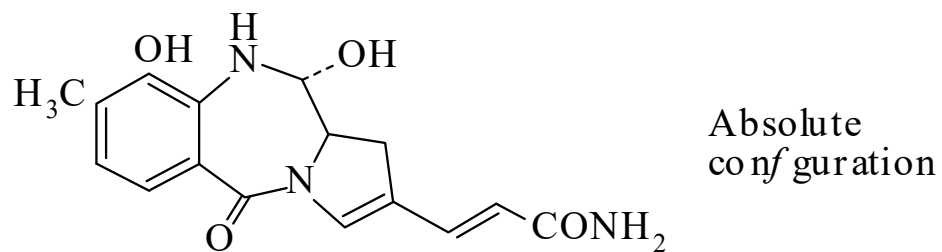




>>Entry Name: Anthramycin, USAN

Synonym(s): 3-(5,10,11,11a-Tetrahydro-9,11-dihydroxy-8-methyl-5-oxo-1*H*-pyrrolo[2,1-*c*][1,4]benzodiazepin-2-yl)-2-propenamide, 9Cl. **Antramycin**, INN. Refuin. Ro 5-9000. Antibiotic Ro 5-9000



CAS Registry Number: 4803-27-4

Molecular Formula: C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>4</sub>

Molecular Weight: 315.328

Accurate Mass: 315.121907

Percentage Composition: C 60.94%; H 5.43%; N 13.33%; O 20.30%

Biological Source: Isol. from *Streptomyces refuineus* var. *thermotolerans* and *Streptomyces spadicogriseus*

Use/Importance: Antibiotic with antineoplastic activity. DNA complexing agent

Physical Description: Small yellow prisms (Me<sub>2</sub>CO aq.)

Melting Point: Mp 188-194°

Optical Rotation: [α]<sub>D</sub><sup>25</sup>+930 (c, 1 in DMF)

Solubility: BERDY SOL: Sol. DMF, DMSO, MeOH, butanol; poorly sol. hexane

Calculated Log P Data: Log P -1.1 (uncertain value) (calc)

UV: [acid] λ<sub>max</sub> 235 (ε 18200); 333 (ε 31800) (MeCN) (Derep) [neutral] λ<sub>max</sub> 220 (ε 34000); 235 (sh) (ε 30000); 335 (ε 39400) (MeOH) (Derep) [neutral] λ<sub>max</sub> 220 (); 336 () (MeOH) (Berdy) [neutral] λ<sub>max</sub> 235 (ε 18200); 333 (ε 31800) (MeCN) (Berdy)

Other Data: Cryst. from hot aq. MeOH gives the Me ether. Epimerises in soln.

Hazard & Toxicity: LD<sub>50</sub> (mus, ipr) 0.65 mg/kg ; BERDY HAZD : LD<sub>50</sub> (mus, ipr) .73 mg/kg

>>Derivative: 11-Me ether

Physical Description: Pale-yellow needles (H<sub>2</sub>O)

Melting Point: Mp 120 dec.°

Optical Rotation: [α]<sub>D</sub><sup>25</sup>+1002 (c, 1 in DMF)

UV: [neutral] λ<sub>max</sub> 218 (ε 30000); 231 (ε 22100); 232 (sh) (ε ); 334 (ε 40800); 360 (sh) (ε ) (MeCN) (Derep)

#### References:

Leimgruber, W. *et al.*, *J.A.C.S.*, 1965, **87**, 5791; 1968, **90**, 5641, (*isol, ir, uv, ms, nmr, struct, synth*)

Kohn, K.W., *Antibiotics (N.Y.)*, 1975, **3**, 3, (*rev*)

Horwitz, S.B., *Handb. Exp. Pharmacol.*, 1975, **38**, 642, (*rev, pharmacol*)

Hurley, L.H., *J. Antibiot.*, 1977, **30**, 349, (*rev, biosynth*)

Mostad, A. *et al.*, *Acta Chem. Scand., Ser. B*, 1978, **32**, 639, (*cryst struct*)

Komatsu, N. *et al.*, *J. Antibiot.*, 1980, **33**, 54, (*isol*)

Hurley, L.H., *Antibiotics (N.Y.)*, 1981, **4**, 262, (*rev*)

Ishikura, M. *et al.*, *Chem. Comm.*, 1982, 741, (*synth*)

Pena, M.R. *et al.*, *J.A.C.S.*, 1989, **111**, 5417, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, API000