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DECIPHERING THE PHYTOCHEMICAL LANDSCAPE OF PURPLE ELEPHANT GRASS GENOTYPES THROUGH INTEGRATED HRMS AND NMR DATA: IMPLICATIONS FOR ANIMAL NUTRITION AND HEALTH

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Elephant grass (*Cenchrus purpureus*) is a strategic forage crop cultivated across tropical regions due to its high biomass yield, nutritional value, and adaptability. This study aimed to compare two Embrapa genotypes (S1 and S2) through untargeted metabolomic profiling and assessment of their antioxidant and anti-inflammatory properties. Hydroalcoholic extracts were analyzed using HRMS Orbitrap ESI (+), ^{1}H-NMR, and voltammetric techniques. Spectrophotometric assays revealed that S1 exhibited the highest antioxidant potential (DPPH IC_{50}: 2.5 µg/mL) and total phenolic content (39.8 mg GAE/100 g), indicating a strong correlation between phenolic abundance and antioxidant capacity. Voltammetric analysis showed anodic peaks at Epa ≈ 0.2 V or lower, characteristic of polyphenolic compounds, with peak intensities suggesting higher concentrations of electroactive species in S1. Metabolomic analysis revealed 142 putatively identified metabolites, including flavonoids, anthocyanins, tannins, phenolic acids, phenylpropanoids, and terpenes, supported by molecular networking and *in silico* fragmentation tools. Pathway enrichment analysis indicated strong activity in the shikimate and phenylpropanoid biosynthetic routes, with high abundance of flavonoid subclasses such as flavones (tricin, luteolin glucosides, apigenin derivatives) and flavonols (kaempferide). Anthocyanins such as delphinidin-3-*O*-galactoside and cyanidin-3-*O*-pentoside were confirmed via ^{1}H-NMR chemical shifts (δ 9–10 ppm for H-4 and δ 3–4 ppm for glycosidic linkages). S2 showed higher anthocyanin content but lower antioxidant activity, likely due to lower levels of redox-active aglycones. Cytokine quantification revealed that both genotypes reduced pro-inflammatory mediators, indicating immunomodulatory potential. These effects are attributed to phenolic acids, flavonoids, and tannins, known to engage in redox cycling and inflammation regulation. Overall, the S1 genotype demonstrated greater metabolic diversity, stronger antioxidant response, and superior bioactivity, highlighting its potential as a multifunctional forage crop with therapeutic and nutritional benefits. Notably, untargeted metabolomics revealed significant qualitative and quantitative differences in the secondary metabolite profiles of the two genotypes. While S2 was richer in anthocyanin glycosides and conjugated polyphenols, S1 exhibited a broader distribution of free phenolics, aglycones, and phenylpropanoids, which correlated more directly with redox activity and anti-inflammatory effects. These findings underscore the application of metabolomic fingerprinting not only in identifying bioactive constituents but also in guiding genotype selection for functional and nutraceutical applications in tropical forage systems.

Keywords: *Untargeted metabolomic, Polyphenols, Anti-inflammatory activity, nutraceutical applications*