

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

Tetsuichi SHIBATA, Tamiko OHKURA and Seichi INAYAMA

Pharmaceutical Institute, School of Medicine, Keio University

35 Shinanomachi, Shinjuku-ku, Tokyo 160, Japan

Reimei MOROI

Research Institute, Daiichi Seiyaku Co. Ltd.

1-16-13, Kitakasai, Edogawa-ku, Tokyo 134, Japan

Displacement of steroid-nonsteroid equilibrium were determined by chemical shift of C₁₀-methyl of ¹³C NMR in the series of 4,10-dimethyldecal-3-ones, especially γ -tetrahydro- β - α -santonin acid (γ -THSA) and its derivatives (shown in Table 1), compared with γ -tetrahydro- β - 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 ¹³C 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 ₂ OH
4	HO-	β -Me	CH ₂ OH
5	$\begin{smallmatrix} \text{O} \\ \diagup \end{smallmatrix} \text{X}$	α -Me	CH ₂ OH
6	$\begin{smallmatrix} \text{O} \\ \diagup \end{smallmatrix} \text{X}$	β -Me	CH ₂ OH
7	$\begin{smallmatrix} \text{S} \\ \diagup \end{smallmatrix} \text{X}$	α -Me	CH ₂ OH
8	$\begin{smallmatrix} \text{S} \\ \diagup \end{smallmatrix} \text{X}$	β -Me	CH ₂ OH

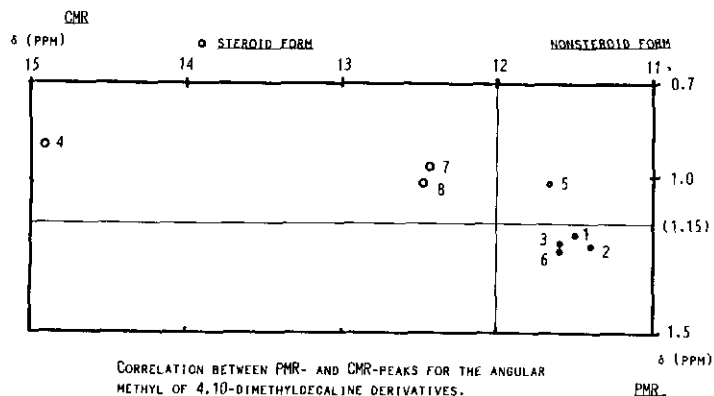


Fig. 1.