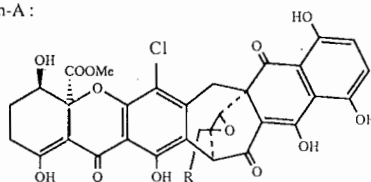


chlorinated Xanthone/Anthraquinone skeleton. Most of these toxins belong to the two families of Beticolin A and B (figure). Both types of toxins differ mainly by the way the two anthraquinone and xanthone moieties are attached together. Beticolin 1 (R=H) and Beticolin 3 (R=OH), part of the beticolin A family, were crystallized from CHCl<sub>3</sub>/methanol mixture as CHCl<sub>3</sub> solvates (the structures are isomorphous) while Beticolin 2 (B type, R=H) and Beticolin 4 (B type, R=OH) were identified by NMR (Millat et al., 1993) to share the cebetin A structure (Jalal et al., 1992).

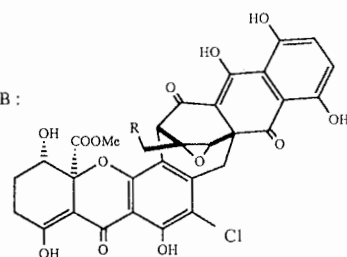
The structure of Beticolin 1 was easily solved by direct methods. In the case of Beticolin 3, the crystals so far obtained were too small (max. size : 0.15mm) to produce enough data for direct methods. The structure was solved by Molecular Replacement technique.

	Beticolin 1	Beticolin 3
Xtal size (mm) :	0.25x0.25x0.5	0.05x0.05x0.15
nb. of Fobs observed :	2480	1027
R factor (%) :	6.0	9.4

Beticolin-A :



Beticolin-B :



## References :

- M.A.F. Jalal, M.B. Bilayet Hossain, D.J. Robeson, D. van der Helm (1992) *J. Amer. Chem. Soc.*, 114, 5967-5971.
- M.L. Millat, J.P. Blein, J. Einhorn, J.C. Tabet, P.H. Ducrot, J.Y. Lallemand (1993) *Tetrahedron Lett.*, submitted.

**PS-04.01.25 THE STRUCTURE OF DUTOMYCIN.** Ming-Qin Chen\* and Jie Liu, Research Center of analysis & Measurement, Fudan University, Shanghai, P.R.China, 200433. Li-Jiang Xuan, Sao-Hua Xu, Hai-Lin Zhang and Ya-Ming Xu, Shanghai Institute of Materia Medica, Academia Sinica, P.R.China.

Dutomycin, a new antitumor antibiotic, has been found in the culture of *Streptomyces* SP1725 (Ya-Ming Xu and Ming-Qin Chen, et al.(1992) *J.Antibiotics*, 45, 715). The antibiotic was active against leukemia P388 and 100% inhibition was achieved as a concentration of 1 µg/ml. We report herewith its molecular structure and absolute configuration.

The empirical formula was established as C<sub>41</sub>H<sub>51</sub>O<sub>11</sub>·2C<sub>2</sub>H<sub>5</sub> on the basis of X-ray diffraction analysis and reconfirmed by elemental analysis, NMR spectral analysis and chemical degradation. The compound crystallized in the orthorhombic space group P2<sub>1</sub>2<sub>1</sub>2, with a=18.045(3), b=18.963(3), c=15.611(3)Å, V=5341.8Å<sup>3</sup>, Z=4. Based on 5223 unique and 1612 observed reflections (I>3σ(I)), the structure was solved by direct methods and refined by full matrix least squares to the final R value of 0.0773. The molecule has a naphthacene carbon skeleton which is structurally related to the tetracycline and Anthracycline antibiotics,

such as SP2575 (Masahiro Hatsu, et al.(1992) *J. Antibiotics*, 45, 325), and is unique by bearing glycosides and 2,4-dimethylheptene-2 acid moieties and containing many carbonyl groups which may relate to its biological activity as shown in Fig. 1.

In the aglycone moiety intramolecular hydrogen bonding between the exocyclic oxygen atoms on neither rings B and C nor C and D has been observed. However, the intramolecular hydrogen bonding O<sub>111</sub>...H<sub>119</sub>...O<sub>3</sub> may exist. This differs from that observed in most anthracycline antibiotics. The rings B, C, D are nearly coplanar (except C<sub>111</sub> atom) because of the configuration among these atoms. It resembles the shape observed in all the anthracycline antibiotics.

The absolute configuration of Dutomycin was elucidated by subsequent chemical degradation (See Fig. 2). Methanolysis of 1 with methanolic hydrochloric acid gave the aglycone 2 and a pair of anomeric isomers 3 and 4. 3 was further methanolized in alkaline methanol and L-axenose methyl glycosides 5 was obtained (Arcamone, F. et al. (1973) *J. Am. Chem. Soc.*, 95, 2008). Since the configuration of 5 was known and consistent with that found in Dutomycin, the determined structure was thus implied absolute meaning due to the retention of the configuration during degradations. The chiral carbon atoms C<sub>11</sub>, C<sub>11'</sub>, C<sub>11''</sub>, C<sub>1'</sub>, C<sub>1''</sub>, C<sub>1</sub>, and C<sub>1'''</sub> thus have the configuration of (S,S,R,R,R,S,R).

Fig. 1 Perspective view of dutomycin (4).

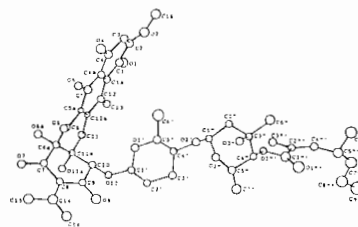
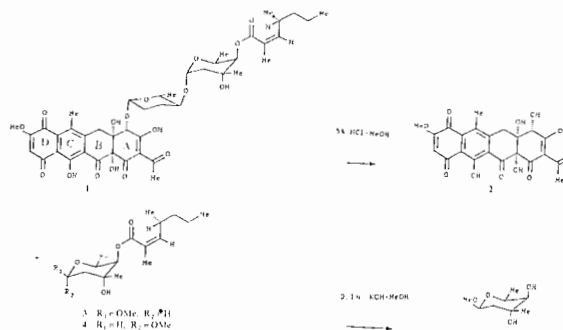


Fig. 2 Structure of dutomycin (1) and its derivatives.



**PS-04.01.26 THE PROTOTYPES OF THE ENNIATIN B CHANNELS IN THE CRYSTAL STRUCTURE OF THIS MEMBRANE-ACTIVE ANTIBIOTIC**

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The crystal structure of the title compound has been determined by a single-crystal three-dimensional X-ray diffraction study. The compound crystallized from heptane in the space group P2<sub>1</sub> with four C<sub>33</sub>H<sub>57</sub>N<sub>3</sub>O<sub>9</sub> molecules in one asymmetric unit. The unit cell dimensions are a=29.178(15), b=28.294(15), c=10.840(5)Å, g=121.12(5)°. The structure was solved by direct