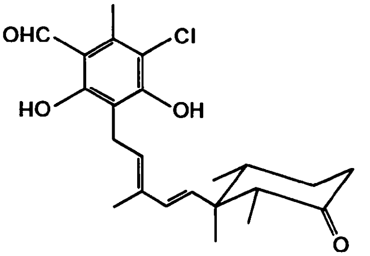
was established mainly on the basis of the two-dimensional ^1H NMR spectrum. The singular rearranged skeleton of the terpenoid part of the molecule shows only a remote similarity with the diterpene alkaloid thelepogine (Fridrichsons & Mathieson, 1960).

The structure determination confirms the general configuration deduced by Bieber *et al.* (1989) from biogenetic pathways. The tetrasubstituted cyclohexanone part of (1) (Fig. 1) has a relative configuration identical with that found in ascochlorin (2), an antibiotic isolated from *Ascochyta viciae* (Nawata, Ando, Tamura, Arima & Iitaka, 1969). Interestingly, cordiaquinone B is dextrorotatory, whereas ascochlorin and all its synthetic precursors containing the same cyclohexanone moiety are levorotatory (Mori & Takechi, 1985).



(2)

The authors thank Professor Brown (URA CNRS 482, Le Mans) for useful discussions.

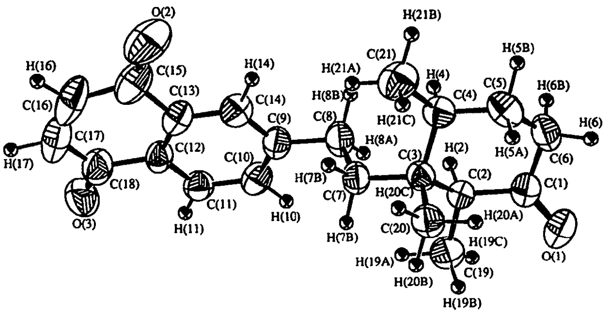


Fig. 1. *ORTEP* plot of the molecule of $C_{21}H_{24}O_3$. For the sake of clarity, the thermal parameters of the H atoms have been divided by ten.

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Structure of 3-(*p*-Chlorophenyl)-1-(3-pyridyl)-2,5-pyrrolidinedione

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Abstract. $C_{15}H_{11}ClN_2O_2$, $M_r = 286{\cdot}72$, monoclinic, $P2_1/c$, $a = 12{\cdot}586$ (2), $b = 6{\cdot}423$ (1), $c = 17{\cdot}186$ (3) Å, $\beta = 92{\cdot}73$ (2)°, $V = 1387{\cdot}7$ (4) Å^3, $Z = 4$, $D_x = 1{\cdot}372$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2{\cdot}7$ cm^{-1}, $F(000) = 592$, room temperature, final $R = 0{\cdot}044$ for 1198 observed reflections (of 2393 unique data). There are no unusual distances or angles. The angles between the plane of the five-membered ring and those of the phenyl and pyridyl rings are 89·1 (1) and 53·9 (1)° respectively.

Experimental. The title compound was recrystallized from ethanol to give colourless block-like crystals. Crystal dimensions 0·15 × 0·25 × 0·2 mm. Preliminary data obtained from a CAD-4 diffractometer. Final lattice parameters from least-squares refinement of 25 reflections ($4 < \theta < 12°$); no absorption correction applied; $\theta < 25°$ (h 0/14, k 0/7, l −20/20); ω–2θ scan technique; Mo $K\alpha$ radiation at room temperature; intensity of three standard reflections monitored every 70 reflections showed no significant fluctuations; 2393 unique reflections measured; 1198 observed reflections with $I > 2\sigma(I)$.

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Structure solved by direct methods [*SHELXS*86 (Sheldrick, 1986)] with $R(E) = 0{\cdot}29$. The E map provided positions for all non-H atoms. All H atoms were located in calculated positions in the riding model; isotropic thermal parameters of H atoms taken as 1·5 times the temperature factors for their parent C atoms. Refinement by full-matrix least squares (on F) with anisotropic temperature factors for all non-H atoms converged to $R = 0{\cdot}044$ {with $w = 2{\cdot}0364/[\sigma(F)^2]$ to $wR = 0{\cdot}036$} with the empirical extinction-correction coefficient $g = 0{\cdot}00143$; changes in all parameters $\Delta/\sigma < 0{\cdot}03$. The minimum and maximum peaks in the final $\Delta\rho$ map were $-0{\cdot}18$ and 0·18 e Å^{-3}; atomic scattering factors from *SHELX76* (Sheldrick, 1976). All calculations performed using *SHELX76* and *CSU* programs (Vicković, 1988) on an Amstrad 1512 PC. The molecule is shown in Fig. 1, coordinates are given in Table 1,* and bond distances and angles are listed in Table 2.

