the values of the angles are comparable with those of ellipticine (Courseille, Busetta & Hospital, 1974) and its derivatives (Aggarwal, Neidle & Sainsbury, 1983; Courseille, Busetta & Hospital, 1982; Kuroda & Sainsbury, 1984; Garlich, Kaiser & Schlemper, 1984, and references therein). It follows that a substituent in position 9 or 11 only exerts a minor influence on the molecular conformation, which is not surprising considering the rigidity of such types of aromatic molecule.

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# Structure of Lumi-arteannuin B

By Judith L. Flippen-Anderson, Richard Gilardi and Clifford George

*Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC* 20375-5000, *USA*

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**Abstract.** $C_{15}H_{20}O_3$, $M_r = 248{\cdot}25$, monoclinic, $P2_1$, $a = 6{\cdot}970\,(1)$, $b = 14{\cdot}004\,(2)$, $c = 14{\cdot}124\,(2)$ Å, $\beta = 104{\cdot}94\,(1)°$, $V = 1332{\cdot}0\,(4)$ Å$^3$, $Z = 4$, $D_x = 1{\cdot}238$ Mg m$^{-3}$, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}54178$ Å, $\mu = 0{\cdot}65$ mm$^{-1}$, $F(000) = 536$, $T = 295$ K, final $R = 0{\cdot}044$, $wR = 0{\cdot}042$ for 1473 independent observed reflections. Formed by rearrangement upon irradiation of arteannuin B. Both molecules in the asymmetric unit have the same conformation. All three O atoms lie on the same side of the best plane through the nine-membered ring and consequently there are close O···O intramolecular approaches (2·82–3·24 Å). The nine-membered ring is flattened on one end with C1—C2···C8—C9 forming a plane. The epoxy ring is at an angle of 105° to this plane.

**Experimental.** Colorless, $0{\cdot}06 \times 0{\cdot}32 \times 0{\cdot}18$ mm crystal, from benzene/cyclohexane. Isolated by N. Roth of the Division of Experimental Therapeutics of the Walter Reed Army Institute of Research, m.p. = 437–439 K. Automated Nicolet $R3m$ diffractometer with incident-beam graphite monochromator; 25 centered reflections within $26 < 2\theta < 60°$ used for determining cell parameters. Data corrected for Lorentz and polarization effects, absorption ignored. $2\theta_{\max} = 110°$; range of $hkl$: $0 \le h \le 7$, $0 \le k \le 14$, $-15 \le l < 13$. Standards, $1\bar{1}0$, 040, 004, monitored every 60 reflections with random variation 2·4% over data collection, $\theta$–$2\theta$ mode, scan width $(2{\cdot}0 + \Delta_{\alpha1,\alpha2})$, scan rate a function of count rate (6° min$^{-1}$ minimum, 60° min$^{-1}$ maximum); 2041 reflections measured, 1763 unique, $R_{\mathrm{int}} = 0{\cdot}019$, 1473 observed $[F_o > 3\sigma(F_o)]$.

Structure solved by direct methods. The least-squares

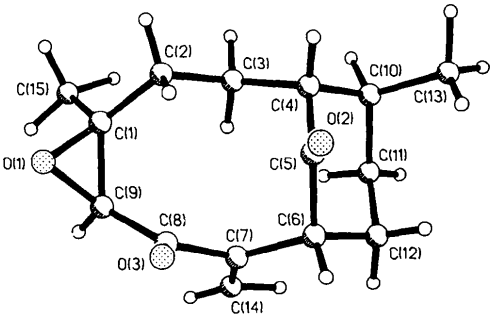

Fig. 1. Perspective drawing of the results of the X-ray study on lumi-arteannuin B. Only one of the two molecules in the asymmetric unit is shown. Numbering of the second molecule was set by adding 20 to the number of the corresponding atom in the illustrated molecule.

