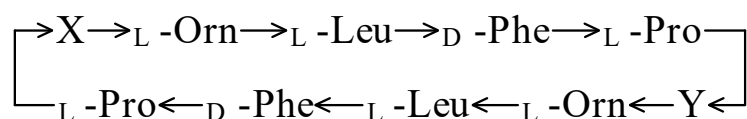




>>Entry Name: Gramicidin S, INN

Synonym(s): Soviet gramicidin. Gramicidin C. Gramicidin J1. Gramicidin J2



S₁ X = Y = _L -Val
S₂ X = 2-Aminobutanoic acid, Y = _L -Val
S₃ X = Y = 2-Aminobutanoic acid

CAS Registry Number: 113-73-5

Source/Synthesis: Prod. by *Bacillus brevis*

Use/Importance: Antibiotic used clinically in topical applications. Active against gram-positive bacteria

Solubility: BERDY SOL: Sol. EtOH, MeOH, CHCl₃; fairly sol. Me₂CO, H₂O; poorly sol. C₆H₆, hexane, Et₂O

UV: [neutral] λ_{max} 249 (); 258 (); 265 () (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, ipr) 17 mg/kg ; BERDY HAZD : LD₅₀ (mus, ipr) 20.8 mg/kg

>>Variant: Gramicidin S₁

Synonym(s): Gramicidin S-A

Molecular Formula: C₆₀H₉₂N₁₂O₁₀

Molecular Weight: 1141.461

Accurate Mass: 1140.705938

Percentage Composition: C 63.13%; H 8.12%; N 14.73%; O 14.02%

Physical Description: Needles (Me₂CO aq.)

Optical Rotation: [α]_D¹⁸ -289 (c, 0.43 in 70% EtOH)

Solubility: Sol. Et₂O, EtOH, Me₂CO, insol. H₂O; BERDY SOL: Sol. MeOH-H₂O, Me₂CO, CHCl₃; fairly sol. EtOH; poorly sol. H₂O, Et₂O, hexane

Other Data: Major component of Gramicidin S complex

Hazard & Toxicity: BERDY HAZD : LD₅₀ (rats, ivn) 17 mg/kg

>>Derivative: Hydrochloride (1:2)

Physical Description: Cryst. + 3H₂O (EtOH/HCl)

Melting Point: Mp 274-279°

Optical Rotation: [α]_D -260 (c, 0.4 in EtOH)

>>Derivative: All-L-analogue

Physical Description: Rods + 4H₂O (as hydrochloride)

Melting Point: Mp 246-247° (hydrochloride)

Optical Rotation: [α]_D²⁴ -76.8 (c, 0.66 in 60% EtOH aq.)

Other Data: Biol. inactive

>>Variant: Gramicidin S₂

CAS Registry Number: 92278-12-1

Molecular Formula: C₅₉H₉₀N₁₂O₁₀

Molecular Weight: 1127.434

Accurate Mass: 1126.690288

Percentage Composition: C 62.86%; H 8.05%; N 14.91%; O 14.19%

Physical Description: No phys. props. reported

Solubility: BERDY SOL: Sol. MeOH, Me₂CO; poorly sol. Et₂O, hexane

UV: [neutral] λ_{max} 219 () (MeOH) (Berdy)