Short Oral Communications

Session 2 Cocoa composition and chemistry

Oral Session Cocoa 02.01

Linking cocoa polyphenol composition to chocolate quality with Average-Mass-Spectra fingerprints

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Text Approaches enabling prediction of chocolate quality from cocoa composition would avoid time- and money-consuming steps to chocolate makers. Average mass spectra of cocoa-polyphenol-extracts led to fingerprints used to select the molecules that discriminate chocolate sensory groups.
16 worldwide cocoa samples were processed into chocolates which were characterized by sensory analysis, allowing sorting of the samples into four sensory groups.
The cocoa polyphenol extracts were analyzed by liquid chromatography−low-resolution mass spectrometry. Averaging each mass spectrum provided polyphenolic fingerprints, which were combined into a matrix and processed with chemometrics (PCA, PLS-DA) to select the most meaningful molecules for discrimination of the chocolate sensory groups[1]. A larger set af 44 cocoa samples was used to validate the previous results. 29 mass signals of known and unknown molecules, mainly flavan-3-ols, were finally targeted, including 2 newly described ethyl-bridged flavan-3-ols[2], enabling sensory-group discrimination.
Average mass spectra fingerprints of cocoa-polyphenol-extracts proved to be quick and efficient to select the molecules that discriminate chocolate sensory groups.
A targeted MRM (Multiple Reaction Monitoring) mass spectrometry method was then developed and validated to routinely analyse large series of cocoa samples.

References:
[1] Fayeulle N, Meudec E, Boulet JC, Vallverdú-Queralt A, Hue C, Boulanger R, Cheynier V, Sommerer N, (2019), Fast Discrimination of Chocolate Quality Based On Average Mass Spectra Fingerprints of Cocoa Polyphenols, Journal of Agricultural and Food Chemistry, 2723-2731, 67, https://doi.org/10.1021/acs.jafc.8b06456
[2] Fayeulle N, Vallverdú-Queralt A, Meudec E, Hue C, Boulanger R, Cheynier V, Sommerer N, (2018), Characterization of new flavan-3-ol derivatives in fermented cocoa beans, Food Chemistry, 207-212, 259, https://doi.org/10.1016/j.foodchem.2018.03.133