

(UT) FINGERPRINTING OF COCOA VOLATILES BY COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY - TIME-OF-FLIGHT MASS SPECTROMETRY AND TANDEM IONIZATION

Alessandro Guglielmetti¹, Carlo Bicchi¹, Erica Liberto¹, Lucie Baroux², Philippe Merle², Stephen E. Reichenbach^{3,4}, Elena Allegrucci⁵, Guido Gobino⁵, Chiara Cordero¹

¹ Dipartimento di Scienza e Tecnologia del Farmaco - University of Turin, Via Pietro Giuria, 9, I-10125 Turin, Italy

² Firmenich SA, Route des Jeunes, 1, 1227 Geneva, Switzerland

³ Computer Science and Engineering Department - University of Nebraska, 1400 R Street, 68588-0115 Lincoln, United States

⁴ GC Image LCC - GC Image LCC, PO Box 57403, 68505-7403 Lincoln, United States

⁵ Guido Gobino srl, Via Cagliari 15/b, 10153 Turin, Italy

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.

[1] E.J. Kongor, M. Hinneh, D. Van De Walle, O.E. Afoakwa, P. Boeckx, K. Dewettinck, *Food Res. Int.* 82 (2016) 44–52.

[2] F. Magagna, L. Valverde-Som, C. Ruíz-Samblás, L. Cuadros-Rodríguez, S.E. Reichenbach, C. Bicchi, C. Cordero, *Anal. Chim. Acta.* 936 (2016) 245–258.