O6—C20	1.482 (19)	C13—C18	1.507 (13)
O7—C19	1.20 (2)	C14—C15	1.536 (12)
C1—C2	1.511 (17)	C15—C16	1.522 (12)
C1—C10	1.501 (15)	C16—C17	1.508 (13)
C2—C3	1.496 (15)	C21—C22	1.44 (2)
C3—C4	1.514 (14)	C21—C23	1.288 (16)
C3—C21	1.535 (14)	C24—C25	1.468 (15)
C4—C5	1.533 (14)	C25—C26	1.414 (14)
C5—C6	1.541 (15)	C25—C30	1.372 (14)
C5—C10	1.526 (13)	C26—C27	1.398 (17)
C6—C7	1.498 (14)	C27—C28	1.364 (16)
C7—C8	1.513 (13)	C28—C29	1.389 (18)
C8—C9	1.555 (12)	C29—C30	1.389 (17)
C8—C14	1.558 (12)		
C17—O4—C24	118.2 (8)	C12—C13—C18	111.2 (7)
C19—O6—C20	113.0 (13)	C14—C13—C17	104.2 (6)
O1—C1—C2	121.2 (10)	C14—C13—C18	113.2 (8)
O1—C1—C10	121.0 (10)	C17—C13—C18	115.8 (7)
C2—C1—C10	117.7 (10)	O3—C14—C8	108.0 (7)
C1—C2—C3	111.1 (10)	O3—C14—C13	105.6 (7)
C2—C3—C4	106.9 (8)	O3—C14—C15	111.0 (6)
C2—C3—C21	110.8 (9)	C8—C14—C13	113.7 (6)
C4—C3—C21	113.2 (9)	C8—C14—C15	114.8 (7)
C3—C4—C5	113.0 (8)	C13—C14—C15	103.4 (7)
C4—C5—C6	113.6 (8)	C14—C15—C16	104.7 (7)
C4—C5—C10	113.7 (8)	C15—C16—C17	108.1 (7)
C6—C5—C10	110.0 (8)	O4—C17—C13	112.1 (8)
C5—C6—C7	110.0 (8)	O4—C17—C16	106.3 (8)
O2—C7—C6	120.5 (9)	C13—C17—C16	106.7 (7)
O2—C7—C8	122.6 (8)	O6—C19—O7	125.5 (13)
C6—C7—C8	116.9 (9)	O6—C19—C10	107.6 (13)
C7—C8—C9	110.2 (7)	O7—C19—C10	126.9 (15)
C7—C8—C14	111.0 (7)	C3—C21—C22	113.4 (10)
C9—C8—C14	113.5 (7)	C3—C21—C23	126.0 (11)
C8—C9—C10	112.6 (7)	C22—C21—C23	120.6 (11)
C8—C9—C11	110.7 (7)	O4—C24—O5	123.8 (10)
C10—C9—C11	113.5 (6)	O4—C24—C25	111.0 (9)
C1—C10—C5	107.0 (7)	O5—C24—C25	125.2 (9)
C1—C10—C9	110.7 (8)	C24—C25—C26	119.3 (9)
C1—C10—C19	111.3 (10)	C24—C25—C30	122.2 (9)
C5—C10—C9	112.3 (7)	C26—C25—C30	118.5 (9)
C5—C10—C19	106.6 (9)	C25—C26—C27	120.6 (10)
C9—C10—C19	109.0 (8)	C26—C27—C28	120.2 (10)
C9—C11—C12	111.1 (6)	C27—C28—C29	119.0 (11)
C11—C12—C13	112.9 (8)	C28—C29—C30	121.7 (11)
C12—C13—C14	107.9 (7)	C25—C30—C29	119.9 (10)
C12—C13—C17	103.8 (8)		

We thank Dr R. Ruel for helpful discussions while writing this paper.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry, together with a stereoview of the unit-cell contents, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71196 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD1040]

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Structure of 3-Epiryanodol: a Heptahydro Diterpene

ANDRÉ G. MICHEL AND MARC DROUIN

Laboratoire de Chimie Structurale et Modélisation Moléculaire, Département de chimie, Faculté des Sciences, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