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Table 1. *Atomic coordinates and equivalent isotropic displacement parameters* (Å$^2$ × 10$^2$)

| | $x$ | $y$ | $z$ | $U_{eq}$* |
|---|---|---|---|---|
| C(1) | 0·3516 (8) | 0·1424 (5) | 0·9627 (4) | 4·6 (2) |
| C(2) | 0·4157 (8) | 0·0397 (5) | 0·9765 (3) | 4·3 (2) |
| C(3) | 0·3532 (8) | −0·0148 (5) | 0·8781 (4) | 4·3 (2) |
| C(4) | 0·2722 (8) | −0·1149 (5) | 0·8861 (3) | 4·2 (2) |
| C(5) | 0·1040 (8) | −0·1147 (5) | 0·9358 (4) | 4·1 (2) |
| C(6) | −0·0957 (8) | −0·0742 (5) | 0·8792 (4) | 4·8 (2) |
| C(7) | −0·0916 (8) | 0·0345 (5) | 0·8707 (4) | 4·5 (2) |
| C(8) | 0·0044 (8) | 0·0845 (5) | 0·9646 (4) | 4·8 (2) |
| C(9) | 0·1451 (9) | 0·1655 (5) | 0·9576 (4) | 5·1 (2) |
| C(10) | 0·2031 (9) | −0·1630 (5) | 0·7851 (4) | 5·5 (3) |
| C(11) | 0·0037 (9) | −0·1212 (5) | 0·7260 (4) | 6·1 (3) |
| C(12) | −0·1561 (9) | −0·1261 (5) | 0·7812 (4) | 5·9 (2) |
| C(13) | 0·1945 (12) | −0·2721 (5) | 0·7966 (5) | 7·7 (3) |
| C(14) | −0·1736 (9) | 0·0842 (6) | 0·7909 (5) | 5·7 (3) |
| C(15) | 0·4689 (9) | 0·2050 (5) | 0·9130 (4) | 6·0 (3) |
| O(1) | 0·2954 (6) | 0·1864 | 1·0451 (3) | 6·1 (2) |
| O(2) | 0·1221 (6) | −0·1508 (4) | 1·0155 (3) | 5·7 (2) |
| O(3) | −0·0163 (7) | 0·0579 (4) | 1·0429 (3) | 7·1 (2) |
| C(21) | −0·0241 (10) | 0·9051 (5) | 0·2747 (4) | 5·5 (3) |
| C(22) | −0·0175 (9) | 0·9162 (5) | 0·3813 (4) | 5·6 (2) |
| C(23) | 0·0034 (8) | 1·0220 (5) | 0·4106 (3) | 4·7 (2) |
| C(24) | 0·1478 (8) | 1·0409 (5) | 0·5112 (3) | 4·6 (2) |
| C(25) | 0·3517 (9) | 1·0013 (5) | 0·5215 (4) | 5·5 (2) |
| C(26) | 0·4786 (9) | 1·0478 (6) | 0·4609 (4) | 6·0 (3) |
| C(27) | 0·4032 (8) | 1·0278 (6) | 0·3509 (4) | 5·3 (2) |
| C(28) | 0·3526 (10) | 0·9249 (6) | 0·3255 (4) | 5·9 (3) |
| C(29) | 0·1615 (11) | 0·9077 (5) | 0·2466 (4) | 6·0 (3) |
| C(30) | 0·1666 (8) | 1·1484 (5) | 0·5362 (4) | 5·1 (2) |
| C(31) | 0·2932 (10) | 1·1980 (5) | 0·4764 (4) | 6·0 (3) |
| C(32) | 0·4944 (10) | 1·1540 (6) | 0·4881 (5) | 6·5 (3) |
| C(33) | 0·2515 (10) | 1·1642 (6) | 0·6468 (4) | 7·2 (3) |
| C(34) | 0·3905 (10) | 1·0926 (7) | 0·2823 (5) | 6·6 (3) |
| C(35) | −0·2100 (10) | 0·9337 (6) | 0·2022 (5) | 7·2 (3) |
| O(21) | 0·0674 (8) | 0·8186 (4) | 0·2499 (3) | 7·8 (2) |
| O(22) | 0·4215 (7) | 0·9402 (4) | 0·5814 (3) | 8·7 (2) |
| O(23) | 0·4495 (8) | 0·8608 (5) | 0·3697 (3) | 9·5 (2) |