Table 1. *Non-*H *fractional atomic coordinates* (× 10^4) *and equivalent isotropic temperature factors* (× 10^3) *with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}(Å^2)
C(1)	262 (3)	−6659 (6)	872 (2)	51 (1)
C(2)	584 (3)	−4419 (6)	1924 (2)	53 (1)
C(3)	1638 (3)	−5533 (6)	1818 (2)	53 (1)
C(4)	1361 (3)	−7174 (6)	1187 (2)	60 (1)
C(5)	−1191 (3)	−4274 (5)	1233 (2)	46 (1)
C(6)	−1376 (3)	−2163 (6)	1120 (2)	53 (1)
C(8)	−3165 (3)	−2672 (8)	1033 (2)	74 (1)
C(9)	−3047 (3)	−4787 (7)	1128 (2)	81 (2)
C(10)	−2040 (3)	−5620 (6)	1241 (2)	66 (1)
C(11)	2453 (3)	−3904 (6)	1603 (2)	51 (1)
C(12)	2396 (3)	−2954 (6)	876 (2)	61 (1)
C(13)	3079 (3)	−1370 (6)	697 (2)	64 (1)
C(14)	3829 (3)	−726 (6)	1249 (3)	61 (1)
C(15)	3926 (3)	−1672 (8)	1963 (2)	81 (1)
C(16)	3234 (3)	−3257 (7)	2140 (2)	72 (1)
C(1)	−232 (2)	−7455 (4)	337 (1)	70 (1)
C(2)	389 (2)	−3192 (4)	2430 (1)	75 (1)
N(1)	−128 (2)	−5031 (4)	1329 (2)	44 (1)
N(2)	−2351 (3)	−1346 (5)	1027 (2)	68 (1)
Cl	4647 (1)	1390 (2)	1036 (1)	98 (< 1)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)	C(4)	1·498 (5)	C(6)	N(2)	1·337 (5)
C(1)	C(1)	1·200 (4)	C(8)	C(9)	1·375 (7)
O(1)	N(1)	1·410 (5)	C(8)	N(2)	1·333 (6)
C(2)	C(3)	1·526 (5)	C(9)	C(10)	1·381 (5)
C(2)	O(2)	1·207 (4)	C(11)	C(12)	1·389 (5)
C(2)	N(1)	1·384 (5)	C(11)	C(16)	1·380 (5)
C(3)	C(4)	1·540 (5)	C(12)	C(13)	1·376 (5)
C(3)	C(11)	1·523 (5)	C(13)	C(14)	1·370 (6)
C(5)	C(6)	1·388 (5)	C(14)	C(15)	1·369 (6)
C(5)	C(10)	1·375 (5)	C(14)	Cl	1·754 (4)
C(5)	N(1)	1·426 (4)	C(15)	C(16)	1·383 (6)

C(4)	C(1)	O(1)	128·2 (3)	C(5)	C(10)	C(9)	117·6 (3)
C(4)	C(1)	N(1)	107·6 (3)	C(3)	C(11)	C(12)	120·9 (3)
O(1)	C(1)	N(1)	124·2 (3)	C(3)	C(11)	C(16)	120·7 (3)
C(3)	C(2)	O(2)	126·9 (3)	C(12)	C(11)	C(16)	118·3 (3)
C(3)	C(2)	N(1)	108·3 (3)	C(11)	C(12)	C(13)	121·3 (3)
O(2)	C(2)	N(1)	124·8 (3)	C(12)	C(13)	C(14)	119·1 (4)
C(2)	C(3)	C(4)	103·7 (3)	C(13)	C(14)	C(15)	121·0 (4)
C(2)	C(3)	C(11)	107·8 (3)	C(13)	C(14)	Cl	118·8 (3)
C(4)	C(3)	C(11)	115·6 (3)	C(15)	C(14)	Cl	120·2 (3)
C(1)	C(4)	C(3)	106·1 (3)	C(14)	C(15)	C(16)	119·6 (4)
C(6)	C(5)	C(10)	119·4 (3)	C(11)	C(16)	C(15)	120·7 (4)
C(6)	C(5)	N(1)	120·0 (3)	C(1)	N(1)	C(2)	113·1 (3)
C(10)	C(5)	N(1)	120·7 (3)	C(1)	N(1)	C(5)	122·6 (3)
C(5)	C(6)	N(2)	123·2 (3)	C(2)	N(1)	C(5)	124·0 (3)
C(9)	C(8)	N(2)	123·6 (4)	C(6)	N(2)	C(8)	116·7 (4)
C(8)	C(9)	C(10)	119·5 (4)				

Related literature. The title compound is a member of a series of compounds with potential anticonvulsant properties. The aim of this work is therefore to collect information for further examination of structure–activity relationships. The compounds have been the subject of pharmacological screening (Łucka-Sobstel, Zejc & Obniska, 1977; Lange, Rump, Ilczuk, Łapiszewicz, Rabsztyn & Walczyna, 1977; Lange, Rump, Gałecka, Ilczuk, Lechowska-Postek, Rabsztyn, Szymańska & Walczyna, 1977; Łapiszewicz, Lange, Rump & Walczyna, 1978; Chmielewska, 1983, 1984; Zejc & Obniska, 1984; Zejc, Obniska, Chojnacka-Wójcik, Tatarczyńska & Wiczyńska, 1987). Some have been subjected to X-ray structure analyses (Kwiatkowski, Karolak-Wojciechowska, Obniska & Zejc, 1990).

