

Isomers of Quinic Acid and Quinides in Roasted Coffee: Indicators for the Degree of Roast?

B. M. SCHOLZ-BÖTTCHER, H. G. MAIER

Institut für Lebensmittelchemie der TU Braunschweig, Schleinitzstr. 20,
D-3300 Braunschweig, Germany

SUMMARY

Quinic acid is one of the dominant acids in the coffee bean. It appears as free acid and as esters, mainly with caffeic acid, i.e. the chlorogenic acids.

Under thermal treatment only the racemisation of (-)-quinic acid and the generation of the corresponding ($\pm$)- γ -quinides have been reported and were already described in roasted coffee.

Under the roasting conditions of coffee as well as in model experiments with (-)-quinic-, n-chlorogenic acid and Potassium-caffeine-chlorogenate, which are not discussed at this time, all possible stereoisomers of quinic acid and quinide are generated. Their isolation, characterisation and identification using GC/MS and NMR-spectroscopy will be briefly discussed. Seven compounds are described for the first time. Pairs of enantiomers could not be separated.

More than 50 coffee samples of different degrees of roast, roasting type and pretreatment were investigated. 6 Quinic acids and 7 quinides (γ and δ) were quantified, 11 of them for the first time. Except for ($\pm$)-quinic acid and ($\pm$)- γ -quinide, the concentrations of all other isomers are increasing during the roasting process.

As a result a quotient IG, the degree of isomerisation, is defined. The IG is closely related to the colour and therefore to the roasting degree of coffee, independent of the origin and of the roasting type. It is possible to estimate the roasting degree of the coffee even from extracts or beverages.