Chirality and numbering of substituted tropane alkaloids

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The strict application of IUPAC rules for the numbering of tropane alkaloids is not always applied by authors and there is hence a lot of confusion in the literature. In most cases, the notation of 3, 6/7-disubstituted derivatives has been chosen arbitrarily, based on NMR and MS data, without taking into account the absolute configuration of these two carbons. This paper discusses the problem and the relevance of CD and NMR to determine molecular configurations. We report on the use of 1H-NMR anisochrony (??) induced by the Mosher's chiral auxiliary reagents (R)-(-)-and (S)-(+)-?-methoxy-?-trifluoromethylphenylacetyl chlorides (MTPA-Cl), to determine the absolute configuration of (3R,6R)-3?-hydroxy-6?- senecioyloxytropane, a disubstituted tropane alkaloid isolated from the aerial parts of Schizanthus grahamii (Solanaceae). These analytical tools should help future works in correctly assigning the configuration of additional 3, 6/7 disubstituted tropane derivatives.