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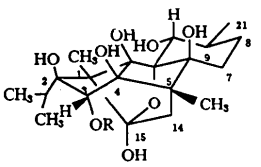
Abstract

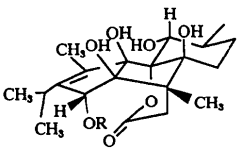
As part of an investigation of structure-activity relationships of ryanoids, the crystal structure of 3-epiryanodol was carried out in order to confirm its stereochemistry Ryanodol has 11 asymmetric C atoms. The C3 atom, which has *R* stereochemistry in the natural product, was inverted to the *S* stereochemistry to give this 3-epimer of ryanodol. The compound makes three inter- and four intramolecular hydrogen bonds.

Comment

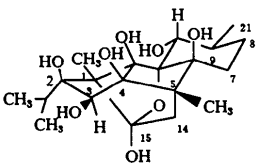
The natural compound ryanoidine (1) isolated from *Ryania speciosa* Vahl (Rogers, Koniuszy, Shavel & Folkers, 1948) is the ester of α-pyrrolecarboxylic acid and the complex diterpene (+)-ryanodol (2). Its crystal structure was reported by Srivastava & Przybylska (1970). It is an interesting and important calcium-release channel modulator in mammalian muscle (Jenden & Fairhurst, 1969).



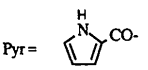
(1) (R = Pyr) Ryanodine
(2) (R = H) Ryanodol



(3) (R = Pyr) Anhydroryanodine



(4) 3-Epiryanodol



In order to identify the structural features which are necessary to retain the biological activity, several of these compounds were prepared (Deslongchamps, Ruest, Welch & Sutko, 1993). The chemical modifications on anhydroryanodine (3) have led to the synthesis of the title compound (4) (Ruest & Deslongchamps, 1993). These authors supplied us with a suitable crystal for X-ray diffraction analysis. We report herein the crystal structure of this new 3-epimer of ryanodol.

An *ORTEP* (Johnson, 1976) perspective view of the molecule is shown in Fig. 1. All the six-membered rings of the skeleton are in the chair form and the five-membered rings are in the envelope form. All of the hydroxyl groups are involved in hydrogen bonding (Fig. 2). The H atoms are directed towards the neighbouring O atoms to optimize the H—O interactions. As viewed in Fig. 2, the O23 atom is an acceptor of two different intramolecular hydroxyl donors, O22 and O25 for hydrogen bonds (*a*) and (*c*) respectively. O23 is also an intermolecular donor to O24 (*b*), which is an intramolecular donor to O25 (*d*). There are two other intermolecular hydrogen bonds, the donors being O26 and O28 for (*e*) and (*g*), respectively. The hydroxyl hydrogen HO27 is oriented towards O26 [Δ = 2.20 (3) Å] constituting a weak interaction (*f*). The donor-acceptor distances range from 2.548 (4) to 2.913 (3) Å with an average value of 2.705 Å.

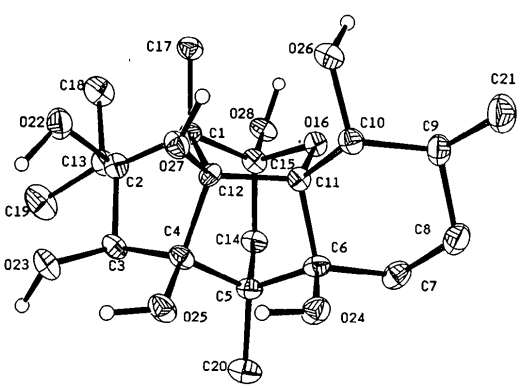


Fig. 1. *ORTEP* perspective view (Johnson, 1976) with crystallographic numbering. Thermal ellipsoids are shown at 50% probability levels for non-H atoms; for clarity only hydroxyl H atoms with arbitrary isotropic thermal parameters are included.

