Structure by 2D NMR and X-ray Crystallography of a Triterpene from *M. imbricate*

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Many specimens of Maytenus (Celastraceae) are used in medicine folk in different Brazilian regions and shown a diversity of secondary metabolites, like as flavonoids, glycosides, maitansinoids, alkaloidic and non alkaloidic sesquiterpenes, friedelanes, oleananes, lupanes, quinonoids triterpenes and pentacyclic triterpenes (PCTTs) of the other series. To PCTTs are attributed pharmacological properties like ant-asthmatic and antimicrobial antiseptic. action. as antispermatogenic, antispasmodic, analgesic and ant-ulcer effect, insecticide, antitumoral, moluscicide, allelopatic and antiinflammatory effect.

The compound was isolated from the powder extract of *Maytenus imbricata*. From the Mass Spectrometry (MS), ¹H and ¹³C NMR and X-ray data it was possible to determine the molecular formula $C_{30}H_{50}O_2$. The structure of the compound were established by two-dimensional NMR spectroscopic techniques and later confirmed by single crystal X-ray diffraction as 3 β ,30-dihydroxy-lup-20(29)-ene.

The crystal structure shows one molecule in the asymmetric unit. The symmetry was examined carefully and it was concluded that $P4_1$ is the correct space group. The crystal packing is stabilized by two intermolecular hydrogen bonds, which give rise to the formation of five infinite helical chain along *c* per unit cell. Analysis with Mogul program showed all bound length and bound angle between corresponding atom in the molecule are in good agreement with expected.

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