

EFFECT OF A 6β -HYDROXY SUBSTITUENT ON THE CHEMICAL SHIFTS OF THE TERTIARY METHYL GROUPS IN THE ^1H -NMR SPECTRA OF SOME LUPANE DERIVATIVES

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It is well known that the introduction of substituents into the steroid¹ and triterpene skeleton^{2,5} is accompanied by systematic changes in the chemical shifts of the tertiary methyl groups. In the ^1H -NMR spectra of lupeol and betulin respectively the chemical shifts of the tertiary methyl protons between $\delta 0.7$ and $\delta 1.05$. In lupenone there is deshielding of the C-23, C-24 and C-25 methyl groups. In the ^1H -NMR spectra of lupeol and betul in respectively the chemical shifts of the tertiary methyl protons^{2,5} but the tertiary methyl resonances are approximately within the same range ($\delta 0.8$ - 1.06). The tertiary methyl, group resonances in the 6β -hydroxy lupanes isolated from *Pleurostyliia opposita* (Celastraceae) appeared between $\delta 0.80$ and $\delta 1.44$.

In 6β , 20-dihydroxy-lupan-3-one (5), $3\beta,6\beta$ -dihydroxy-lup-20 (29)-ene-3-one (6), the 6β -hydroxy group is in a 1,3-diaxial relationship with the C-24, C-25 and C-26 methyl groups and is expected to deshield each of them strongly.⁴ The deshielding observed in the above examples was about 0.40- 0.45 p.p.m. Deshielding due to such 1,3-diaxial interactions has been reported for lupene diol with an 11β -hydroxy substituent³.

References :

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