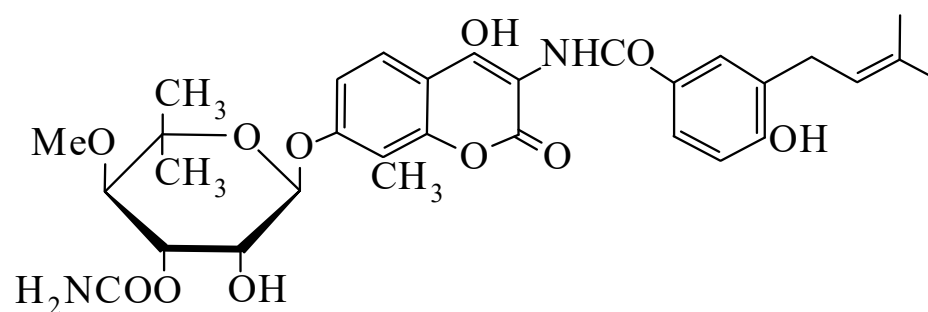




>>Entry Name: **Novobiocin**, BAN, INN

Synonym(s): Albamycin. Biotexin. Cardelmycin. Cathocin. Cathomycin. Inamycin. Spheromycin. Streptonivicin. Vulcamycin. PA 93. Antibiotic PA 93. WS 6629. Antibiotic WS 6629. Griseoflavin. Antibiotic S 800. S 800



CAS Registry Number: 303-81-1

Molecular Formula: C₃₁H₃₆N₂O₁₁

Molecular Weight: 612.632

Accurate Mass: 612.231913

Percentage Composition: C 60.78%; H 5.92%; N 4.57%; O 28.73%

Biological Source: Prod. by *Streptomyces niveus*, *Streptomyces spheroides*, *Streptomyces griseoflavus* and *Streptomyces griseus*

Biological Use/Importance: Active against gram-positive bacteria; used clinically. Leukotriene B₄ antagonist

Physical Description: Light-sensitive pale yellow cryst. (EtOH)

Melting Point: Mp 152-156° (159-161°) (dimorph.). Mp 174-178°

Optical Rotation: [α]_D²⁵ -62 (c, 1 in EtOH)

pKa Value: pK_{a1} 4.3; pK_{a2} 9.1

Calculated Log P Data: Log P 3.84 (calc)

UV: [acid] $\lambda_{\max}$ 334 (ϵ 24900) (0.1N HCl) (Derep) [base] $\lambda_{\max}$ 310 (ϵ 32600) (0.1N NaOH) (Derep) [neutral] $\lambda_{\max}$ 248 (ϵ 22200); 308 (ϵ 20100) (EtOH/pH 7.5) (Derep)

Hazard & Toxicity: Hypersensitivity reactions and haemopoietic effects reported when used therapeutically. LD₅₀ (mus, orl) 1500 mg/kg

>>Derivative: Na salt

CAS Registry Number: 1476-53-5

Melting Point: Mp 210-215° (dec.)

Optical Rotation: [α]_D²⁵ -34 (c, 1.08 in H₂O)

Hazard & Toxicity: LD₅₀ (mus, orl) 962 mg/kg

Fluka: 74675

Sigma: N1628

>>Derivative: O-Decarbamoyl

Synonym(s): Decarbamoylnovobiocin

CAS Registry Number: 10544-02-2

Molecular Formula: C₃₀H₃₅NO₁₀

Molecular Weight: 569.607

Accurate Mass: 569.226099

Percentage Composition: C 63.26%; H 6.19%; N 2.46%; O 28.09%

Biological Source: Prod. by *Streptomyces spheroides*

Melting Point: Mp 130-140°

Optical Rotation: [α]_D²⁴ -17.7 (MeOH)

>>Derivative: O^{3'}-Decarbamoyl, O^{2'}-carbamoyl

Synonym(s): Isonovobiocin

CAS Registry Number: 10543-94-9

Molecular Formula: C₃₁H₃₆N₂O₁₁

Molecular Weight: 612.632

Accurate Mass: 612.231913

Percentage Composition: C 60.78%; H 5.92%; N 4.57%; O 28.73%

Biological Source: Prod. by *Streptomyces spheroides*

References: