Modeling anthocyanin composition during grape berry development:
another way of phenotyping

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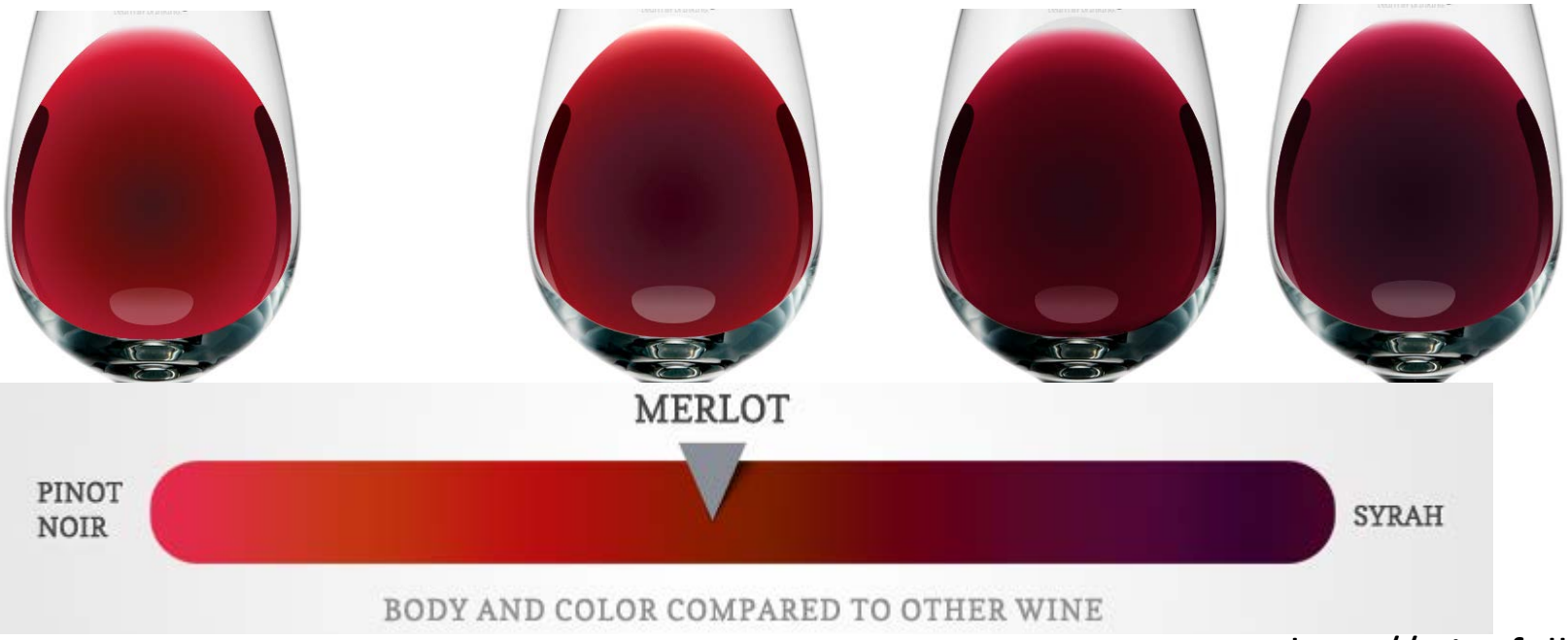
Anthocyanins are important quality indicator for grapes

Pinot Noir

Merlot

Cabernet Sauvignon

Syrah

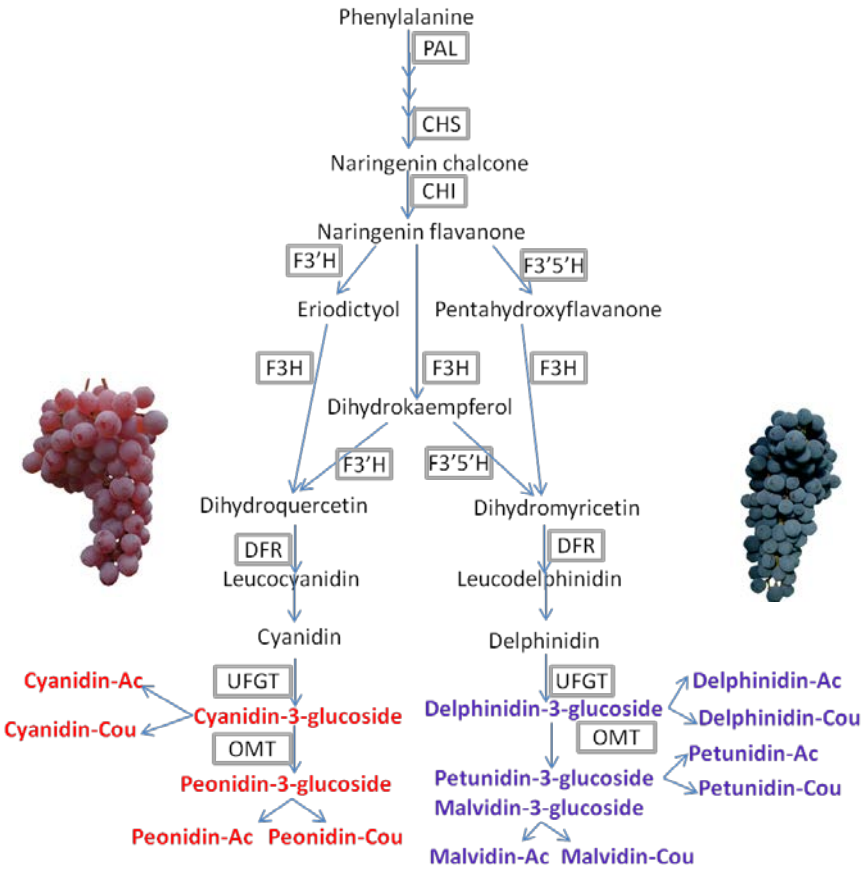


http://winefolly.com/

Genetic diversity of anthocyanin content and composition

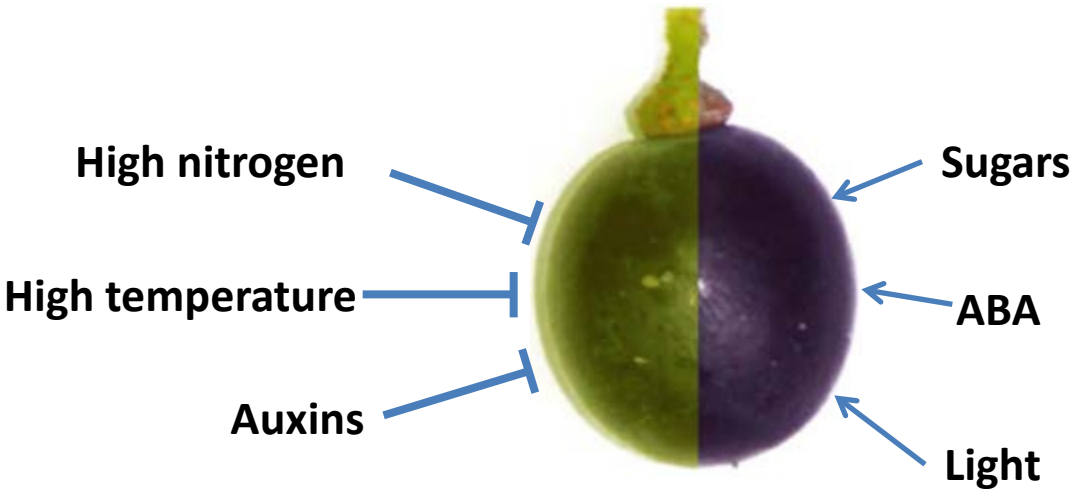
- Wide variation in total anthocyanin content and composition;