* Equivalent isotropic $U$ defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

refinement used the full-matrix program provided with the MicroVAX versions of the *SHELXTL* system (Sheldrick, 1980). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1/[\sigma^2(|F_o|) + g(F_o)^2]$, $g = 0{\cdot}00025$. 348 parameters refined: atom coordinates and anisotropic temperature factors for all non-H atoms; for H atoms, coordinates riding (C—H distance held constant at 0·96 Å) on covalently bonded atoms and isotropic thermal parameters fixed at final isotropic values of covalently bonded atoms; $(\Delta/\sigma)_{\max} = 0{\cdot}304$, $R = 0{\cdot}044$, $wR = 0{\cdot}042$, $S = 1{\cdot}28$. Final difference Fourier excursions 0·16 and −0·17 e Å$^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).* Atom numbering for Tables 1 and 2, atom coordinates, bond distances and bond angles, follows that shown in Fig. 1.

Table 2. *Bond lengths* (Å) *and angles* (°)

| | | | |
|---|---|---|---|
| C(1)–C(2) | 1·504 (8) | C(1)–C(9) | 1·459 (7) |
| C(1)–C(15) | 1·492 (8) | C(1)–O(1) | 1·456 (6) |
| C(2)–C(3) | 1·547 (7) | C(3)–C(4) | 1·527 (7) |
| C(4)–C(5) | 1·514 (7) | C(4)–C(10) | 1·538 (7) |
| C(5)–C(6) | 1·524 (7) | C(5)–O(2) | 1·211 (5) |
| C(6)–C(7) | 1·528 (8) | C(6)–C(12) | 1·524 (7) |
| C(7)–C(8) | 1·496 (8) | C(7)–C(14) | 1·322 (8) |
| C(8)–C(9) | 1·519 (8) | C(8)–O(3) | 1·210 (6) |
| C(9)–O(1) | 1·430 (6) | C(10)–C(11) | 1·539 (8) |
| C(10)–C(13) | 1·539 (8) | C(11)–C(12) | 1·516 (8) |
| C(21)–C(22) | 1·502 (7) | C(21)–C(29) | 1·448 (9) |
| C(21)–C(35) | 1·485 (8) | C(21)–O(21) | 1·453 (7) |
| C(22)–C(23) | 1·534 (8) | C(23)–C(24) | 1·538 (6) |
| C(24)–C(25) | 1·498 (8) | C(24)–C(30) | 1·544 (8) |
| C(25)–C(26) | 1·526 (8) | C(25)–O(22) | 1·214 (6) |
| C(26)–C(27) | 1·531 (8) | C(26)–C(32) | 1·533 (9) |
| C(27)–C(28) | 1·504 (9) | C(27)–C(34) | 1·315 (8) |
| C(28)–C(29) | 1·519 (8) | C(28)–O(23) | 1·198 (7) |
| C(29)–O(21) | 1·416 (7) | C(30)–C(31) | 1·536 (8) |
| C(30)–C(33) | 1·537 (7) | C(31)–C(32) | 1·502 (9) |

