Comptes Rendus
Chimie
Supplementary material to the article available at:
https://doi.org/10.5802/crchim.241

Supplementary material: Volatile organic compound emissions from almond shoots during spring—dissociation between reproductive and vegetative organs

Anjélica Leconte *, [a], **Nicolas Barthes** [a], **Bruno Buatois** [a], **Eugénie Coutagne** [b], **Henri Duval** [c], **Philippe Lucas** [d] and **Michael Staudt** [a]

[a] CEFE, CNRS, Univ Montpellier, EPHE, IRD, Montpellier, France

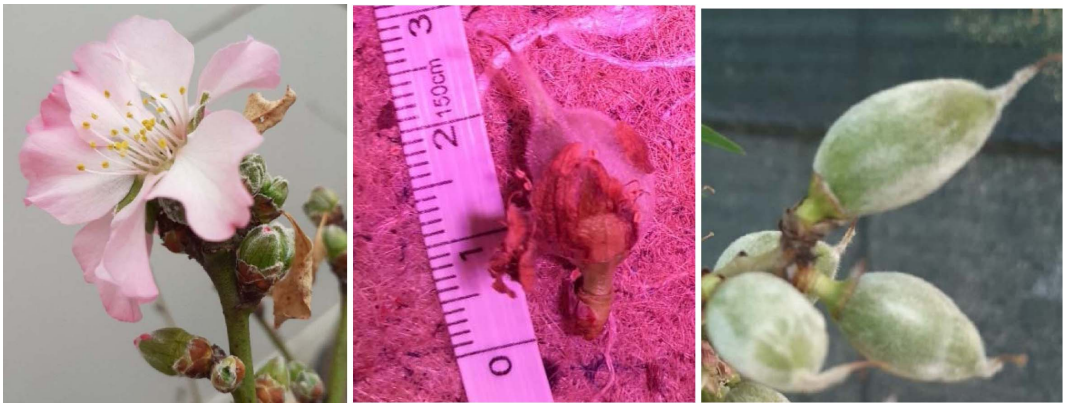
[b] Compagnie des amandes, Aix-en-Provence, France

[c] GAFL, INRAE, Montfavet, France

[d] iEES Paris, INRAE, Sorbonne Université, CNRS, UPEC, IRD, Université P7, Paris, France

E-mails: anjelica.leconte@gmail.com (A. Leconte), nicolas.barthes@cefe.cnrs.fr (N. Barthes), bruno.buatois@cefe.cnrs.fr (B. Buatois), ec@compagniedesamandes.com (E. Coutagne), henri.duval@inrae.fr (H. Duval), philippe.lucas@inrae.fr (P. Lucas), michael.staudt@cefe.cnrs.fr (M. Staudt)

Not yet published



Supplementary Figure S1. Simplified phenological stages in our experiments, inspired by Socias i Company *et al.* (2017) for an almond tree: flowering (left), young (middle) and mature (right).

