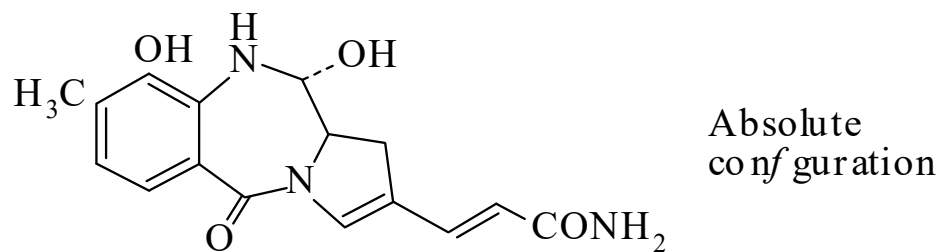




>>Entry Name: Anthramycin, USAN

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: C₁₆H₁₇N₃O₄

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 (Me₂CO aq.)

Melting Point: Mp 188-194°

Optical Rotation: [α]_D²⁵+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_{max} 235 (ε 18200); 333 (ε 31800) (MeCN) (Derep) [neutral] λ_{max} 220 (ε 34000); 235 (sh) (ε 30000); 335 (ε 39400) (MeOH) (Derep) [neutral] λ_{max} 220 (); 336 () (MeOH) (Berdy) [neutral] λ_{max} 235 (ε 18200); 333 (ε 31800) (MeCN) (Berdy)

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

Hazard & Toxicity: LD₅₀ (mus, ipr) 0.65 mg/kg ; BERDY HAZD : LD₅₀ (mus, ipr) .73 mg/kg

>>Derivative: 11-Me ether

Physical Description: Pale-yellow needles (H₂O)

Melting Point: Mp 120 dec.°

Optical Rotation: [α]_D²⁵+1002 (c, 1 in DMF)

UV: [neutral] λ_{max} 218 (ε 30000); 231 (ε 22100); 232 (sh) (ε); 334 (ε 40800); 360 (sh) (ε) (MeCN) (Derep)

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