| | | | |
|---|---|---|---|
| C(9)–C(1)–C(2) | 118·3 (5) | C(15)–C(1)–C(2) | 116·2 (5) |
| C(15)–C(1)–C(9) | 120·0 (5) | O(1)–C(1)–C(2) | 115·7 (4) |
| O(1)–C(1)–C(9) | 58·7 (3) | O(1)–C(1)–C(15) | 114·9 (5) |
| C(3)–C(2)–C(1) | 110·5 (4) | C(4)–C(3)–C(2) | 114·3 (4) |
| C(5)–C(4)–C(3) | 112·2 (4) | C(10)–C(4)–C(3) | 111·5 (4) |
| C(10)–C(4)–C(5) | 109·7 (4) | C(6)–C(5)–C(4) | 118·0 (4) |
| O(2)–C(5)–C(4) | 121·5 (5) | O(2)–C(5)–C(6) | 120·3 (5) |
| C(7)–C(6)–C(5) | 112·3 (5) | C(12)–C(6)–C(5) | 107·4 (5) |
| C(12)–C(6)–C(7) | 114·2 (5) | C(8)–C(7)–C(6) | 114·2 (5) |
| C(14)–C(7)–C(6) | 125·3 (6) | C(14)–C(7)–C(8) | 120·4 (6) |
| C(9)–C(8)–C(7) | 116·1 (5) | O(3)–C(8)–C(7) | 122·3 (5) |
| O(3)–C(8)–C(9) | 121·3 (5) | C(8)–C(9)–C(1) | 118·5 (5) |
| O(1)–C(9)–C(1) | 60·5 (3) | O(1)–C(9)–C(8) | 116·0 (5) |
| C(11)–C(10)–C(4) | 111·0 (5) | C(13)–C(10)–C(4) | 110·3 (5) |
| C(13)–C(10)–C(11) | 112·3 (5) | C(12)–C(11)–C(10) | 112·6 (5) |
| C(11)–C(12)–C(6) | 112·2 (5) | C(9)–O(1)–C(1) | 60·7 (3) |
| C(29)–C(21)–C(22) | 118·3 (6) | C(35)–C(21)–C(22) | 117·3 (6) |
| C(35)–C(21)–C(29) | 119·1 (5) | O(21)–C(21)–C(22) | 115·2 (5) |
| O(21)–C(21)–C(29) | 58·4 (4) | O(21)–C(21)–C(35) | 114·7 (5) |
| C(23)–C(22)–C(21) | 110·2 (4) | C(24)–C(23)–C(22) | 114·2 (5) |
| C(25)–C(24)–C(23) | 113·8 (4) | C(30)–C(24)–C(23) | 112·1 (5) |
| C(30)–C(24)–C(25) | 108·5 (5) | C(26)–C(25)–C(24) | 117·4 (5) |
| O(22)–C(25)–C(24) | 121·9 (6) | O(22)–C(25)–C(26) | 120·4 (6) |
| C(27)–C(26)–C(25) | 113·2 (5) | C(32)–C(26)–C(25) | 106·7 (5) |
| C(32)–C(26)–C(27) | 114·6 (5) | C(28)–C(27)–C(26) | 114·6 (5) |
| C(34)–C(27)–C(26) | 124·1 (6) | C(34)–C(27)–C(28) | 121·2 (6) |
| C(29)–C(28)–C(27) | 115·8 (5) | O(23)–C(28)–C(27) | 121·8 (6) |
| O(23)–C(28)–C(29) | 122·2 (6) | C(28)–C(29)–C(21) | 118·6 (5) |
| O(21)–C(29)–C(21) | 61·0 (4) | O(21)–C(29)–C(28) | 116·2 (5) |
| C(31)–C(30)–C(24) | 110·0 (5) | C(33)–C(30)–C(24) | 111·1 (5) |
| C(33)–C(30)–C(31) | 111·7 (5) | C(32)–C(31)–C(30) | 114·0 (5) |
| C(31)–C(32)–C(26) | 111·4 (5) | C(29)–O(21)–C(21) | 60·6 (4) |

**Related literature.** The structures of other materials isolated from the plant *Artemesia annua* have been reported (Luo, Yeh, Brossi, Flippen-Anderson & Gilardi, 1984; Lin, Klayman, Hoch, Silverton & George, 1985).

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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 44393 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.