Shimazaki et al. 2011



Castellarin and Di Gaspero, 2007

Factors affect anthocyanin synthesis



adapted from Böttcher and Davies, 2012

Anthocyanins: a complex trait

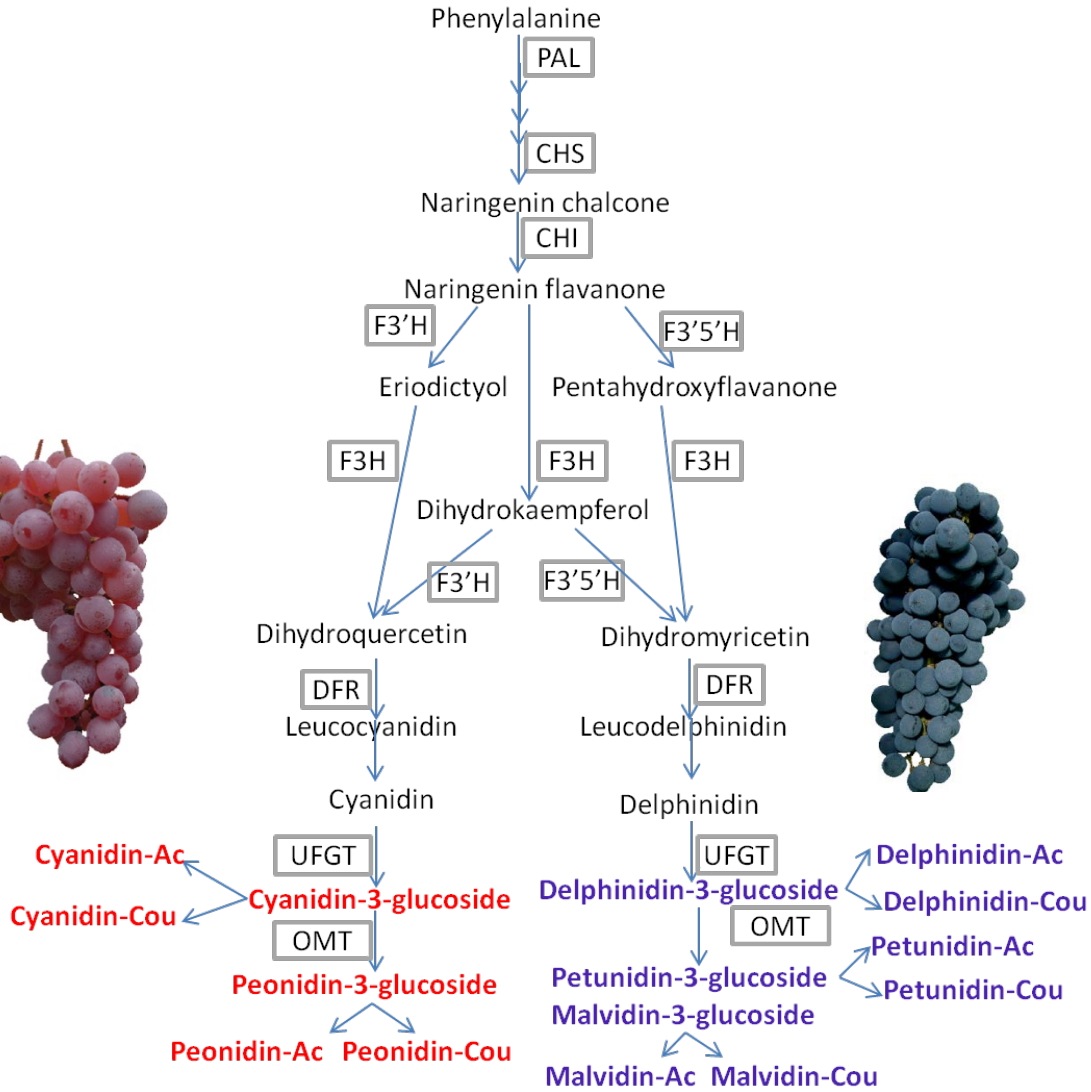
Phenotype= f (genotype, environment, development)

high instability of a trait turns into a bottleneck in identifying reliable molecular markers to genetically improve the trait

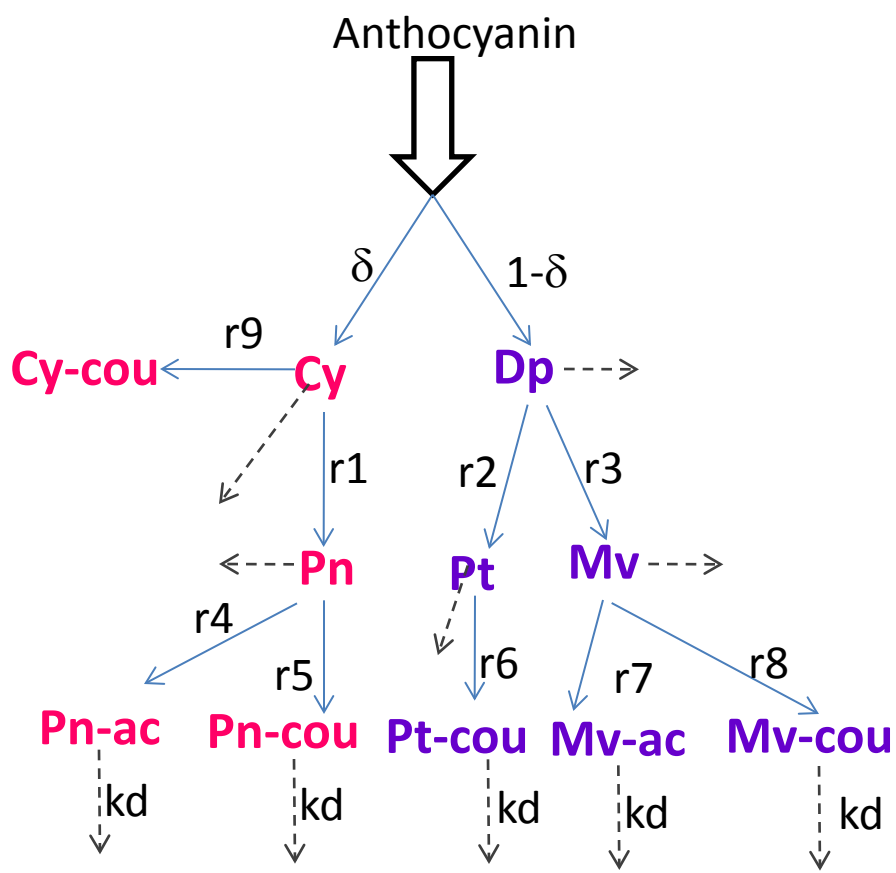
How to dissect a complex trait into more simple and stable ones?

Mathematic models can integrate multiple processes and quantify the relative contribution of each to a trait.

Anthocyanin model: Anthocyanin metabolism pathway



A dynamic model of anthocyanin composition



$$Ai = \int_{t0}^{tmax} \frac{dAi}{dt} \qquad CAi = \frac{100Ai}{FW}$$

$$TA = \sum_{i=1}^{11} Ai = Cy + Dp + Pn + Pt + Mv + Pn_{ac} + Pn_{cou} + Pt_{cou} + Mv_{ac} + Mv_{cou} + Cy_{cou}$$

$$\frac{dTA}{dt} = \frac{dTAobs}{dt} + kdTA$$

$$\frac{dCy}{dt} = \delta\frac{dTA}{dt} - (r1 + r9 + kd)Cy$$

$$\frac{dDp}{dt} = (1-\delta)\frac{dTA}{dt} - (r2 + r3 + kd)Cy$$

$$\frac{dPn}{dt} = r1Cy - (r4 + r5 + kd)Pn$$

$$\frac{dPt}{dt} = r2Dp - (r6 + kd)Pt$$

$$\frac{dMv}{dt} = r3Dp - (r7 + r8 + kd)Mv$$

$$\frac{dPn\_ac}{dt} = r4Pn - kdPn\_ac$$

$$\frac{dPn_{cou}}{dt} = r5Pn - kdPn_{cou}$$

$$\frac{dPt_{\_cou}}{dt} = r6Pt - kdP\_cou$$

$$\frac{dMv_{\_ac}}{dt} = r7Mv - kdMv_{\_ac}$$

$$\frac{dMv\_cou}{dt} = r8Mv - kdMv\_cou$$

$$\frac{dCy\_cou}{dt} = r9Cy - kdCy\_cou$$

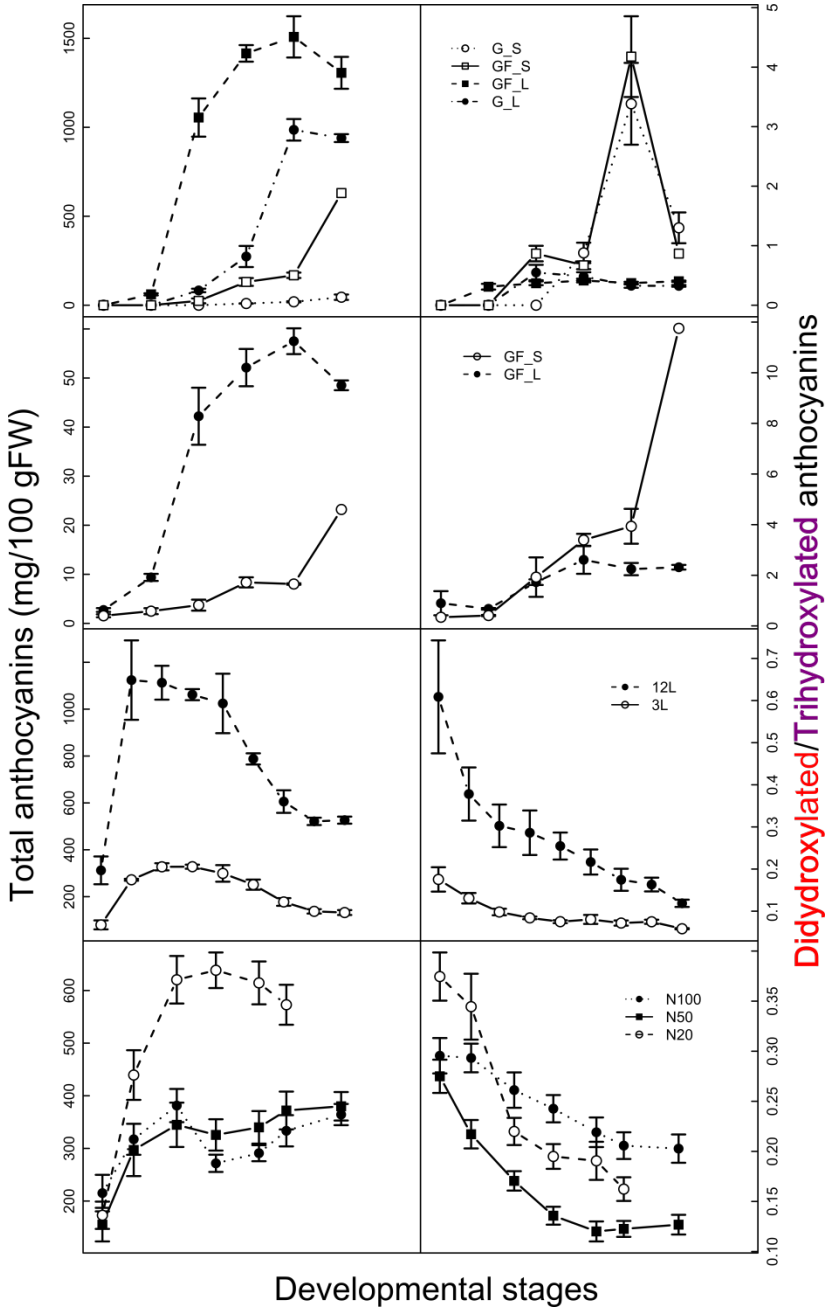
Plasticity of anthocyanin content and composition

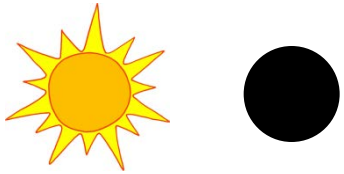
Skin
Gamay Freaux

Pulp
Gamay Freaux

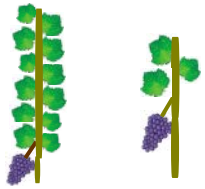
Cabernet Sauvignon

Merlot





Guan et al., 2015 submitted

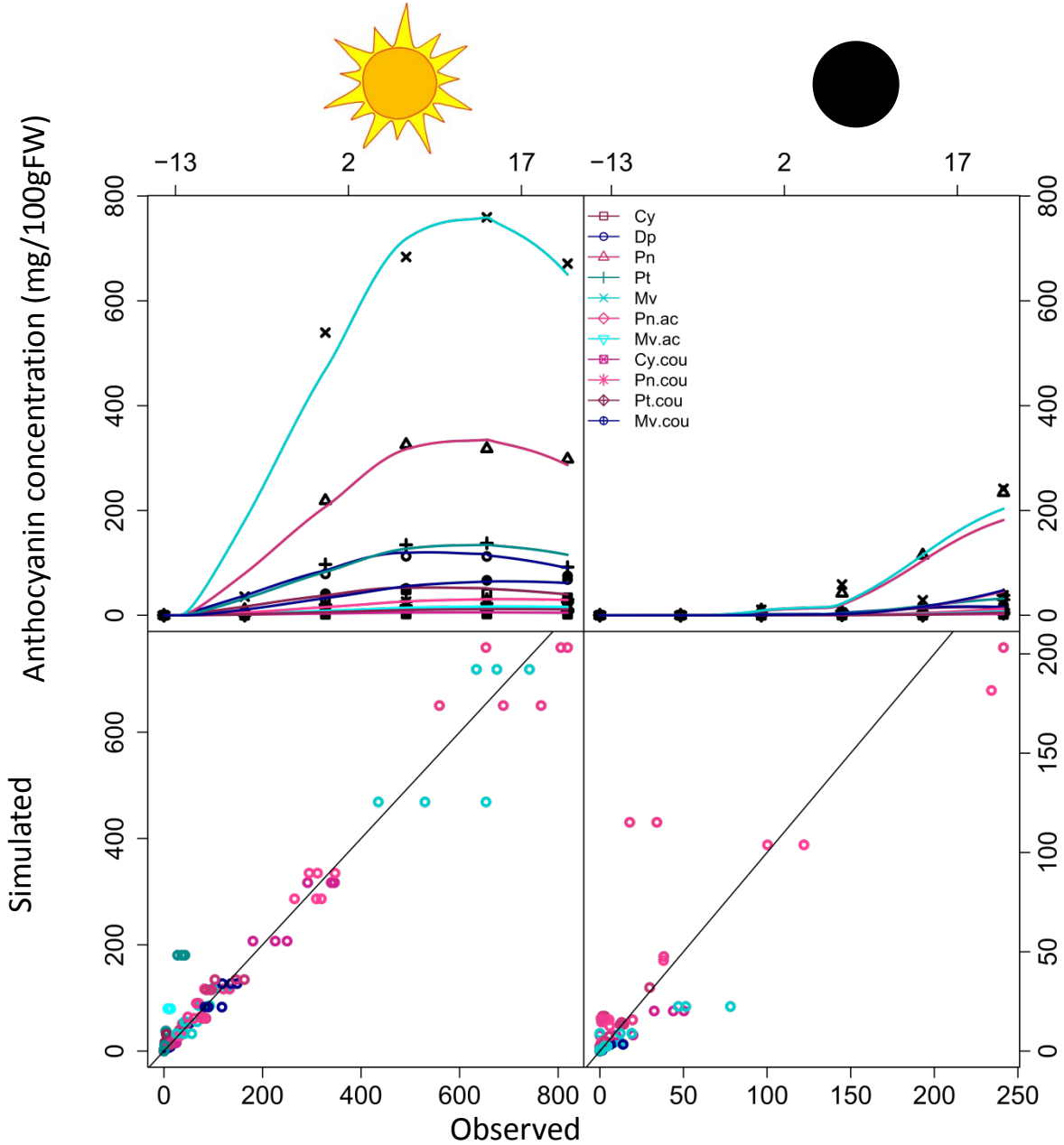


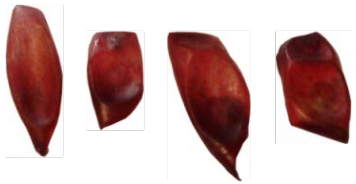
Bobeica et al., 2015

N N

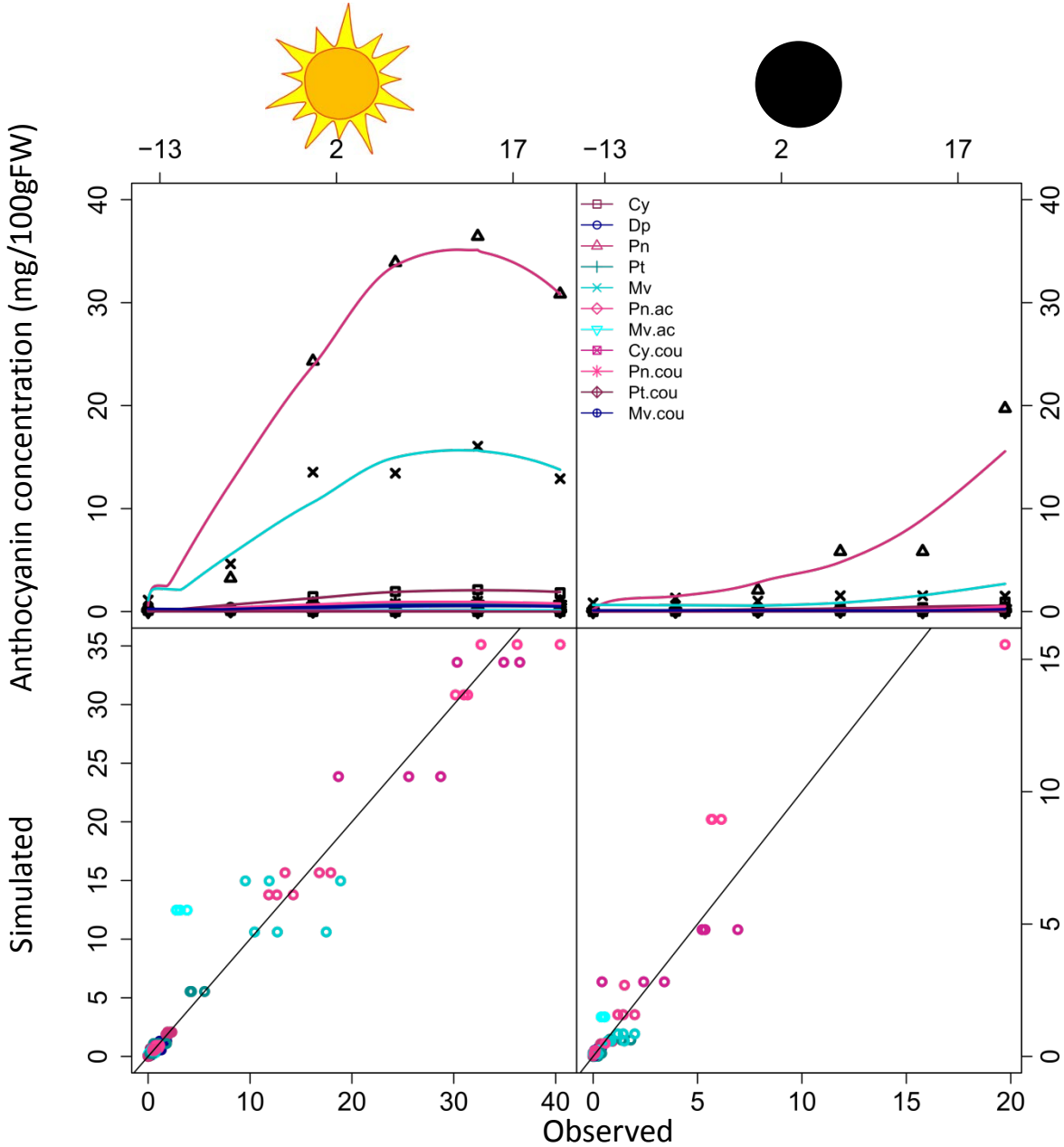
Hilbert et al., 2003

Simulating the effect of light on anthocyanin composition

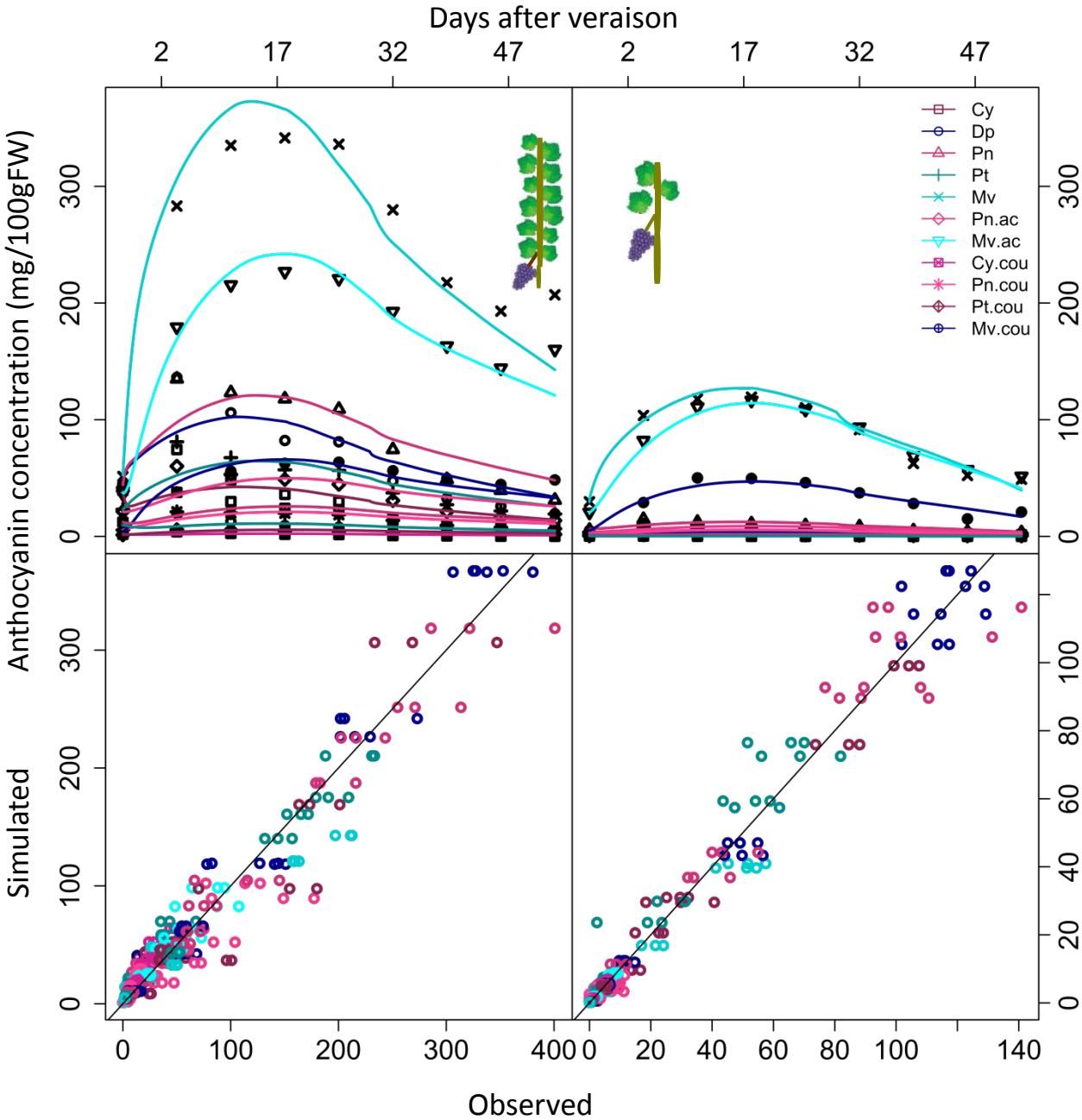




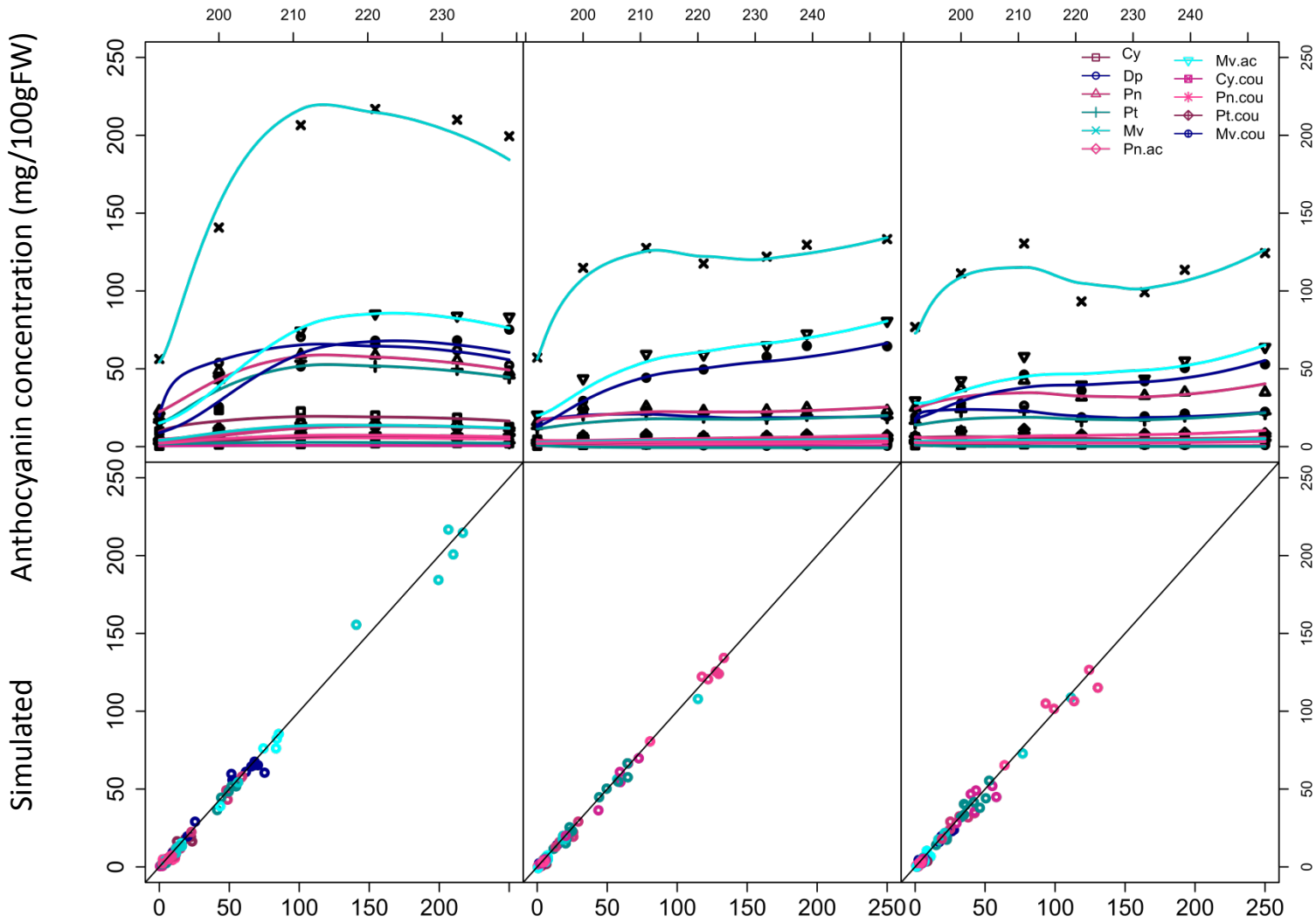
Simulating the effect of light on anthocyanin composition



Simulating the effect of carbon supply on anthocyanin composition

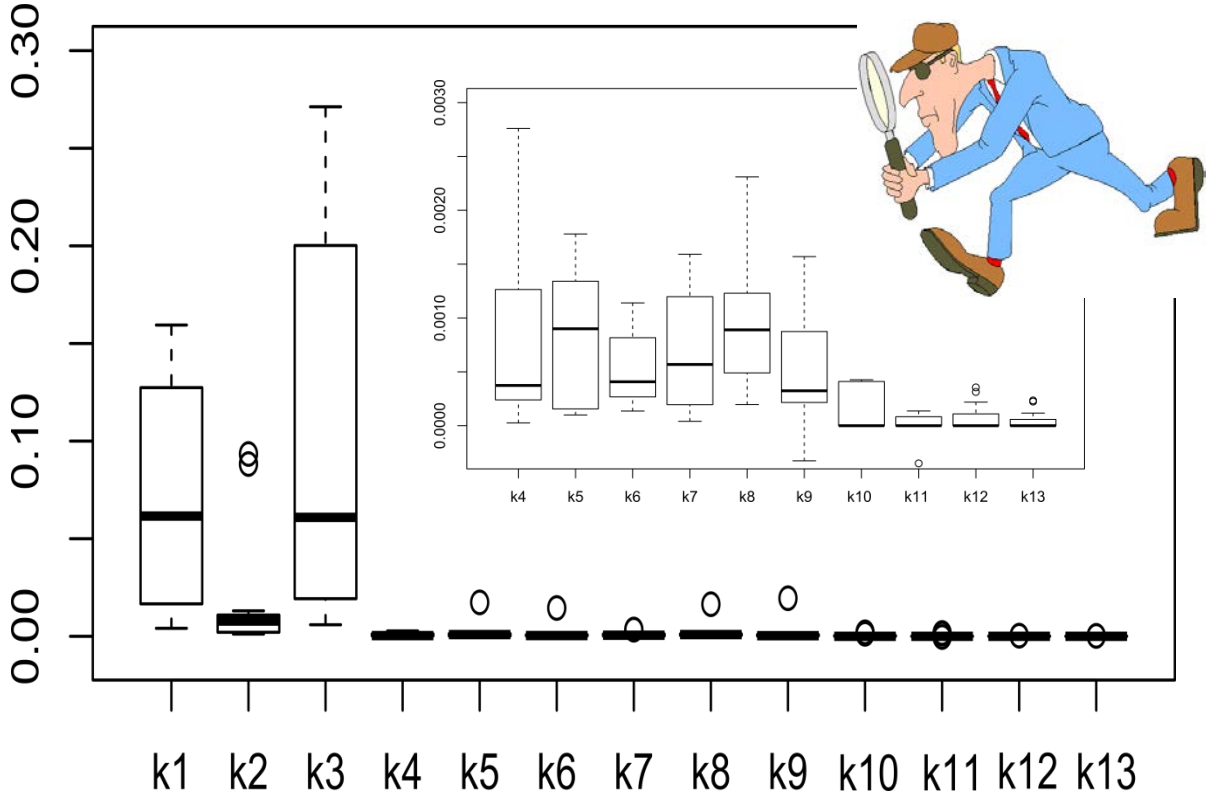


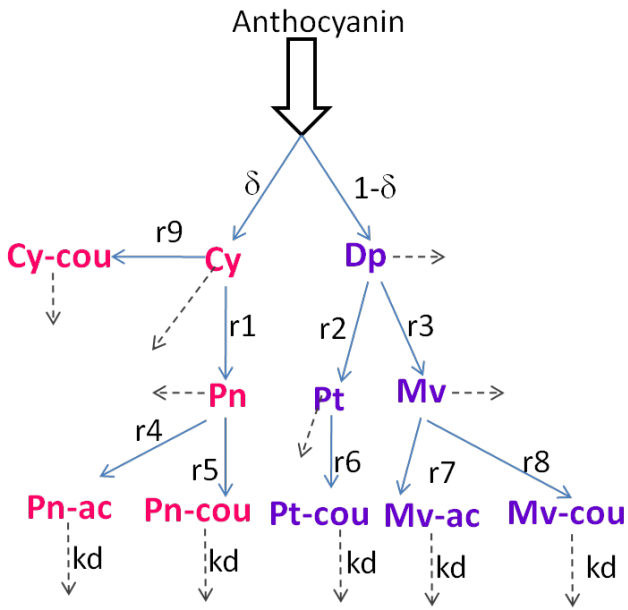
Simulating the effect of nitrogen on anthocyanin composition



