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DEVELOPMENT OF AN EFFICIENT, HIGH-THROUGHPUT AND GREEN PROCEDURE FOR METABOLIC PROFILING OF Capsicum spp.

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Fruits of Capsicum spp. are largely consumed worldwide. Chemical investigations have focused on few commercial species, neglecting local varieties and green chemistry principles. This work aimed to develop a sustainable, optimized analytical process for untargeted metabolomics of Brazilian *Capsicum* spp. Nineteen varieties were supplied by Embrapa Hortaliças and analysed by UHPLC-MS following the reference analytical procedure of Cervantes-Hernández et al., (2019). A principal component analysis (PCA) was performed separating the varieties in five clusters according to their metabolomic resemblance. A mixture with one sample of each of the five clusters was used to statistically develop a new, green and mathematically optimized analytical procedure (DoE), from sample preparation (dynamic maceration) to UHPLC-DAD/UV-MS metabolite profiling. The new analytical procedure demonstrated greater metabolite coverage, increasing the average number of chromatographic peaks from 151,0 ± 5,0 to 158,3 ± 1,52. Furthermore, the relative greenness of the new procedure was measured by the Analytical GREEnness Metric Approach and Software (AGREE), which assigned to the new procedure a score of 0.69, greener than that of the reference one (0.53). This was achieved mainly because the new sample preparation employed miniaturised, simultaneous extractions, allowing high sample throughput with recommended solvents (400 mg of plant/4 mL of EtOH:H2O) followed by a syringe filtration before injection. The developed procedure proved to be advantageous for metabolite profiling *Capsicum* spp. from a comprehensive perspective, while being in line with the recommendations for a greener natural products chemistry (Funari et al., 2023) as well as with the goals 9, 12,13, 14 and 15 of United Nations Sustainable Development Goals. This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Number #2024/06494-0

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