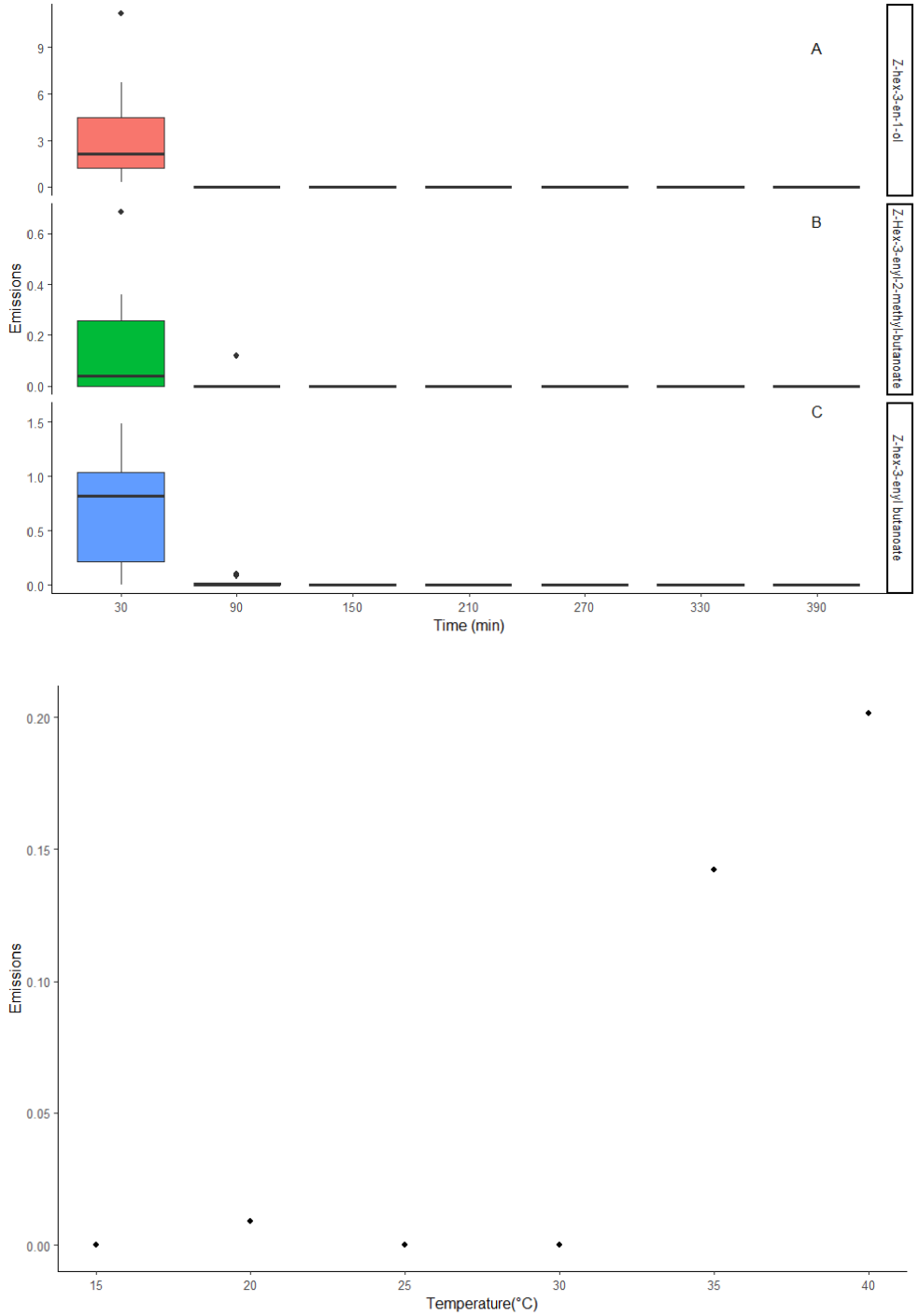
* Corresponding author.

Supplementary Table S1. Parameters chosen in MZMine software to process the chromatograms and obtain the area under the curve (AUC)

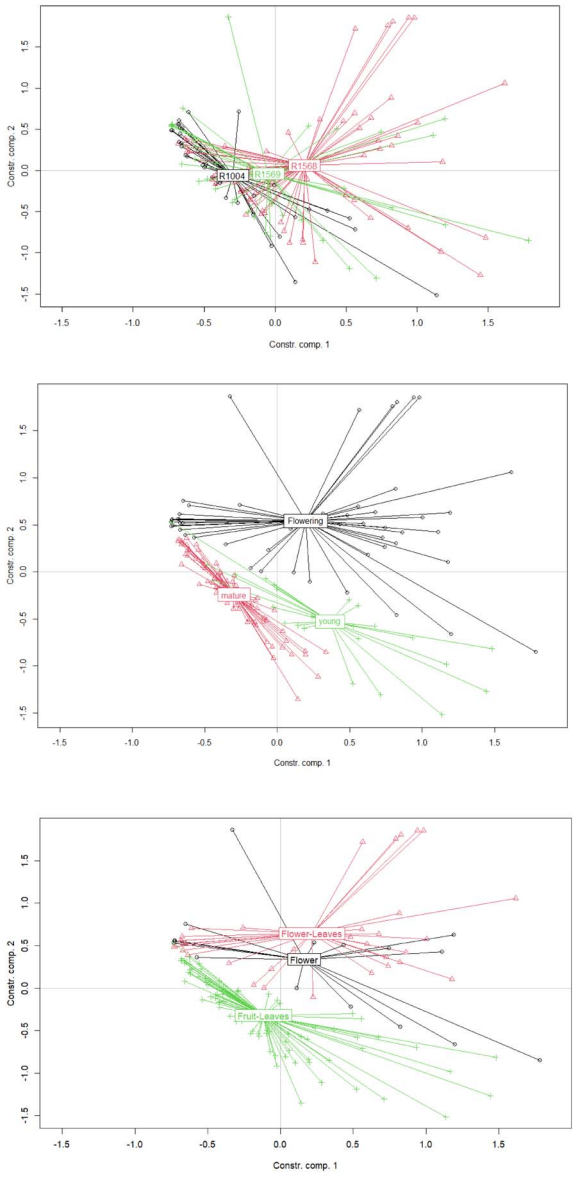
Parameter	Value
Scan-by-scan filtering	Round resampling filter
Crop filter	m/z 38–350
Baseline correction module	RollingBall baseline correction (wm = 100, ws = 12)
Mass detection parameters	Centroid; noise = 4×10^2
ADAP chromatogram builder	Min group size = 5; group intensity threshold = 10^2; min highest intensity = 3×10^2; m/z tolerance = 0.3 or 1000 ppm
ADAP Chromatogram deconvolution	S/N = 7; Wavelet Coeff. SN; min feature height = 200, coefficient = 50; peak duration range: 0.02–0.6; RT wavelet range = 0–0.05
MCR Spectral deconvolution parameter	Window = 0.2; RT tolerance = 0.15; min peaks = 1
ADAP aligner	Min confidence = 0.7; RT tolerance = 0.5 min; m/z tolerance = 0.001 or 5 ppm; m/z score threshold = 0.75; score weight = 0.1; RT difference (fast)