N20 **N50** **N100**

Model parameter represents enzyme properties





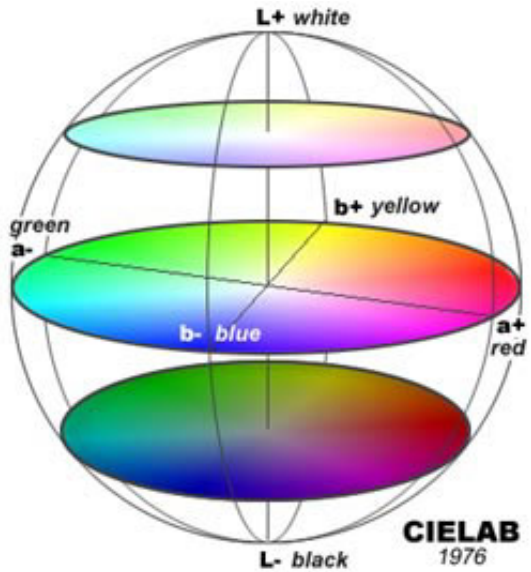
$$v = \frac{v_{\max}[S]}{[S] + K_m}$$

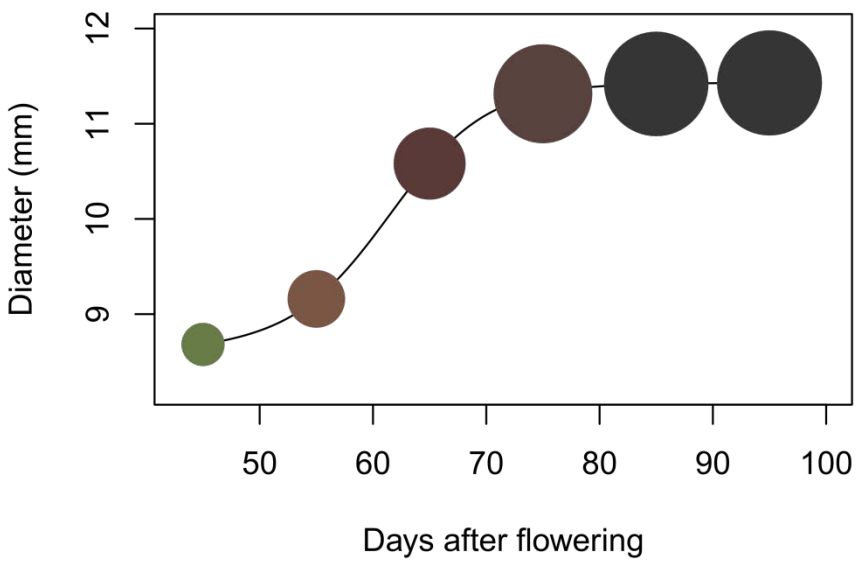
Michaelis-Menten equation

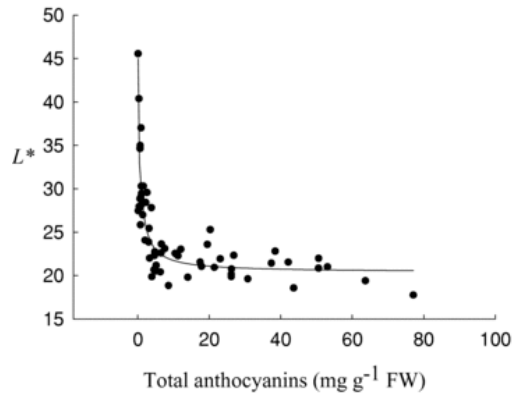
Model parameter can be considered as dissected traits.

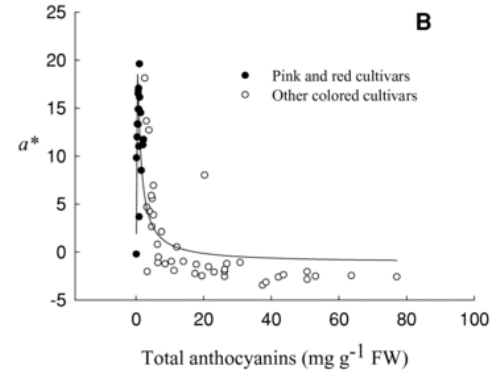
From anthocyanin content and composition to berry color

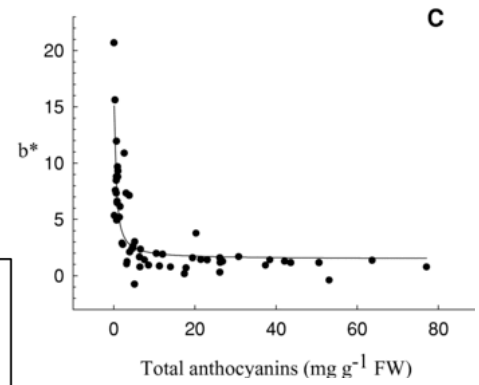
CIELAB coordination











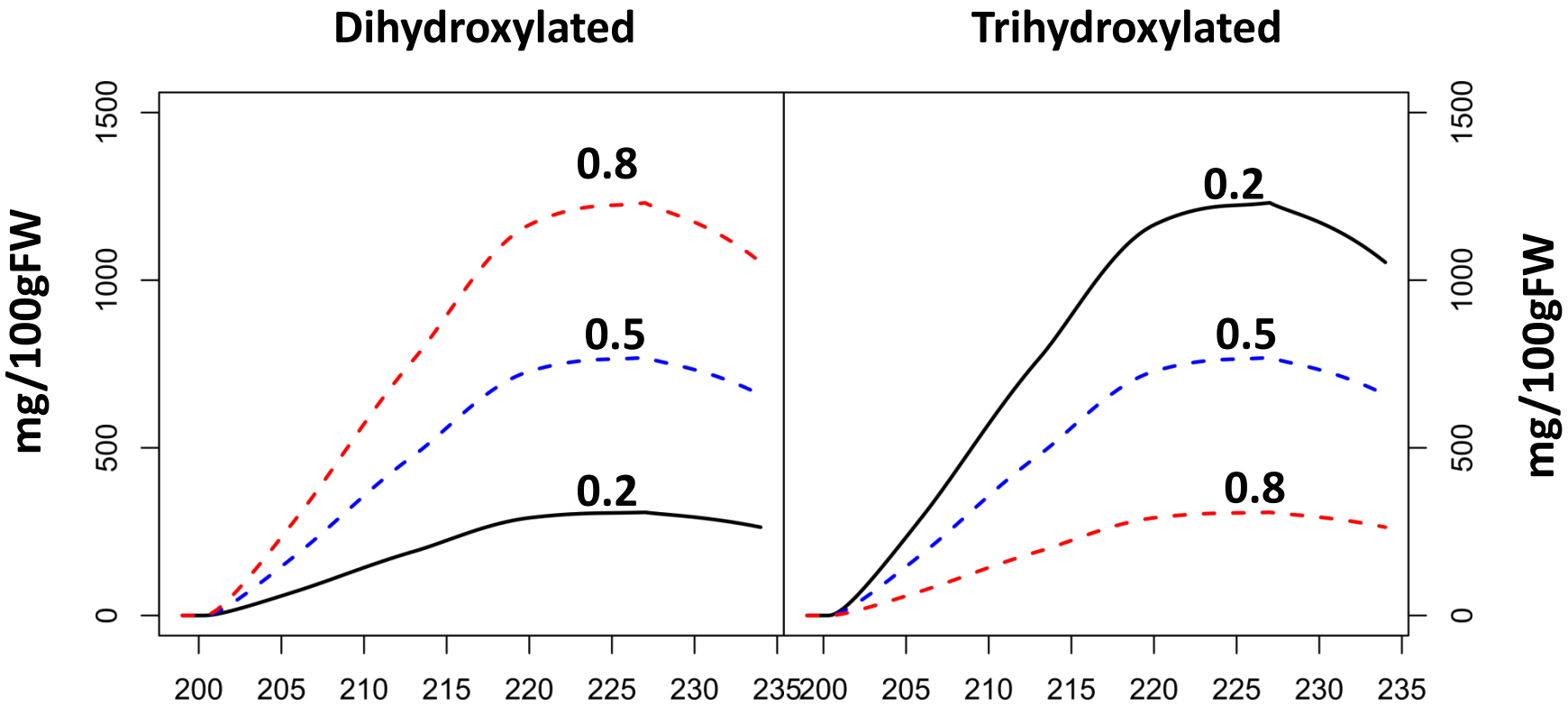
$$L^* = 25.761 + 0.086\mathrm{Cy} - 0.061\mathrm{Dp} - 0.048\mathrm{Mv} - 0.1\mathrm{Pt}\ (r = 0.551)$$

