Salvitriol—A New Triterpene from *Salvia leucantha* Cav.

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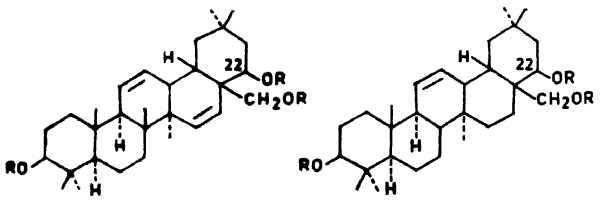
In continuation of our studies on the triterpenes from *Salvia leucantha* Cav. (Labiatae)[1], we report here the isolation and characterisation of another new minor triterpene from the benzene extract of the whole plant (aerial parts and roots).

The dried and powdered deffated whole plant (1.5 kg) was extracted with benzene in a Soxhlet apparatus for 56 h. It was then concentrated to give a dark brown gummy mass. The crude extract was then subjected to column chromatography over Si-gel (60—120 mesh) using solvents of increasing polarity. Elution of the column with a mixture of petroleum ether (b.p. 60—80°)-benzene (1 : 3) afforded (salvitriol (1), $C_{30}H_{48}O_3$, m.p. 240— 41°, $[M]^+$ *m/z* 456. It gave positive Liebermann-Burchardt test for triterpenes and developed a yellow colour with tetranitromethane. It exhibited ir bands at ν_{max} (KBr) 3 400 (hydroxyl) and 1 670 cm^{-1} (unsaturation). On acetylation with acetic anhydride and pyridine at room temperature, 1 readily afforded a triacetate (2), $C_{36}H_{54}O_6$, m.p. 190°, having no free hydorxyl group as revealed from its ir spectrum. This suggests that all the three oxygens in salvitriol are present as hydroxyl functions. The appearance of signals at δ 0 70 (3H, s), 0.75 (3H, s), 0.90 (9H, s), 0.98 (3H, s) and 1.20 (3H, s) in the ^1H nmr (100 MHz; $CDCl_3$) spectrum indicates the presence of seven tertiary C-methyls in 1; a pair of doublets around δ 3.20 (2H, *J* 10 Hz) is due to CH_2OH while a triplet at δ 3.65 and a quartet around δ 3 75 for one proton each are due to the presence of two CHOH groups. The signals at δ 5.15 (2H, d, *J* 6 Hz) and 5.40 (1H, m) are attributed to di- and trisubstituted double bonds respectively.

The mass spectral fragmentation pattern of salvitriol is typical of Δ^{12}-oleanene skeleton[2] (Δ^{12}-ursene skeleton being excluded from the basis of the ^1H nmr spectrum which does not exhibit any signal for secondary methyl group) and recorded peaks at *m/z* 425, 248(A), 217, 207(B), 199, 189 and 148 besides the molecular ion peak at *m/z* 456. From the above mass fragmentation it is evident that in salvitriol, one of the hydroxyl groups is present in the part containing rings A/B while the other two hydroxyl groups are located in the rings C/D/E. Hydrogenation of the triacetate (2) over platinum and acetic acid yielded an amorphous triacetate, $C_{36}H_{56}O_6$ (3) which on hydrolysis with KOH yields a triterpene, m.p. 215°, which was found to be completely identical with leucanthol (4)[2] (m.m.p., co-ir and co-tlc), establishing thereby that salvitriol is dehydro-3β, 22β-28-trihydroxy-Δ^{12}-oleanene. In an oleanene skeleton probable sites[3] for the reducible double bonds are C_2-C_3, C_6-C_7, $C_{15}-C_{16}$ and $C_{21}-C_{22}$. Presence of hydroxyl functions at C_3 and C_{22} excludes the possibility of location of this reducible unsaturation either at C_2-C_3 or at $C_{21}-C_{22}$ positions. Out of the other two positions, $C_{15}-C_{16}$ was found to be more probable and was strongly supported

from mass spectral analysis. The mass values of retro-Diels-Alder fragment ion peaks at *m/z* 248(A) and 207(B) as well as other peaks originated from A and B at *m/z* 217 (A-CH_3OH), 199 (A-CH_3OH—H_2O), 189 (B-H_2O) clearly locates the reducible double bond in C/D/E rings portion, i.e. at the C_{15}—C_{16} position. Further, the appearance of an intense peak at *m/z* 148 by the loss of 100 mass units ($C_6H_{12}O$) containing C_{19}, C_{20}, C_{21} and C_{22} atmos from the ion (A) clearly indicates the presence of an unsaturation at C_{15}—C_{16} position in salvitriol.



(1) R = H
(2) R = Ac
(3) R = Ac
(4) R = H

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