Supplementary Table S2. Pairwise comparisons between group levels with false discovery rate correction for the temperature model. Only factors with a significant effect on the model are presented

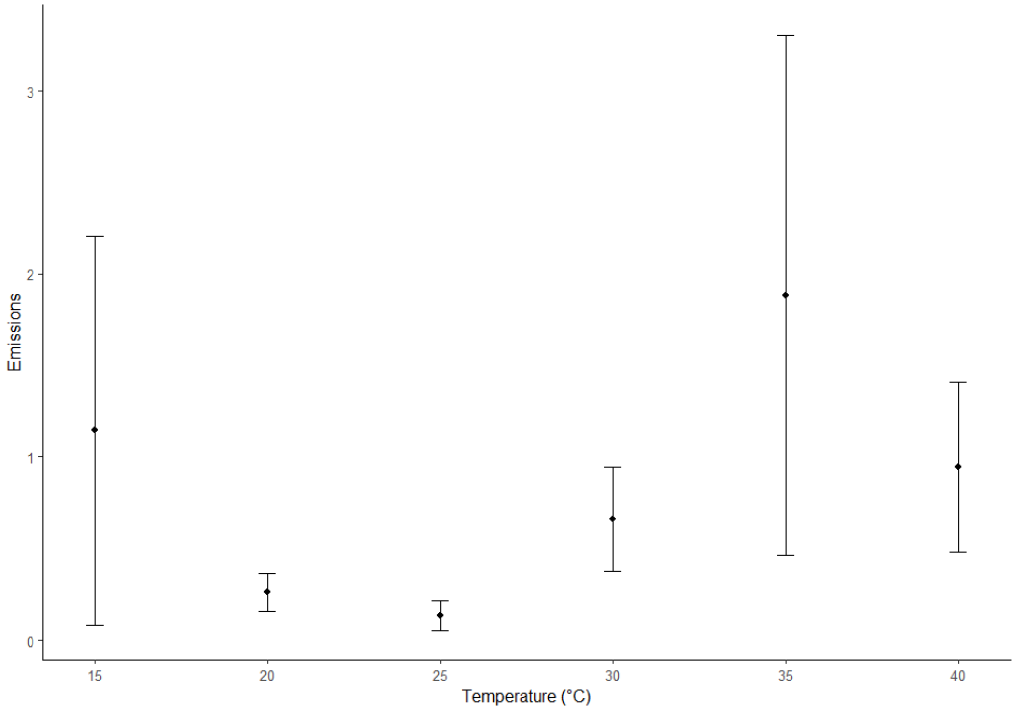
Variety		R1004		R1568	
R1568		0.003		-	
R1569		0.152		0.13	
Temperature	15	20	25	30	35
20	0.061	-	-	-	-
25	0.107	0.853	-	-	-
30	0.003	0.061	0.061	-	-
35	0.003	0.061	0.085	0.853	-
40	0.003	0.003	0.003	0.057	0.129
Branch composition		Flower		Flower-leaves	
Flower-leaves		0.267		-	
Fruit-leaves		0.0015		0.0015	
Phenology		Flowering		Mature	
Mature		0.001		-	
Young		0.001		0.001	



Supplementary Figure S2. (A) Green leaf volatiles emitted at the start of the experiment regardless of temperature and light effect. Emissions were given in $ng{\cdot}m^{-2}{\cdot}s^{-1}$ depending on the time. One time step corresponds to 30 min of sampling. (B) Unknown SQT 6 emissions according to temperature.



