Secokahweol – A New Diterpene Degradation Product in Roasted Coffee

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SUMMARY

During the roasting process, the diterpenes cafestol and kahweol are decomposed to several degradation products: dehydrocafestol and dehydrokahweol, cafestal and kahweal as well as isokahweol and dehydroisokahweol. With secokahweol, another peak was now elucidated in roasted Arabica coffee, intensifying with increasing roasting degree. The molecular mass was determined to 314.1901, and the empirical formula was calculated as C₂₀H₂₆O₃. The IUPAC-name for this substance is 6-(hydroxymethyl)-1-[2-(5-methyl-1-benzofuran-4-yl) ethyl] bicycle [3.2.1] octan-6-ol.

INTRODUCTION

The pentacyclic diterpenes of Coffea arabica and Coffea canephora var. Robusta are well known: Arabica coffee beans contain the diterpenes cafestol and kahweol whereas Robusta coffee beans contain cafestol, small amounts of kahweol and, in addition, 16-O-methylcafestol and 16-O-methylkahweol (Speer and Kölling-Speer, 2006; Kölling-Speer and Speer, 2006).

During the roasting process, cafestol is decomposed to dehydrocafestol and cafestal whereas the degradation products of kahweol are dehydrokahweol, kahweal and, furthermore, isokahweol and dehydroisokahweol. All of these degradation products were identified by our work group for the first time a few years ago (Tewis et al., 1993; Speer et al., 2000; Kölling-Speer et al., 2005).

While analysing various commercial roasted coffees on containing Robusta parts by using DIN method No. 10779 (1999), a further additional peak was discovered in the HPLC chromatograms (Peak ? in Figure 1). It was clearly noticeable in Arabica coffees of a higher roasting degree, which was determined via the cafestol/dehydrocafestol ratio (Kölling-Speer and Speer, 1997).

METHODS

Using semi-preparative HPLC, the peak was isolated and subsequently elucidated by means of GC-MS, high-resolution mass spectrometry and different NMR and 2D-NMR experiments.
Figure 1. HPLC chromatogram of a commercial strong roasted Arabica coffee.

RESULTS

We named the new diterpene secokahweol (Figure 2), due to its apparent derivation from kahweol and due to the cleavage of the ring. The compound had been unknown up to now.

The elucidation is presented in the following.

The molecular mass was determined to 314.1901, and the empirical formula was calculated as $C_{20}H_{26}O_{3}$. Therefore, secokahweol has the same molecular mass and formula as kahweol, however the mass spectra are clearly different (Figure 3).

Structural information in detail is given from the $^1$H-NMR (Figure 4) and, in particular, from the 2D-NMR experiments below.

Figure 2. Structural formulae of kahweol and secokahweol.
Figure 3. EI-mass spectra of secokahweol and kahweol.

Figure 4. $^1$H-NMR spectrum of secokahweol.

The 2D-NMR experiment NOESY (Figure 5) shows the correlations between H-7/H-20, H-7/H-18 und H-8/H-18, which prove the ring opening between C-5 and C-10.

Figure 5. NOESY spectrum of secokahweol.

In addition, the cross signals in the HMBC experiment (Figure 6) between the CH$_2$-protons of H-7 and the C-1, C-5 und C-6-atoms as well as between the H-20 protons of the CH$_3$ group and the C-5 and C-6 atoms are only explicable with the ring opening.
Figure 6. Cut-out of HMBC spectrum of secokahweol.

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REFERENCES


