



CAS Registry Number: 50-76-0

Related CAS Registry Numbers(s): 1402-43-3 1402-51-3 1402-58-0 54650-01-0

Molecular Formula: C₆₂H₈₆N₁₂O₁₆

Molecular Weight: 1255.432

Accurate Mass: 1254.628478

Percentage Composition: C 59.32%; H 6.90%; N 13.39%; O 20.39%

Biological Source: Isol. from *Actinomyces* spp.

Biological Use/Importance: Active against gram-positive bacteria and malignant neoplasms

Physical Description: Red rhomboids + 3H₂O (EtOH)

Melting Point: Mp 246-247°

Optical Rotation: [α]_D²⁸ -315 (c, 0.25 in MeOH)

Calculated Log P Data: Log P 7.32 (uncertain value) (calc)

UV: [base] $\lambda_{\max}$ 288 (ϵ 12500); 342 (ϵ 21200); 445 (ϵ 5770) (pH 13/5 h) (Derep) [neutral] $\lambda_{\max}$ 240 (ϵ 30000); 426 (ϵ 21000); 427 (sh) (ϵ); 442 (ϵ 22300) (MeOH) (Derep)

Other Data: Intercalates DNA and can cause single strand breaks in DNA

Hazard & Toxicity: Skin irritant. Dermatitis, gastrointestinal effects and bone-marrow depression reported when used therapeutically. LD₅₀ (rat, orl) 7.2 mg/kg. Exp. carcinogenic, reprod. and teratogenic effects

Aldrich: 85625-8

Fluka: 1815

Sigma: D6049

>> **Derivative:** *N,N'*-Di-de-Me

Synonym(s): *N,N'*-Didemethylactinomycin D. Auranthin 3B

Molecular Formula: C₆₀H₈₂N₁₂O₁₆

Molecular Weight: 1227.379

Accurate Mass: 1226.597178

Percentage Composition: C 58.72%; H 6.73%; N 13.69%; O 20.86%

Biological Source: Prod. by *Streptomyces* sp.

Physical Description: Orange-yellow powder

Solubility: Sol. MeOH, C₆H₆; poorly sol. H₂O, hexane

UV: [neutral] $\lambda_{\max}$ 240 (); 442 () (MeOH)

References: