



METABOLIC PROFILE STUDY OF DIFFERENT SORGHUM GENOTYPES BY ¹H NMR

Jéssika Thayanne da Silva^{1*}, Pablo Batista Mendes¹, Maria Lúcia Ferreira Simeone², Alan Rodrigues Teixeira Machado³, Valéria Aparecida Vieira Queiroz², Cícero Beserra de Menezes², Lúcia Pinheiro Santos Pimenta¹

jessikats@gmail.com

1-CerQBio, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 2-Embrapa Milho e Sorgo, Rod MG 424, Sete Lagoas, MG, 35701-970, Brazil. 3-Departamento de Ciências Exatas, Universidade do Estado de Minas Gerais, Unidade João Monlevade, João Monlevade, Minas Gerais, 35930-314, Brazil.

Among the United Nations' seventeen Sustainable Development Goals (SDGs), one ensures access to affordable, reliable, sustainable, and modern energy. Using renewable biomass in products or biofuels as an alternative to fossil fuels meets this goal directly. In Brazil, we can highlight ethanol as one of the main renewable fuel sources. Lately, the ethanol industry has become the focus of attention in searching for new raw materials to optimize its production. *Sorghum* is a wide-world cereal crop known due to its wide adaptability to hard climate conditions, short life cycle, good adaptation to most regions of Brazil, and multiple uses (human food, animal feed, biofuel, and industrial uses). Moreover, all parts of *Sorghum* can be used as a sustainable feedstock for biofuel production. Four Sorghum genotypes were obtained to increase the productivity and sanity of grains used in bioethanol production. The main differences among them are the tannin contents (SC084, BRS305) and origin: lines (SC084, CMSXS180) or hybrid (BRS501, BRS305). This work aimed to use ¹H NMR-based metabolic profiling coupled with chemometric tools to characterize and distinguish four Sorghum genotypes: SC084, CMSXS180, BRS501, and BRS305. Sample preparation was carried out according to Kim et al. Protocol (2010), the spectroscopic measurements were done using the Bruker Avance Neo 600 MHz NMR equipment, and the chemometrics analysis was performed by the MetaboAnalyst platform. The genotype SC084 showed a metabolic profile quite different from the others by the enhanced presence of flavan-3-ols/anthocyanins, the lower sucrose content compared to BRS501 and BRS305, and the lipid content and composition. ¹H NMR data and PCA analysis also showed that it was possible to differentiate defatted and *in natura* grains. The authors thank the support from their institutions and the financial support of ANP/FINEP for the PRH program, especially PRH-1.1

Keywords: *Sorghum bicolor*, bioethanol, chemometrics, ¹H NMR-based metabolomics, bioenergy, biomass

