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TATRIDIN A FROM *ARTEMISIA ARBUSCULA* SSP. *ARBUSCULA*: CRYSTAL STRUCTURE OF TATRIDIN A DIACETATE AND THE IDENTIFICATION OF DEACETYLTULIRINOL

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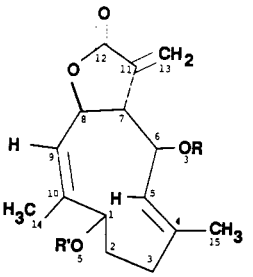
ABSTRACT.—Tatridin A [**1**], isolated from *Artemisia arbuscula* Nutt. ssp. *arbuscula*, has been identified as deacetyltulirinol [**1**] on the basis of the crystal structure determination of the derivative, tatridin A diacetate [**2**]. Tatridin A diacetate displays a *trans*-4,5-*cis*-9,10-cyclodecadiene ring structure; hence, tatridin A may be termed a 4,5-*trans*-9,10-*cis*-germacranolide.

The germacranolide tatridin A [**1**], which has been isolated from different species of the genus *Artemisia*, big sagebrush [*A. tridentata* Nutt. ssp. *tridentata* (1), *A. tridentata* ssp. *vaseyana* f. *spiciformis* (Osterhout) Beetle (1), and *A. arbuscula* Nutt. ssp. *arbuscula* (2,3)] was assigned structure **1** on the basis of nmr spectral assignments (1).

In these earlier works (1–3), tatridin A was incompletely characterized with the position of lactonization (C-6 or C-8) in question. The X-ray crystal structure of tulirinol acetate, isolated from the leaves of *Liriodendron tulipifera* L. (Magnoliaceae), commonly known as tulip poplar, has been published (4). Comparison of the physical properties of tulirinol acetate with tatridin A diacetate [**2**] indicated the two compounds might be similar in structure. The need to clarify the direction of lactonization, to determine conformation of tatridin A, and to compare tulirinol acetate with tatridin A diacetate [**2**] that had been isolated from a completely different plant source, provided the justification for the X-ray crystallographic analysis of the derivative, tatridin A diacetate. This work is part of a continuing project to identify duplicate compounds in the literature isolated from diverse plant sources (5).

RESULTS AND DISCUSSION

The perspective view of tatridin A diacetate or its mirror image is represented in Figure 1. Tatridin A diacetate crystallizes in the monoclinic space



1 R,R′=H

2 R=$\overset{16}{C}\overset{17}{C}H_3$ (O at 4), R′=$\overset{18}{C}\overset{19}{C}H_3$ (O at 6)

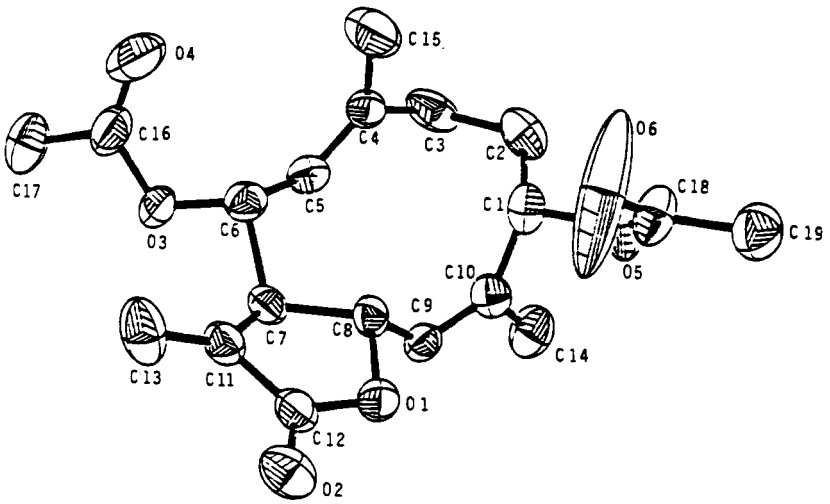


FIGURE 1. The structure and numbering scheme for tatridin A diacetate [2]. Non-hydrogen atoms are represented as thermal ellipsoids scaled to enclose 50% probability. The hydrogen atoms are omitted for clarity (6).

group $P2_1$, and the unit cell parameters are: $a = 6.698$ (1), $b = 7.967$ (1), $c = 17.530$ (3) Å, and $\beta = 93.59$ (2)°. Tulirinol acetate also crystallizes in the monoclinic space group $P2_1$ with $a = 17.470$ (2), $b = 7.966$ (8), $c = 6.799$ (5) Å, and $\beta = 86.63°$ (4). The bond distances and angles for both compounds agree quite well.[1,2] On the basis of the X-ray crystallographic data and mass spectral data, tulirinol acetate, originally isolated from the tulip poplar, is identical to tatridin A diacetate, isolated from sagebrush.

ACKNOWLEDGMENTS

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[1]Full details of the X-ray structure determination may be obtained from the senior author.

[2]Atomic coordinates for this structure have been deposited with the Cambridge Crystallographic Data Centre and can be obtained on request from Dr. Olga Kennard, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK.