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HIGH QUALITY COCOA FINGERPRINTING - PART I UNTARGETD AND TARGETED (UT) FINGERPRINTING OF COCOA VOLATILES BY COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY - TIME-OF-FLIGHT MASS SPECTROMETRY AND TANDEM IONIZATION

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Cocoa, produced from cocoa beans (*Theobroma cacao* L. Malvaceae family), is a crop of great economic relevance as raw ingredient for chocolate manufacturing. Cocoa quality and economic value are related to its unique and complex flavour. The sensory profile (aroma, taste, mouth feeling, and texture) is a key-factor for premium quality products suited to consumer preferences. Flavors develop from complex biochemical and chemical reactions occurring at post-harvesting and vary with genotype, geographical origin, farming practices, and technological processing [1]. Above all, post-harvest treatments and, in particular, fermentation and roasting are key steps in the formation of the characteristic cocoa aromas.
The present study investigates volatile organic compounds (VOCs) peculiar signatures from commercial grade, high-quality cocoa with novel pattern recognition strategies that combine untargeted and targeted fingerprinting on GC×GC-TOF-MS and tandem ionization (*UT fingerprinting*) [2]. Samples are from different origins and stages of processing. Advanced pattern recognition is tested to validate its effectiveness in highlighting the chemical information encrypted in VOCs signatures. Furthermore tandem ionization data (70 and 12 eV) are mined to explore different issues such as origin/process characteristics and sensory profile(s) quality. The beneficial role of thermal modulation on band compression is also exploited at supporting GC-O screenings to target potent odorants within detectable VOCs.

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