

NMR SPECTRAL ASSIGNMENT OF 6,13-DIHYDRO-5-
OXO-5H-ISOQUINOLINO[1,2-b][1,3]BENZOXAZINE

Robert John Bass and Michael Kinns

Pfizer Central Research, Sandwich, Kent, England

Tetsuji Kametani,* Chu Van Loc, Masataka Ihara,

and Keiichiro Fukumoto

Pharmaceutical Institute, Tohoku University, Aobayama,

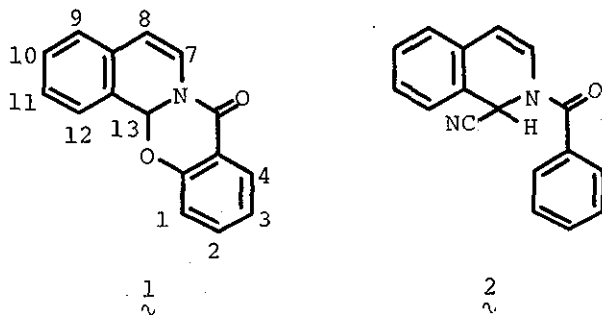
Sendai 980, Japan

A revision of nmr spectral assignment of the title compound is described.

We have recently reported the synthesis of 6,13-dihydro-5-oxo-5H-isoquinolino[1,2-b][1,3]benzoxazine (1)¹ by a condensation of isoquinoline with salicyl chloride. On the basis of the coupling constant ($J = 7.0$ Hz) the signal at 7.95δ was assigned as the low field doublets arising from proton C_7 -H.¹ Comparison of this assignment with that reported by Uff² (2) for a proton in a similar environment; C_3 -H, 6.65δ (the Reissert compound 2) suggested that the assignment for 1 was too low.

Therefore careful reinvestigation of the nmr spectrum of 1 revealed that the resonance at 7.95δ showed a double doublet having $J = 2$ and 7.0 Hz which suggested this resonance should be assigned

as C₄-H. This was confirmed by irradiation of the upfield part of the doublet at 5.85 δ ($J = 7.0$ Hz) when part of the aromatic multiplet at 7.42 δ collapsed to a singlet. No effect was discernible on the low field doublet at 7.95 δ . Thus a doublet at 7.95 δ reported earlier should be assigned as C₄-H.



REFERENCES

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