

REFERENCES

1. Kunimine, S. and Suzuki, S. (1937) *Yakugaku Zasshi* **57**, 902; (1938) *Yakugaku Zasshi* **58**, 572; Kuku, T., Ri, H. and Hra, N. (1939) *Yakugaku Zasshi* **59**, 248, A. Sosa (1947) *Bull. Soc. Chim. Biol.* **29**, 918; (1948) *Chem. Abstr.* **42**, 6415.
2. Thiem, H. and Winkler, H. J. (1968) *Pharmazie* **23**, 402, 519; **24**, 117 (1969). Matuo, K., Tokoroyama, T. and Kubota, T. (1972) *Phytochemistry* **11**, 1522.
3. Blair, J. and Newbold, G. T. (1955) *J. Chem. Soc.* 2871.

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ENT-16-KAUREN-19-OL FROM COFFEE

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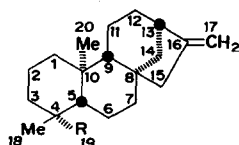
On examination of the sterols of coffee beans (*Coffea arabica* L.) a small amount of a diterpene alcohol in the form of its acetate was encountered [1]. Its structure was tentatively suggested as being 15-abieten-13 β ,19-diyl diacetate. However, its CMR spectrum was not in harmony with the proposed structure. Thus, the compound proved to contain 22 carbon atoms, two of which constituted an acetoxy group (singlet at 171.4 ppm and quartet at 21.0 ppm) attached to a methylene group (triplet at 67.2 ppm). Furthermore, the presence in the CMR spectrum of resonances due to two additional methyl groups (quartets at 27.6 and 18.1 ppm), an exocyclic methylene group (singlet at 155.8 ppm, triplet at 103.0 ppm) and three tetrasubstituted non-oxygenated carbon atoms (singlets at 44.2, 39.2 and 37.1 ppm) implied that the unknown diterpene acetate was 16-kauren-19-yl acetate. This was confirmed by direct comparison with an authentic sample (mmp, $[\alpha]_D$, IR, PMR, CMR and MS).

Ent-16-kauren-19-ol has not been detected in coffee before. From a biogenetic point of view its presence is of interest, since the major diterpenoids of coffee, cafestol [2,3] and kahweol [4], are of the kaurene type. It is also interesting to note that *ent*-16-kauren-19-ol, previously isolated from a few natural sources, e.g. barley [5] and *Abrotanella nivigena* [6], is an intermediate in the biosynthesis of the gibberellins [7,8] and shows a gibberellin-like biological activity [9].

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REFERENCES

1. Nagasampagi, B. A., Rowe, J. W., Simpson, R. and Goad, L. J. (1971) *Phytochemistry* **10**, 1101.
2. Finnegan, R. A. and Djerassi, C. (1960) *J. Am. Chem. Soc.* **82**, 4342.
3. Scott, A. I., Sim, G. A., Ferguson, G., Young, D. W. and McCapra, F. (1962) *J. Am. Chem. Soc.* **84**, 3197.
4. Kaufmann, H. P. and Sen Gupta, A. K. (1964) *Chem. Ber.* **97**, 2652.
5. Petridis, C., Verbeck, R. and Massart, L. (1966) *Naturwissenschaften* **53**, 331.
6. Anthonsen, T. and Chantharasakul, S. (1971) *Acta Chem. Scand.* **25**, 1925.
7. Galt, R. H. B. (1965) *J. Chem. Soc.* 3143.
8. Graebe, J. A., Dennis, D. T., Upper, C. D. and West, C. A. (1965) *J. Biol. Chem.* **240**, 1847.
9. Katsumi, M., Phinney, B. O., Jeffries, P. R. and Henrick, C. A. (1964) *Science* **144**, 849.



- (1) R = CH₂OAc
(2) R = CH₂OH