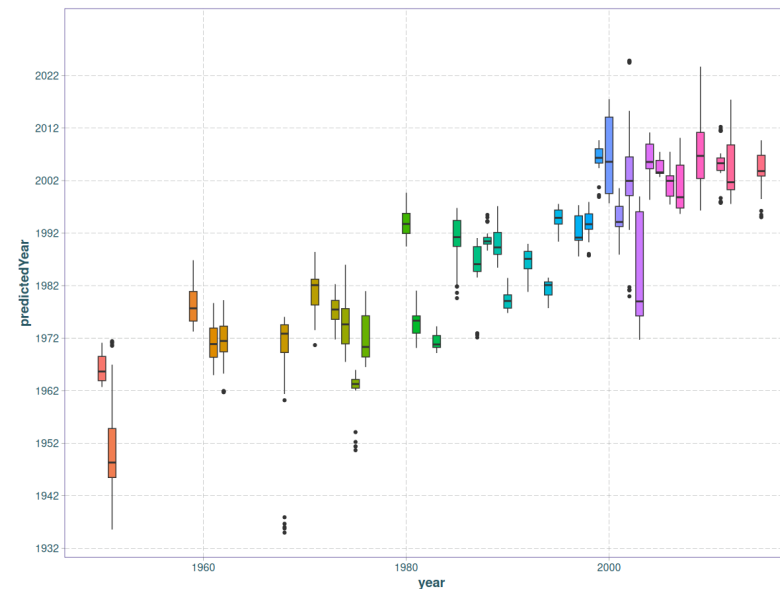


80% of the data to construct the models, 20% to test them (100X)

Models were successfully built for traits measured at PhenoArch

It also worked for the **year of release** of the hybrids

Validation: models were built with all years of release except one, which was used to test them

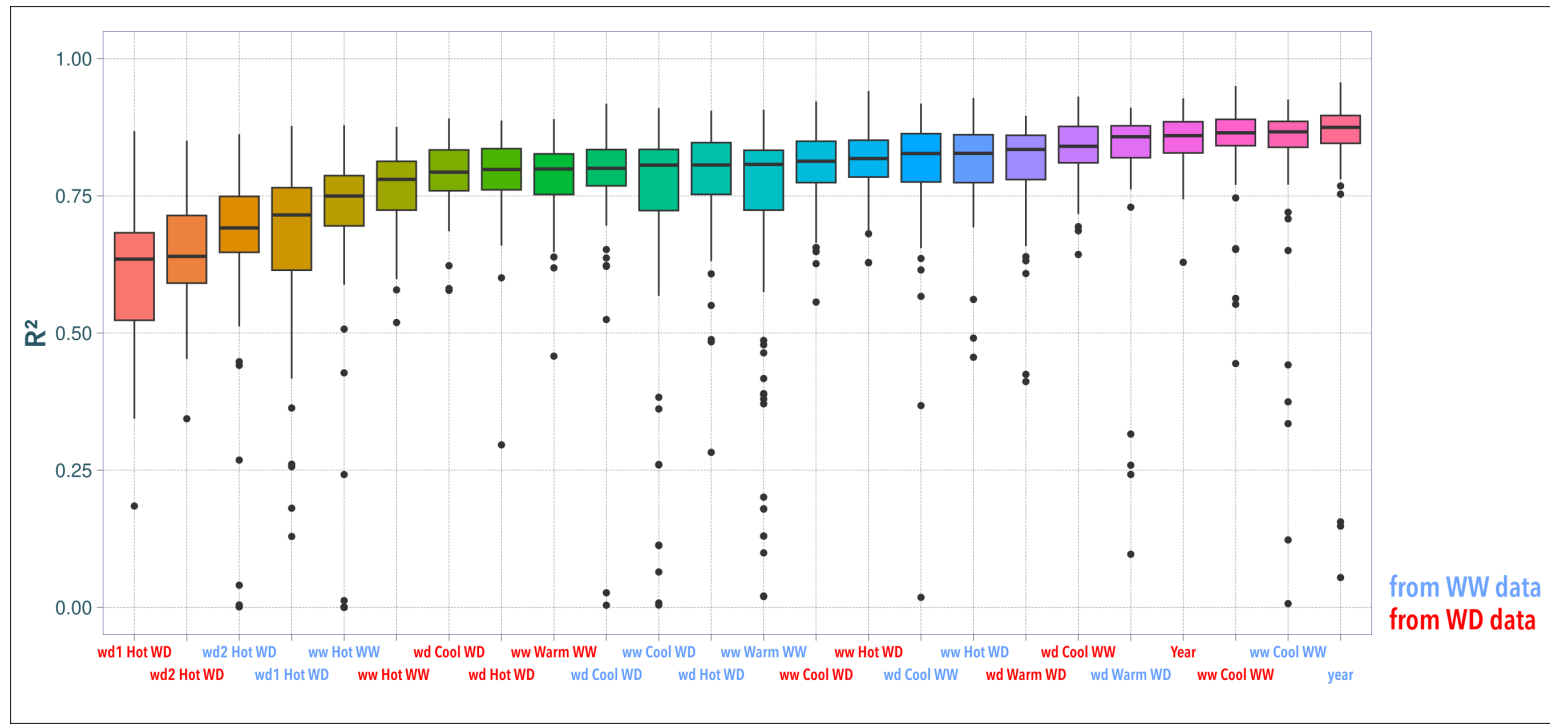


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➤ Modelling yield of the “genetic progress” panel



Distributions of R^2 obtained for yield measured in various field experiments



➤ Conclusion - Outlook

Metabolomics have progressed

- Sampling remains a bottleneck
- Interoperability can be a problem

Trade-off between prediction value and costs

- Costs decrease when throughput increases (most of the costs are linked to the acquisition of equipment). Less than 5€ per sample possible
- Metabolomics can provide good predictions from plants at early growth stages

When to use predictive metabolomics?

- Niche species
- Multi-species (agroecology)

