Crystallographic data of pimaricin and rimocidin crystals, two polyene macrolide antifungal antibiotics

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The structure of pimaricin (GOLDING et al., 1966) and rimocidin (FALKOWSKI et al., 1976) were established on the basis of chemical and spectroscopic evidences. However, three-dimensional structures of these polyenes remain still unknown. An X-ray investigation were undertaken to elucidate crystal and molecular structure of the title compounds. In a long run an explanation of the molecular structure-biological activity relationship will be endeavoured.

Preliminary crystallographic studies were performed on a precession camera with $CuK\alpha$ radiation. The results are:

	pimaricin	rimocidin
Formula	$C_{33}H_{47}NO_{13}$	$C_{39}H_{61}NO_{14}$
Crystal system	monoclinic	monoclinic
Space group	$P2_1$	$P2_1$
Cell dimensions	$a = 7.68\,(1)$ Å	$a = 9.60\,(1)$ Å
	$b = 8.75\,(1)$ Å	$b = 9.31\,(1)$ Å
	$c = 26.90\,(2)$ Å	$c = 27.76\,(2)$ Å
	$\beta = 92.3\,(2)°$	$\beta = 95.0\,(2)°$
Unit cell volume	1805 Å^3	2472 Å^3
Z	2	2

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The number of molecules in the unit cell was calculated from the unit cell volume (KEMPSTER and LIPSON, 1972). The $P2_1$ space group was assumed for both crystals as each of the unit cell contains only two identical asymmetric molecules.

References

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