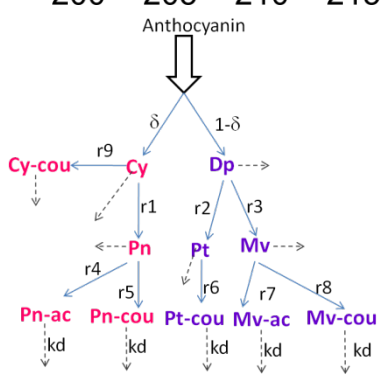
$$a^* = 9.856 + 0.085\mathrm{Dp} - 0.063\mathrm{Cy} - 0.119\mathrm{Mv} - 0.149\mathrm{Pt}\ (r = 0.742)$$

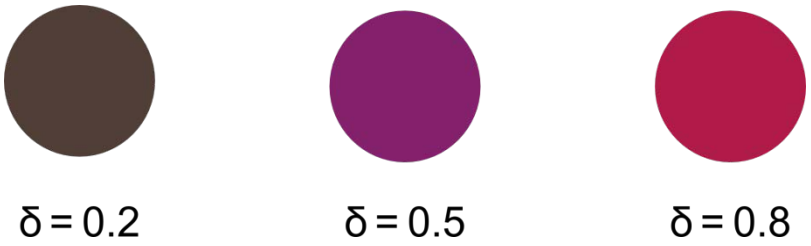
$$b^* = 5.536 + 0.064\mathrm{Cy} - 0.052\mathrm{Dp} - 0.05\mathrm{Mv} - 0.03\mathrm{Pt}\ (r = 0.64)$$

Liang et al., 2011

Model simulation for virtual genotypes







Conclusions and perspectives

- Anthocyanin composition can be dissected into a set of stable parameters, which can be considered as stable traits.

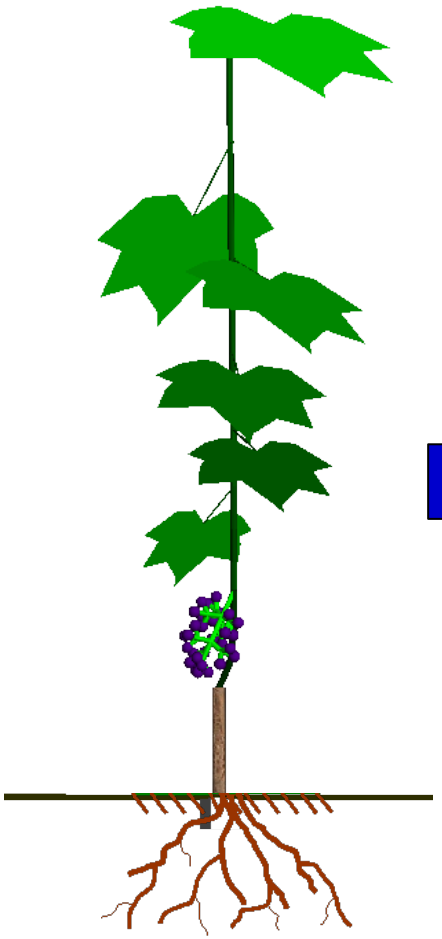
- The model will be tested in more cultivars and different environment combinations (KBBE Innovine project);

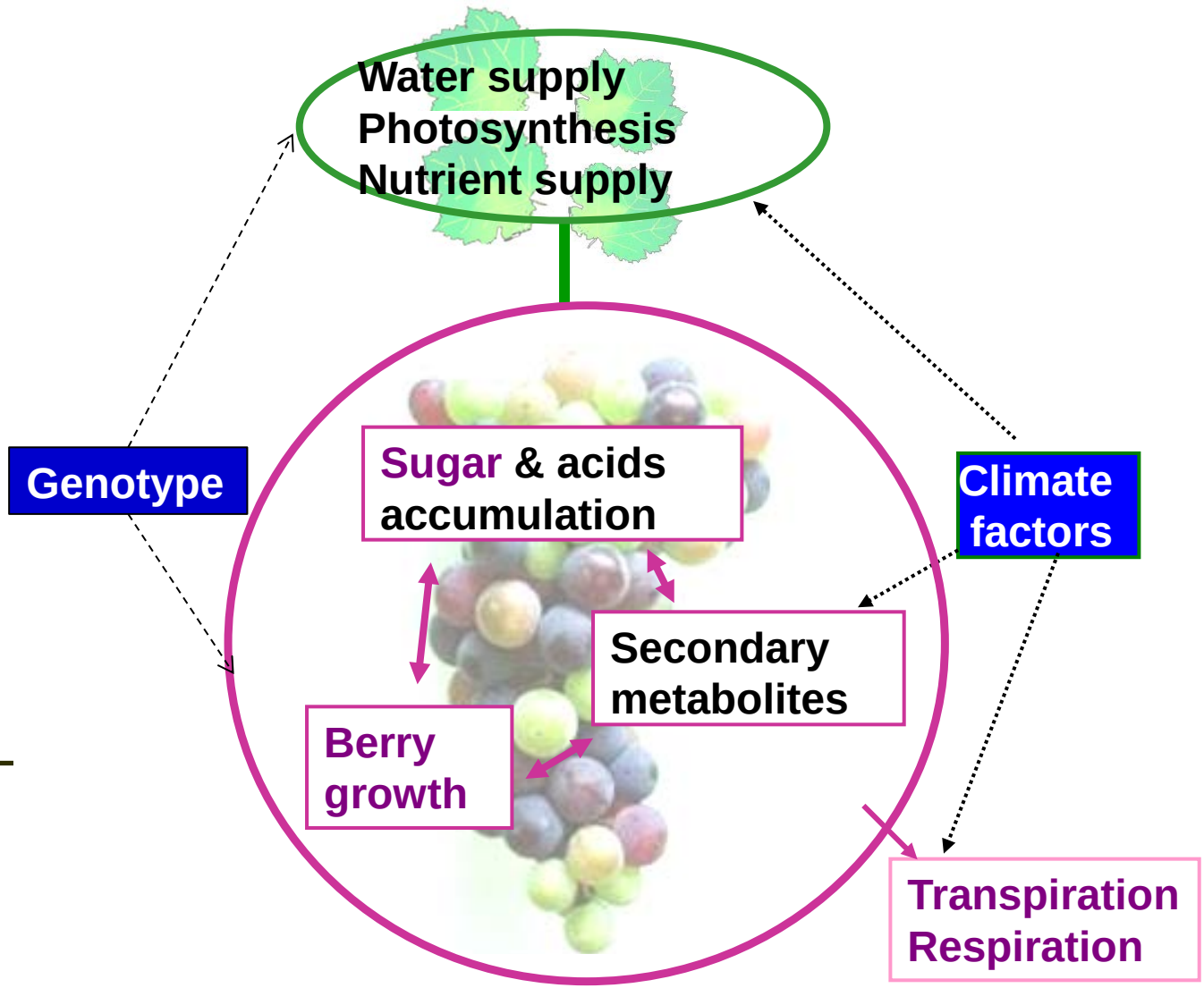
- Update the model to take into account gene expression to make parameters stable for a given genotype;

$$v = \frac{v_{\max}[S]}{[S] + K_m} \qquad v_{\max} = k_{cat}[E_t]$$

- Apply the model to cross populations to identify genetic markers of parameters.

Perspectives—modeling berry quality under climate change





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Thank you for your attention!