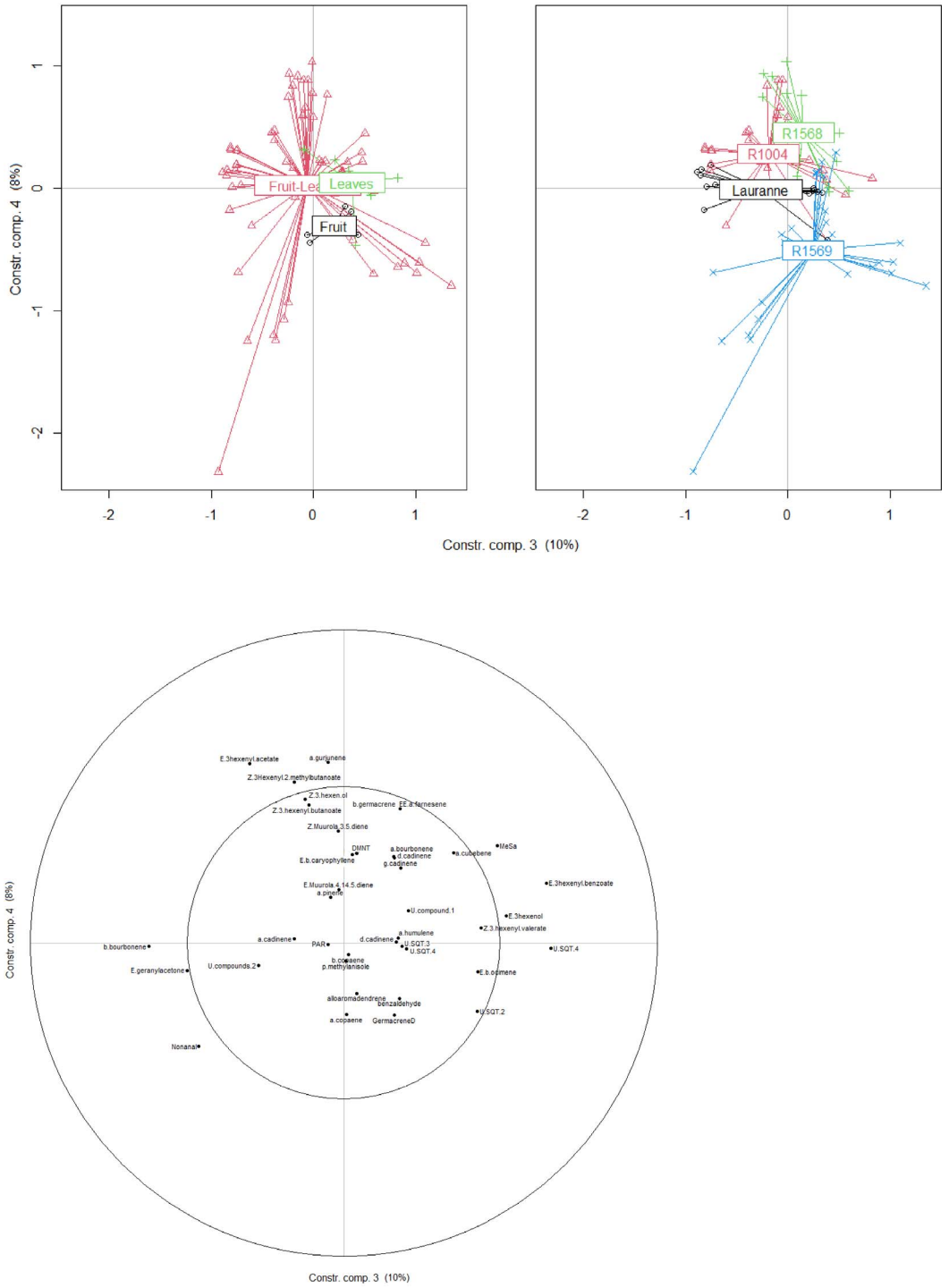
Supplementary Figure S3. Correlation and scores plot for the constrained components 1 and 2 in the temperature model. The profile of VOC emissions from top to bottom depends on varieties, phenological stage, and the composition of the measured branch.



Supplementary Figure S4. Phenolic compounds emissions according to the temperature with error bars (standard errors) for the fruit and leaf development. Emissions were summed by sample and averaged by class.

Supplementary Table S3. Pairwise test with a false discovery rate correction for the effect with a significant effect on the model. Variety and branch composition of VOC emissions are presented

Variety	Lauranne	R1004	R1568
R1004	0.002	-	-
R1568	0.002	0.002	-
R1569	0.009	0.032	0.02
Branch composition		Fruit	Fruit-Leaves
Fruit-leaves		0.0015	-
Leaves		0.0015	0.009



Supplementary Figure S5. Correlation and scores plot for the constrained components 3 and 4 in the light model.