ELSEVIER

Forensic Science International
87 (1997) 175–177

Forensic Science International

Erratum

Erratum to 'Proton and Carbon-13 NMR assignments of 3,4-methylenedioxyamphetamine (MDA) and some analogues of MDA' (*Forensic Sci. Int.*, 86 (1997) 15–24)[1]

Terry A. Dal Cason[a,*], John A. Meyers[a], David C. Lankin[b]

[a]*Drug Enforcement Administration, US Department of Justice, North Central Laboratory, 536 South Clark Street, Suite 800, Chicago, IL 60605-1526, USA*
[b]*G.D. Searle and Company, Skokie, IL 60077, USA*

Received 22 May 1997

Incomplete versions of Tables 1 and 2 were printed for the above paper. Correct versions of these tables follow.

*Corresponding author.

[1]PII of original article: S0379-0738(97)02102-6.

PII S0379-0738(97)02219-6

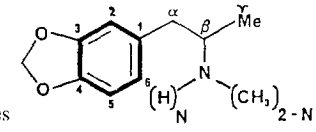
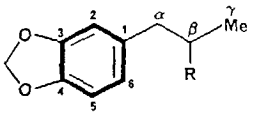


Table 1
3,4-Methylenedioxyamphetamines — ^{1}H-NMR data ($CDCl_3$, 25°C) free bases

Proton	Proton chemical shifts, ppm (coupling constants, Hz)		
	(*N*=2)	(*N*=1)	(*N*=0)
H-2	6.61 d	6.65 d	6.66 d
	(1.2)	(1.2)	(1.6)
H-5	6.67 d	6.67 d	6.66 d
	(7.8)	(7.8)	(7.9)
H-6	6.56 dd	6.56 dd	6.60 dd
	(7.8, 1.2)	(7.8, 1.2)	(7.9, 1.6)
H-α	2.54 dd		3.41 dd
	(5.2, −13.4)		(3.1, −12.8)
H-α	2.36 dd	2.4–2.7 m	2.46 dd
	(8.2, −13.4)		(11.0, −12.8)
H-β	3.03 br.m.		3.39 br.m.
	(6.2, 5.2, 8.2)		
H-γ	1.03 d	1.00 d	1.19 d
	(6.2)	(6.2)	(7.0)
$-O-CH_2-O-$	5.85 s	5.88 s	5.86 s
$N-CH_3$	—	2.34 s	2.74 s
			2.72 s
			2.71 s
			2.69 s
N–H	1.4 br.s.	1.7 br.s.	—

Table 2
3,4-Methylenedioxyamphetamines — ^{1}H-NMR data ($CDCl_3$, 25°C) hydrochloride salts



R	Chemical shifts, ppm (coupling constants, Hz)										
	H-2	H-5	H-6	H-α	H-α	H-β	H-γ	$-OCH_2O-$	-NH	$-N-CH_3$	Other
$-N^+H_3\ Cl^-$ [a]	6.66 d (1.4)	6.72 d (7.8)	6.62 dd (7.8, 1.4)	2.89 dd (7.5)	2.81 dd (7.0)	3.58 br.m.	1.37 d (6.6)	5.90 (s)	7.1 br.s.	—	—
$-N^+H_2-CH_3\ Cl^-$	6.65 d (1.6)	6.69 d (7.8)	6.61 dd (7.8, 1.6)	3.30 dd (−13.0) (4.0)	2.70 dd (−13.0) (4.0)	3.22 br.m.	1.28 d (6.5)	5.88 (s)	9.6 br.s.	2.65 (s)	—
$-N^+H(CH_3)_2\ Cl^-$	6.66 d (1.5)	6.66 d (7.8)	6.60 dd (7.8, 21.5)	3.40 dd (−12.4) (2.9)	2.45 dd (−12.4) (10.9)	3.35 br.m.	1.18 d (6.8)	5.86 (s)	12.3 br.s.	2.72 s 2.73 s 2.71 s 2.70 s	—
$-N^+H_2-CH_2CH_3\ Cl^-$	6.66 d (1.5)	6.68 d (7.9)	6.62 dd (7.9) (1.5)	3.42 dd (−13.0) (3.6)	2.72 dd (−13.0) (11.0)	3.22 br.m	1.29 d (6.5)	5.89 (s)	9.65 br.s	—	CH_3, 1.48 d (7.3) CH_2, 3.35 br.m
$-N^+H_2-CH_2CH_2CH_3\ Cl^-$	6.70 dd (1.8, 0.5)	6.15 dd (7.8, 0.5)	6.66 dd (7.8, 1.8)	3.48 dd (−12.8) (3.5)	2.76 dd (−12.8) (11.0)	3.30 br.m.	1.34 d (6.5)	5.90 (s)	9.64 br.s.	—	CH_3, 0.99 d (7.4) CH_2, 1.99 dq (7.4, 7.8) CH_2, 2.98 br.m.
$-N^+H_2-CH(CH_3)_2\ Cl^-$	6.36 dd (1.8, 0.8)	6.68 dd (7.8, 0.8)	6.62 dd (7.8, 1.8)	3.43 dd (−13.0) (3.5)	2.80 dd (−13.0) (11.0)	3.30 br.m.	1.29 d (6.4)	5.87 (s)	9.39 br.s.	—	CH, 3.35 br.m. CH_3, 1.51 d (6.5) CH_3, 1.43 d (6.5)

[a] CF_3CO_2H added to enhance solubility in $CDCl_3$ solution.