Molecular definition of the taste of roasted cocoa nibs (Theobroma cacao) by means of quantitative studies and sensory experiments

Abstract:
Sensory-guided decomposition of roasted cocoa nibs revealed that, besides theobromine and caffeine, a series of bitter-tasting 2,5-diketopiperazines and flavan-3-ols were the key inducers of the bitter taste as well as the astringent mouthfeel imparted upon consumption of roasted cocoa. In addition, a number of polyphenol glycopyranosides as well as a series of N-phenylpropenoyl-l-amino acids have been identified as key astringent compounds of roasted cocoa. In the present investigation, a total of 84 putative taste compounds were quantified in roasted cocoa beans and then rated for the taste contribution on the basis of dose-over-threshold (DoT) factors to bridge the gap between pure structural chemistry and human taste perception. To verify these quantitative results, an aqueous taste reconstitute was prepared by blending aqueous solutions of the individual taste compounds in their natural concentrations. Sensory analyses revealed that the taste profile of this artificial cocktail was very close to the taste profile of an aqueous suspension of roasted cocoa nibs. To further narrow down the number of key taste compounds, finally, taste omission experiments and human dose/response functions were performed, demonstrating that the bitter-tasting alkaloids theobromine and caffeine, seven bitter-tasting diketopiperazines, seven
bitter- and astringent-tasting flavan-3-ols, six puckering astringent N-phenylpropenoyl-l-amino acids, four velvety astringent flavonol glycosides, gamma-aminobutyric acid, beta-aminoisobutyric acid, and six organic acids are the key organoleptics of the roasted cocoa nibs.