ON THE STRUCTURE OF AJMALINOL

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Abstract - The recently proposed structure for ajmalinol cannot be correlated with the reported ^{13}C NMR spectral data.

Recently the isolation of ajmalinol from Rauwolfia vomitoria Afzuela was reported.[1] Based on analytical and spectroscopic data, the structure 1 was proposed for the compound, the position of the hydroxyl group derived from ^{1}H- and ^{13}C-NMR spectra. However, it must be stated that the ^{13}C NMR spectrum reported[1] can not be assigned for the structure. Besides being misinterpreted for the most part, the chemical shifts reported for the aromatic carbons fit too well for the parent compound ajmaline 2 to ignore the close similarity.

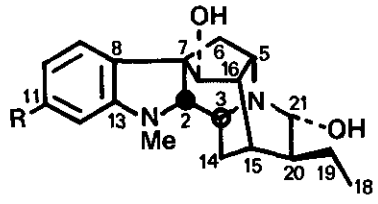
On these grounds , the exact position of the hydroxyl group can by no means be taken as being confirmed. The reported ^{13}C NMR chemical shifts for "ajmalinol"[1], ajmaline[2] and the data for "ajmalinol" rearranged (1') are presented in the table along with the calculated[3] (ipso +26.9,o -12.7,m +1.4,p -7.3)[4] values for the aromatic portion of an 11-hydroxyindoline alkaloid. It should also be noted, that no signals attributable to C_5, C_{14} and C_{15} were reported in the original paper and that two signals at 75.0 and 50.3 can not be fit for either structure 1 or 2.

TABLE ^{13}C NMR DATA

C	calc.[3,4]	1	2	1'
2		77.65 d*	79.3 d	79.4 d
3		77.16 d*	43.0 d	43.2 d
5		75.04 d*	52.8 d	
6		34.91 t	34.8 t	34.9 t
7		56.22 s	56.1 s	56.2 s
8	126.0	127.31 s	133.3 s	133.5 s
9	124.2	122.94 d	122.8 d	122.9 d
10	106.3	119.18 d	119.0 d	119.2 d
11	154.0	153.90 s	127.1 d	127.3 s(?)
12	96.8	109.52 d	109.5 d	109.5 d
13	155.0	133.5 s	153.6 s	153.9 s
14		34.12 t	31.4 t	
15		43.17 d	28.3 d	
16		48.14 d	45.2 d	45.4 d
17		a)	77.3 d	77.7 d or 77.2 d
18		12.2 q	12.2 q	12.2 q
19		25.38 t	25.4 t	25.4 t
20		45.35 d	48.0 d	48.1 d
21	79.41 d	88.1 d	88.1 d	88.1 d
N-Me		50.53 q	34.0 q	34.1 t(?)

a) *not given in the original paper*

* signals left indifferentiated



1 R = OH

2 R = H

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