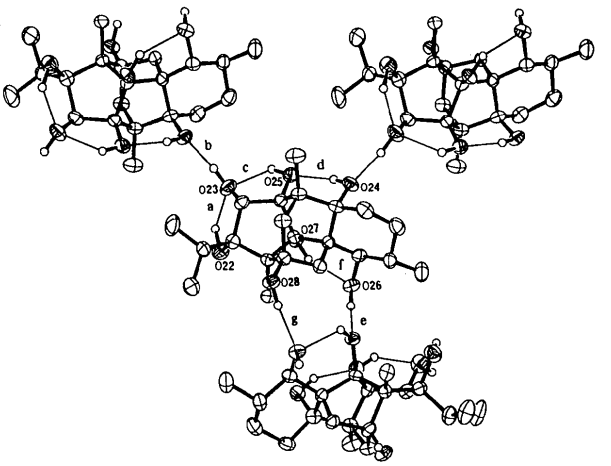


Fig. 2. *ORTEP* perspective view (Johnson, 1976) of the hydrogen-bonding network.

Experimental

Crystal data

$C_{20}H_{32}O_8$	Mo $K\alpha$ radiation
M_r = 400.46	λ = 0.70930 Å
Orthorhombic	Cell parameters from 24 reflections
$P2_12_12_1$	θ = 15.00–20.00°
a = 9.0995 (6) Å	μ = 0.10 mm^{-1}
b = 13.0675 (7) Å	T = 293 K
c = 16.3219 (7) Å	Prismatic
V = 1940.80 (18) Å^3	0.30 × 0.30 × 0.10 mm
Z = 4	Colorless
D_x = 1.371 Mg m^{-3}	

Data collection

Nonius CAD-4 diffractometer	R_{int} = 0.015
$\omega/2\theta$ scans	θ_{max} = 22.43°
Absorption correction: none	h = 0 → 9
4257 measured reflections	k = 0 → 13
2524 independent reflections	l = 0 → 17
2162 observed reflections [$I_{net} > 2.0\sigma(I_{net})$]	3 standard reflections frequency: 60 min intensity variation: none

Refinement

Refinement on F	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
Final R = 0.034	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
wR = 0.029	Extinction correction: Larson (1970)
S = 1.44	Extinction coefficient: 0.30 (3)
1226 reflections	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)
254 parameters	
Only coordinates of H atoms refined	
$w = 1/[\sigma^2(F)+0.0001F^2]$	
$(\Delta/\sigma)_{max}$ = 0.001	

The structure was solved using direct methods. All non-H atoms were located in the first *E* map. All of the hydroxyl H atoms were located from a difference Fourier map. All other H atoms were geometrically placed and the positional parameters of all H atoms were refined. Each H atom was given the isotropic thermal parameter of its respective attached atom, which was not refined. Refinement was by full-matrix least-squares methods. Data collection: *NRCCAD DATCOL* (Le Page, White & Gabe, 1986). Cell refinement: *NRCCAD TRUANG*. Data reduction: *NRCVAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *ORTEP* (Johnson, 1976). Software used to prepare material for publication: *NRCVAX TABLES*.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C1	0.2973 (4)	0.9203 (3)	0.91935 (22)	0.0282 (22)
C2	0.2316 (5)	1.0257 (3)	0.89249 (22)	0.0333 (24)
C3	0.1206 (4)	0.9981 (3)	0.82303 (24)	0.0326 (22)
C4	0.1074 (4)	0.8806 (3)	0.82204 (24)	0.0300 (23)
C5	0.2094 (4)	0.8278 (3)	0.75830 (20)	0.0321 (23)
C6	0.2155 (4)	0.7171 (3)	0.79239 (22)	0.0320 (23)
C7	0.3182 (5)	0.6369 (3)	0.75804 (22)	0.0403 (24)
C8	0.3082 (5)	0.5400 (3)	0.81008 (23)	0.0440 (25)
C9	0.3332 (5)	0.5568 (3)	0.90255 (23)	0.0368 (24)
C10	0.2339 (4)	0.6440 (3)	0.93349 (21)	0.0309 (23)
C11	0.2552 (4)	0.7387 (3)	0.88263 (23)	0.0265 (22)
C12	0.1738 (4)	0.8401 (3)	0.90364 (21)	0.0264 (22)
C13	0.3412 (5)	1.1102 (3)	0.86656 (24)	0.0388 (25)
C14	0.3639 (4)	0.8757 (3)	0.76960 (22)	0.0335 (23)
C15	0.4116 (4)	0.8722 (3)	0.86006 (24)	0.0305 (23)
O16	0.4103 (3)	0.76673 (18)	0.88453 (15)	0.0284 (15)
C17	0.3510 (4)	0.9191 (3)	1.00791 (21)	0.0348 (22)
C18	0.4439 (5)	1.1460 (3)	0.93418 (25)	0.057 (3)
C19	0.2619 (5)	1.2027 (3)	0.8302 (3)	0.066 (3)
C20	0.1594 (4)	0.8374 (3)	0.66916 (22)	0.050 (3)
C21	0.3065 (5)	0.4588 (3)	0.95017 (24)	0.053 (3)
O22	0.1501 (3)	1.06466 (20)	0.96144 (16)	0.0484 (17)
O23	−0.0202 (3)	1.04131 (21)	0.83862 (16)	0.0460 (17)
O24	0.0713 (3)	0.67056 (19)	0.78794 (15)	0.0370 (15)
O25	−0.0410 (3)	0.85036 (19)	0.80904 (16)	0.0380 (16)
O26	0.25299 (24)	0.66463 (21)	1.01952 (14)	0.0348 (15)
O27	0.0638 (3)	0.83071 (19)	0.96432 (14)	0.0319 (15)
O28	0.55438 (25)	0.90980 (20)	0.86458 (15)	0.0367 (15)
HO22	0.041 (3)	1.0819 (24)	0.9396 (16)	0.0586
HO23	−0.050 (3)	1.0843 (23)	0.7949 (17)	0.0560
HO24	0.004 (3)	0.7202 (22)	0.8022 (16)	0.0478
HO25	−0.101 (3)	0.9071 (22)	0.8175 (16)	0.0484
HO26	0.356 (3)	0.6689 (22)	1.0348 (15)	0.0450
HO27	0.097 (3)	0.7934 (20)	1.0091 (16)	0.0419
HO28	0.603 (3)	0.8903 (22)	0.9122 (16)	0.0468

Table 2. *Geometric parameters* (Å, °)

