DETERMINATION OF STEROID-NONSTEROID EQUILIBRIUM AND ANALYSIS OF ITS FACTORS USING DITHIOLANE AND DIOXOLANE

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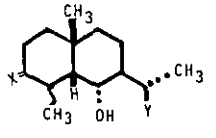
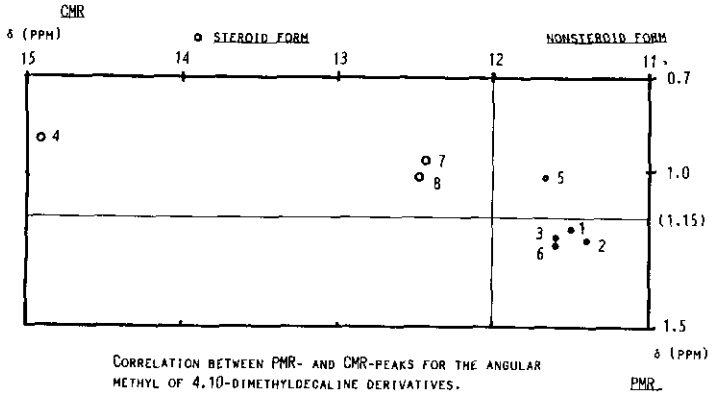
Displacement of steroid-nonsteroid equilibrium were determined by chemical shift of C_{10}-methyl of ^{13}C NMR in the series of 4,10-dimethyldecal-3-ones, especially γ-tetrahydro-ℓ-α-santonic acid (γ-THSA) and its derivatives (shown in Table 1), compared with γ-tetrahydro-ℓ-α-santonin (THS) derivatives with trans- or cis-γ-lactones as the model compounds for typical steroid or nonsteroid types.

It has turned out from the analysis of ^{13}C NMR data in the compounds 5,6, 7 and 8 that not only carbonyl but also acetal (dioxalane) groups are satisfactory groups to take nonsteroid type conformation as shown Fig 1.

Table 1.



No.	X=	C_4	Y-
1	O=	α-Me	COOH
2	O=	α-Me	COOMe
3	O=	α-Me	CH_2OH
4	HO-	β-Me	CH_2OH
5	$[^{O}_{O}X$	α-Me	CH_2OH
6	$[^{O}_{O}X$	β-Me	CH_2OH
7	$[^{S}_{S}X$	α-Me	CH_2OH
8	$[^{S}_{S}X$	β-Me	CH_2OH



CORRELATION BETWEEN PMR- AND CMR-PEAKS FOR THE ANGULAR METHYL OF 4,10-DIMETHYLDECALINE DERIVATIVES.

Fig. 1.