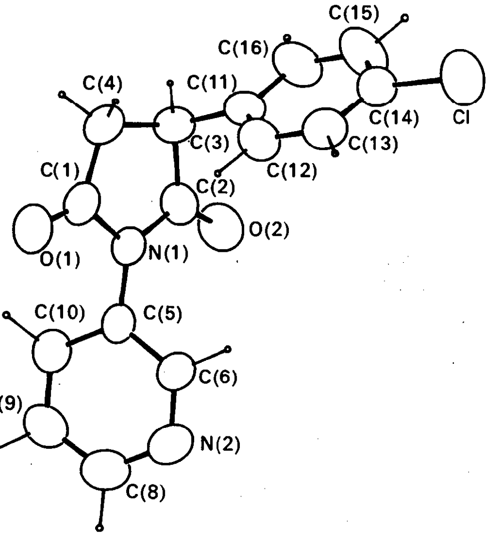

Fig. 1. Numbering scheme and conformation of the title compound.

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* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52443 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Room-Temperature Structure of *α*–*β* Ethylenic Sulfoxide $C_{15}H_{18}OS$: (−)-4,5-Dimethyl-1-*p*-tolylsulfinyl-1,4-cyclohexadiene

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Abstract. $C_{15}H_{18}OS$, $M_r = 246{\cdot}37$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}263\,(2)$, $b = 7{\cdot}965\,(2)$, $c = 26{\cdot}51\,(1)$ Å, $V = 1323\,(1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}24$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}18$ mm^{-1}, $F(000) = 528$, room temperature, $R = 0{\cdot}048$, 701 unique reflections, crystal growth from toluene solution. The structure determination shows that the ground-state conformation of the molecule is S-*trans*.

Experimental. Crystal specimens were obtained from toluene solution by slow evaporation of the solvent giving rise to a prismatic $0{\cdot}20 \times 0{\cdot}10 \times 0{\cdot}10$ mm crystal.

Data were collected on a Siemens AED2 four-circle diffractometer, ω–θ step-scan mode in N steps of 0·035°, $37 \le N \le 41$, time per step: 4 s. Aperture $D = 3{\cdot}5$ mm. Lattice constants were based on 36 reflections measured in double step scan mode at $\pm(2\theta \simeq 28°)$; no correction for absorption. Intensity measurement to $2\theta \le 50°$ within range $0 \le h \le 7$, $0 \le k \le 8$, $0 \le l \le 30$. Standard reflections $1\bar{1}1$, $00\bar{8}$, 111, intensity variation 0·8%; 1419 independent reflections measured, 701 reflections used for refinements $[|F| > 6\sigma(|F|)]$.

Structure was solved from direct methods with the *TANG* option of the *SHELX76* program (Sheldrick, 1976). F magnitudes were used in least-squares refinements: 186 parameters refined; mean $\Delta/\sigma = 0{\cdot}034$, max. $\Delta/\sigma = 0{\cdot}21$; secondary-extinction factor: $x = 4{\cdot}0 \times 10^{-8}$; atomic scattering factors for O, C, H and S were from *International Tables for X-ray Crystallography* (1974); calculations were with the *SHELX76* program (Sheldrick, 1976).

The multisolution tangent direct method of *SHELX76* gives a solution with all non-hydrogen atoms. Successive refinements and Fourier maps were allowed to distinguish oxygen from carbon atoms. Hydrogen atoms were then found from difference Fourier maps and geometric constraints were applied to CH_3, CH_2 or CH groups ($d_{C—H} = 1{\cdot}08$ Å). A unique isotropic thermal parameter was refined for all hydrogen atoms. The residuals decreased to $R = 0{\cdot}048$, $wR = 0{\cdot}041$; $w = 1{\cdot}84/[\sigma^2(|F_o|) + 0{\cdot}00007F_o^2]$. Max. and min. heights in final difference Fourier map: $+0{\cdot}24$ and $-0{\cdot}28$ e Å^{-3}. The absolute configuration of the molecule was not determined.

The final atomic coordinates and equivalent isotropic temperature factors are listed in Table 1.* Selected bond lengths and angles are listed in Table

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52466 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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