C1—C2	1.564 (5)	C13—C18	1.520 (6)
C1—C12	1.557 (5)	C13—C19	1.528 (6)
C1—C15	1.553 (5)	C14—C15	1.540 (5)
C1—C17	1.526 (5)	C15—O16	1.435 (5)
C2—C3	1.560 (5)	C15—O28	1.391 (4)
C2—C13	1.547 (6)	O22—HO22	1.08 (3)
C2—O22	1.441 (5)	O23—HO23	0.95 (3)
C3—C4	1.541 (5)	O24—HO24	0.92 (3)
C3—O23	1.423 (5)	O25—HO25	0.93 (3)
C4—C5	1.556 (5)	O26—HO26	0.97 (3)
C4—C12	1.555 (5)	O27—HO27	0.93 (3)
C4—O25	1.423 (4)	O28—HO28	0.93 (3)
C5—C6	1.551 (5)		
C5—C14	1.550 (5)	O22···O23	2.552 (4)
C5—C20	1.530 (5)	O24···O25	2.585 (4)
C6—C7	1.511 (6)	O25···O23	2.548 (4)
C6—C11	1.542 (5)	O27···O26	2.913 (3)
C6—O24	1.448 (4)	O23···O24^{i}	2.709 (4)
C7—C8	1.528 (6)	O26···O27^{ii}	2.841 (3)
C8—C9	1.542 (5)	O28···O26^{ii}	2.791 (3)
C9—C10	1.539 (5)	HO22···O23	1.82 (3)
C9—C21	1.518 (5)	HO23···O24^{i}	1.77 (3)
C10—C11	1.503 (5)	HO24···O25	1.76 (3)
C10—O26	1.440 (4)	HO25···O23	1.93 (3)
C11—C12	1.557 (5)	HO26···O27^{ii}	1.89 (3)
C11—O16	1.459 (5)	HO27···O26	2.20 (3)
C12—O27	1.413 (4)	HO28···O26^{ii}	1.90 (3)
C2—C1—C12	105.7 (3)	C11—C10—O26	111.6 (3)
C2—C1—C15	115.9 (3)	C6—C11—C10	110.3 (3)
C2—C1—C17	113.4 (3)	C6—C11—C12	104.8 (3)
C12—C1—C15	96.3 (3)	C6—C11—O16	107.0 (3)
C12—C1—C17	112.4 (3)	C10—C11—C12	121.2 (3)
C15—C1—C17	111.8 (3)	C10—C11—O16	108.7 (3)
C1—C2—C3	104.3 (3)	C12—C11—O16	104.0 (3)
C1—C2—C13	117.4 (3)	C1—C12—C4	101.1 (3)
C1—C2—O22	106.8 (3)	C1—C12—C11	105.4 (3)
C3—C2—C13	112.5 (3)	C1—C12—O27	117.0 (3)
C3—C2—O22	108.4 (3)	C4—C12—C11	106.6 (3)
C13—C2—O22	107.0 (3)	C4—C12—O27	110.8 (3)
C2—C3—C4	106.7 (3)	C11—C12—O27	114.6 (3)
C2—C3—O23	111.2 (3)	C2—C13—C18	114.7 (3)
C4—C3—O23	109.1 (3)	C2—C13—C19	111.5 (3)
C3—C4—C5	113.7 (3)	C18—C13—C19	109.2 (3)
C3—C4—C12	107.4 (3)	C5—C14—C15	111.0 (3)
C3—C4—O25	110.6 (3)	C1—C15—C14	113.4 (3)
C5—C4—C12	101.0 (3)	C1—C15—O16	102.1 (3)
C5—C4—O25	110.1 (3)	C1—C15—O28	116.7 (3)
C12—C4—O25	113.7 (3)	C14—C15—O16	107.0 (3)
C4—C5—C6	101.3 (3)	C14—C15—O28	107.7 (3)
C4—C5—C14	106.4 (3)	O16—C15—O28	109.4 (3)
C4—C5—C20	115.0 (3)	C11—O16—C15	104.1 (3)
C6—C5—C14	107.5 (3)	C2—O22—HO22	106.8 (15)
C6—C5—C20	115.4 (3)	C3—O23—HO23	111.1 (17)
C14—C5—C20	110.5 (3)	C6—O24—HO24	107.2 (17)
C5—C6—C7	122.4 (3)	C4—O25—HO25	108.1 (17)
C5—C6—C11	100.4 (3)	C10—O26—HO26	112.1 (15)
C5—C6—O24	109.9 (3)	C12—O27—HO27	111.7 (17)
C7—C6—C11	109.7 (3)	C15—O28—HO28	113.3 (17)
C7—C6—O24	104.5 (3)		
C11—C6—O24	109.7 (3)	O22—HO22···O23	121.0 (20)
C6—C7—C8	109.4 (3)	O23—HO23···O24^{i}	169.0 (30)
C7—C8—C9	114.7 (3)	O24—HO24···O25	149.0 (20)
C8—C9—C10	109.9 (3)	O25—HO25···O23	122.0 (20)
C8—C9—C21	111.0 (3)	O26—HO26···O27^{ii}	165.0 (20)
C10—C9—C21	111.3 (3)	O27—HO27···O26	132.0 (20)
C9—C10—C11	110.6 (3)	O28—HO28···O26^{ii}	159.0 (20)
C9—C10—O26	112.8 (3)		

Symmetry codes: (i) $-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $\frac{1}{2}+x, \frac{3}{2}-y, 2-z$.

