



>>Derivative: 21ξ-Hydroxy

Synonym(s): 21-Hydroxyoligomycin A, 9Cl. **Nemadectin** ω. LL-F 28249ω. Antibiotic LL-F 28249ω

CAS Registry Number: 102042-09-1

Molecular Formula: C₄₅H₇₄O₁₂

Molecular Weight: 807.072

Accurate Mass: 806.51803

Percentage Composition: C 66.97%; H 9.24%; O 23.79%

Biological Source: Prod. by *Streptomyces cyanogriseus noncyanogenus* and *Streptomyces thermoarchaensis*

Physical Description: Powder

Optical Rotation: [α]_D −49 (Me₂CO)

UV: [neutral] λ_{max} 225 (ε 27400); 232 (ε 25700) (MeOH)

>>Derivative: 28-Oxo

Synonym(s): Oligomycin B

CAS Registry Number: 11050-94-5

Molecular Formula: C₄₅H₇₂O₁₂

Molecular Weight: 805.057

Accurate Mass: 804.50238

Percentage Composition: C 67.14%; H 9.01%; O 23.85%

Biological Source: Isol. from *Streptomyces diastatochromogenes*

Biological Use/Importance: Antifungal agent, inhibitor of oxidative phosphorylation

Physical Description: Platelets (MeOH)

Melting Point: Mp 160-161°

Optical Rotation: [α]_D²³ −49.5 (c, 1.03 in MeOH)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; fairly sol. EtOH; poorly sol. H₂O, hexane

UV: [neutral] λ_{max} 219 (sh) (ε); 224 (ε 29100); 232 (ε 27100); 240 (sh) (ε) (MeOH) (Derep) [neutral] λ_{max} 218 (ε 31700); 224 (ε 32000); 233 (ε 29300); 242 (ε 17700); 285 (ε 230) (MeOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 2.9 mg/kg

Fluka: 75354

Sigma: O5126

>>Derivative: 28-Oxo, 12,13-di-Ac

Molecular Formula: C₄₉H₇₆O₁₄

Molecular Weight: 889.131

Accurate Mass: 888.52351

Percentage Composition: C 66.19%; H 8.62%; O 25.19%

Melting Point: Mp 135.5-136.5°

Optical Rotation: [α]_D −66.6 (c, 0.63 in dioxan)

>>Derivative: 26-De-Me

References:

- Masamune, S. *et al.*, *J.A.C.S.*, 1958, **80**, 6092, (*isol, ir, uv*)
Chamberlain, J.W. *et al.*, *Biochem. Biophys. Res. Commun.*, 1969, **34**, 448, (*struct, ms*)
Prouty, W.F. *et al.*, *Biochem. Biophys. Res. Commun.*, 1969, **34**, 511, (*struct*)
v.Glehn, M. *et al.*, *CA*, 1973, **78**, 97462, (*cryst struct*)
Carter, G.T., *Diss. Abstr. Int., B*, 1976, **37**, 766, (*struct*)
Eur. Pat., 1986, 170 006; *CA*, **104**, 205525n, (*21-Hydroxyoligomycin A*)
Evans, D.A. *et al.*, *J.O.C.*, 1990, **55**, 6260, (*synth, abs config*)
Thomas, D.I. *et al.*, *J. Gen. Microbiol.*, 1991, **137**, 2331-2337, (*21-Hydroxyoligomycin A*)
Szilagyi, L. *et al.*, *J. Mol. Struct.*, 1998, **471**, 195-207, (*pmr, cmr, conformn*)
PANEK, J.S. *et al.*, *J.O.C.*, 2001, **66**, 2747-2756, (*Oligomycin C, synth*)