DYNAMIC METABOLOMICS REVEALS PHENOLIC PROFILES IN SORGHUM: FROM FLOWERING TO FINAL PRODUCT

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Sorghum grains (*Sorghum bicolor* L.) are becoming more common in human diets because of their agronomic benefits and the potential health benefits associated with their phenolic compounds (PC). Despite significant advances in metabolomics for understanding the synthesis of PC in cereals, substantial gaps remain in our knowledge of non-conventional cereals, such as sorghum grains. This work aims to provide deep information about PC accumulation throughout sorghum grain maturation; and their changes after biological, physical and thermal processing in Dutch and French sorghum genotypes. Two sorghum genotypes, contrasting in pericarp colors and tannin levels, were harvested at five different stages: from 10 to 40 days after flowering (DAF); from cellular division, grain filling, physiological maturity until harvest (total of 10 samples). Mature grains from diverse genotypes were subjected to three technological processes: germination (16 °C for 72 and 144 h, 60% relative humidity; total of 9 samples), dehulling (whole grain, ~ 15% decorticated grain, and bran; total of 12 samples), and cooking (1:6 sample-to-water ratio; 30 min; total of 24 samples). PC were sequentially extracted and analyzed using high-resolution untargeted metabolomics (UHPLC-ESI-QTOF/MS). Commercial standards and quality control were also injected. The raw data was preprocessed by using Progenesis QI and Metabolomics Standards Initiative levels was applied by using a customized database built from PubChem and Phenol-Explorer to enable annotation and relative quantification of detected features. The software XLSTAT and Metaboanalyst 6.0 were applied to statistical and multivariate analysis. Globally, 318 PC were tentatively identified in all samples. Sorghum PC are synthesized throughout grain growth (40DAF PC content was nine-fold higher than 10DAF). The phenolic profile also changed: in the early stages (10-17DAF), phenolic acids were predominant (50% of total ion abundance); however, from 25 DAF, the flavonoids biosynthesis pathway seems to be prioritized. Dimer/trimer procyanidins (eight isomers) were annotated at all stages, indicating the presence of tannins even in immature grains (10DAF) and in tannin-free genotypes. For mature grains, PCA provided an overview of phenolic changes post-processing. Dehulling had a significant impact on sorghum phenolic content (-45%) and profile, *i.e.*, decorticated grains and bran showed distinct separation in the PCA biplot. After germination, 25 PC were found differentially abundant: 4-hydroxybelzaldehyde increased (+64% and +4-folds) after 72h and 144h; while important sorghum PC (daidzin, caffeic acid, isoferulic acid and p-coumaric acid) decreased during germination. Both germination and dehulling proved to be effective processes for procyanidins depolymerization. Cooking had a minimal impact on the phenolic profile of mature sorghum grains, resulting in a modest increase in phenolic levels (+24%). Such variation may be due to heat-induced disruption of the grain\'s cellular structure, which facilitates the release of bound PC. The genetic effect showed a significant variation in both the number and profile of PC. The only common outcome among the three processing methods was a reduction in flavonoid levels. These findings reveal the rich phenolic profile of sorghum grains and suggest processing techniques or optimal maturity stages that could enhance their consumption and expand their cultivation.

Agradecimentos: The authors are grateful to “AGAP Institute Joint Research Unit\" and \"Maatschap de Milliano-Meijer” for providing and collecting samples. This work was financed by FAPERJ, CNPq and CAPES - Finance Code 001.