Lists of structure factors, anisotropic thermal parameters and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71206 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD1044]

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Structures of the Natural Alkaloids Vincadifformine and 8-Oxotabersonine

GIOVANNI PALMISANO

Dipartimento di Chimica Organica e Industriale, Università degli Studi di Milano and Centro per lo Studio delle Sostanze Organiche Naturali del CNR, Via Venezian, 21, I-20133 Milano, Italy

TULLIO PILATI

Centro per lo Studio delle Relazioni fra Struttura e Reattività Chimica del CNR, Via Golgi, 19, I-20133 Milano, Italy

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Abstract

The structures of two indole alkaloids, vincadifformine [methyl (5′*R*,12a*R*,19′*R*)-2,3-didehydroaspidospermidine-3-carboxylate] and 8-oxotabersonine [methyl (5′*R*,12a*R*,19′*R*)-2,3,6,7-tetradehydro-8-oxoaspidospermidine-3-carboxylate] have been established and are compared. The main difference between the two molecules is in the conformation of the six-membered heterocyclic ring which exhibits a chair conformation in vincadifformine but presents a more flattened sofa conformation in 8-oxotabersonine as a result of the presence of a double bond and an oxo group.

Comment

The *Apocynaceae* family has been known for some time now to be a rich source of complex and intriguing indole alkaloids. In particular, the widespread occurrence of aspidospermine alkaloids has attracted considerable attention over the past several decades (Saxton, 1983). By far the most common structural feature that occurs throughout this subtype of indole alkaloids is that found in vincadifformine (1), a crystalline base existing in nature in both enantiomers, which is a member of a distinct group of aspidospermine-like alkaloids bearing an extra C atom in the form of a CO_2Me group (Plat, Le Men, Janot, Budzikiewicz, Wilson, Durham & Djerassi, 1962).

The crystal structures of naturally occurring and synthetic indoles embodying the same chromophore, for example ervafoline, epiervafoline and 19′-hydroxyervafolidine (Henriques, Kan, Chiaroni, Riche, Husson, Kan & Lounasmaa, 1982), dibromovobtusine (Lefebvre-Soubeyran, 1973) and cathovalinine (Chiaroni, Riche, Diatta, Andriamialisoa, Langlois & Potier, 1976), have been well established. As vincadifformine is the most abundant of all these alkaloids, it is surprising to discover that no X-ray investigations have been recorded to date.

Here we report the structures of vincadifformine and 8-oxotabersonine (2), a related alkaloid first isolated from *Amsonia elliptica* (Aimi, Asada, Sakai & Haginiwa, 1978) and subsequently from *Hazunta modesta* (Bui, Das & Potier, 1980). Table 1 gives the atomic coordinates of both structures while Fig. 1 shows the two molecules with the numbering scheme. Selected bond lengths, bond angles and torsion angles are listed in Table 2. The bond distances of (1) and (2) do not display any particular features, all being comparable with values in the literature (see for example Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). Table 3 gives the conformational parameters of the non-aromatic rings of the two compounds.

The skeletons of vincadifformine and 8-oxotabersonine are quite similar, the main difference being found in

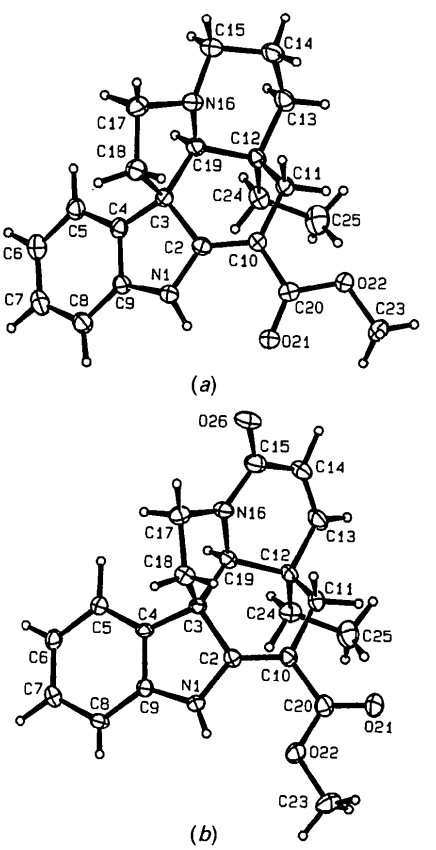

Fig. 1. (*a*) Vincadifformine and (*b*) 8-oxotabersonine; probability level 20%, H atoms not to scale.