Targeted and untargeted metabolomics for the valorisation of *Coffea anthonyi*

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Introduction: This study focuses on three *Coffea* species: *C. arabica* (arabica coffee), C. *canephora* (robusta coffee) and C. *anthonyi*. The two first species are currently used for coffee making while the third one is closely related to *C. arabica* genetically. Leaves and fruit extracts of the three species were compared in a targeted and an untargeted metabolomics approach. The phloem sap of the three species has also been analyzed in order to better explain their biochemical properties. An expression study of genes involved in the biosynthesis of the main xanthines and polyphenols found in coffee genus was also performed.

Materials/Methods:
Leaf and fruit extraction has been performed by suspending dry matter in milliQ water. Phloem sap extracts have been obtained using the phloem exudation technique.
Semi-polar metabolite fingerprints were monitored using RP/LC-HRMS method in positive ionization mode. Data treatment has been performed by the W4M infrastructure. Total RNA was extracted with the Maxwell RSC Plant RNA Kit and reverse transcription was done with the GoScript Reverse cDNA Synthesis Kit (Promega).
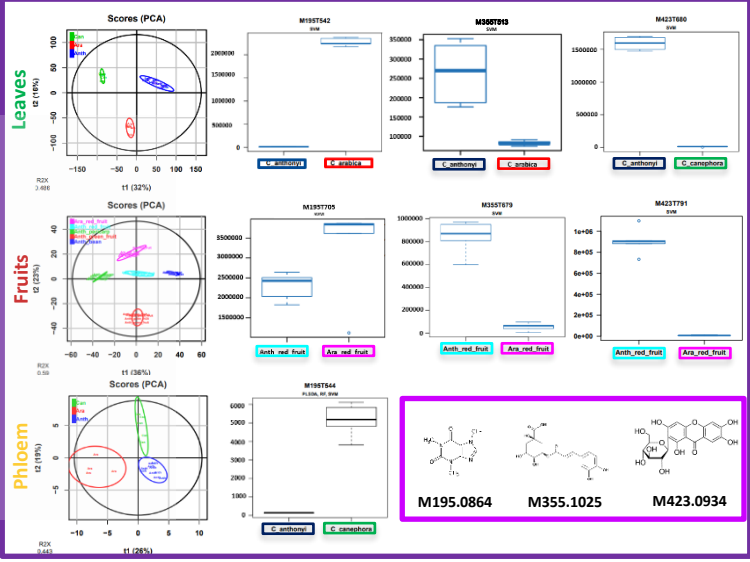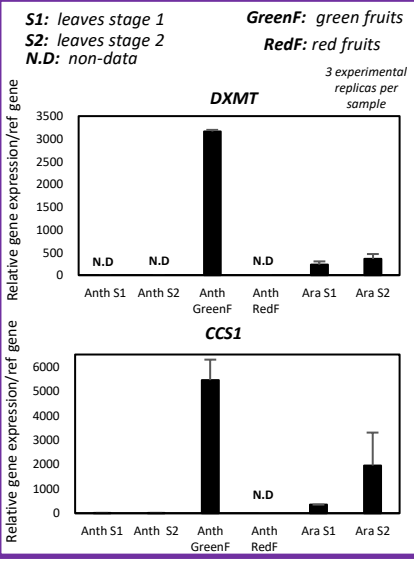

Figure 1: Metabolomic analysis

Figure 2: qPCR results

S1: leaves stage 1
S2: leaves stage 2
N.D: non-data
GreenF: green fruits
RedF: red fruits
3 experimental replicas per sample

Results: Unsupervised multivariate analyses showed a good inter species discrimination. Caffeine, chlorogenic acids and xanthone derivatives appeared as the strongest discriminant metabolites in the leaves, in the fruits and in the phloem sap. Caffeine was abundant in fruits but almost absent in leaves of *C. anthonyi*. The highest content of caffeoylquinic acids and xanthones was detected in *C. anthonyi* leaves and fruits. The very low content of caffeine in *C. anthonyi* leaves can be explained by the low expression of caffeine synthase genes in this organ.

Conclusion: Due to the low *CCS1* and *DXMT* expression in the youngest leaves (stage S1) of *C. anthonyi* and to the absence of caffeine in its phloem, a possible translocation of this xanthine from the leaves to the fruits through the phloem sap can be excluded. Due to the highest content of xanthones and chlorogenic acids in its leaves and fruits *C. anthonyi* could be a good sources of healthy polyphenols.

References: Souard *et al.* Metabolomics fingerprint of coffee species determined by untargeted-profiling study using LC-HRMS. *Food Chemistry* 245, 603-612 (2018).