

SHORT COMMUNICATION

THE IDENTITY OF CALENDULADIOL AND THURBERIN: A LUPENEDIOL FOUND IN MARIGOLD FLOWERS AND ORGAN PIPE CACTUS

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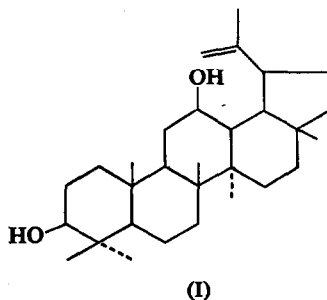
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A NEW triterpene diol, calenduladiol, was recently isolated¹ from the flowers of *Calendula officinales* (marigold) (Compositae) and characterized by degradation, i.r., u.v. and optical rotatory spectral methods. Shortly after this report, the new compound, thurberin,² was isolated from *Lemaireocereus thurberi* (organ pipe cactus) (Cactaceae) and was shown to be Δ -20,30-lupen-3 β ,12 β -diol on the basis of optical spectra, NMR, ORD and m.s. methods.

Comparison of the diacetates of calenduladiol and thurberin were made at the University of Arizona. The mixed melting points were undepressed and the mass spectra of both compounds were superimposable.



We propose that the trivial name, calenduladiol (I), be assigned to Δ -20,30-lupen-3 β ,12 β -diol³ and that the name, calenduladione, be assigned to its oxidation product, Δ -20,30-lupen-3,12-dione.

¹ Z. KASPRZYK and J. PYREK, *Phytochem.* 7, 1631 (1968).

² S. D. JOLAD and C. STEELINK, *J. Org. Chem.* 34, 1367 (1969).

³ A lupene-3,12-diol has also been reported by M. MANZOOR-I-KHUDE, *Tetrahedron* 22, 2377 (1966) as a degradation product of naturally occurring lupane derivative; however, it has different physical constants than calenduladiol.

The physical constants for (I) $C_{30}H_{50}O_2$ are:

M.p.: 206–208° (from methanol),² 213–219° (from ethanol).¹

Diacetate: 191–92°.

$[\alpha]_D^{25} = +12^\circ$ (methanol);² $+17^\circ$ ($CHCl_3$).¹

I.r.: λ_{max} , 2.88, 6.1, 6.99, 7.22 μm .

NMR ($CDCl_3$): τ 8.24 (singlet, 3H), 6.76 (quartet, 1H), 6.37 (quartet, 1H), 5.34 (doublet, 2H).

Mass spectrum: m/e 442 (25.3), 424 (8.16), 399 (9.12), 234 (34.5), 216 (10.9), 207 (74.1), 189 (100), 147 (81.0), 107 (74.1).