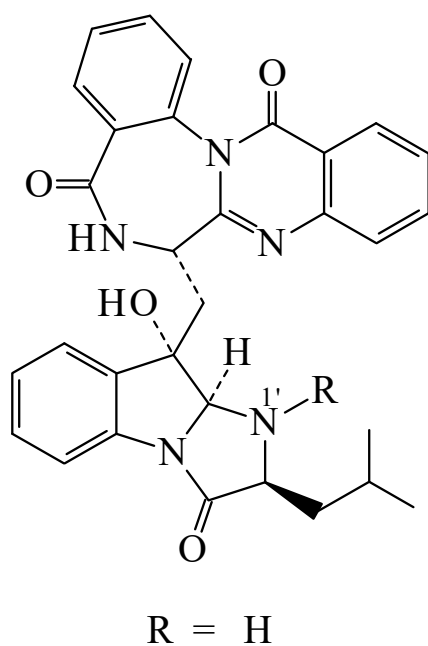




>>Entry Name: Asperlicin



CAS Registry Number: 93413-04-8

Molecular Formula: C₃₁H₂₉N₅O₄

Molecular Weight: 535.601

Accurate Mass: 535.221955

Percentage Composition: C 69.52%; H 5.46%; N 13.08%; O 11.95%

Source/Synthesis: Isol. from *Aspergillus alliaceus*

Use/Importance: A nonpeptide cholecystikinin antagonist used for treatment of gastrointestinal and CNS disorders

Physical Description: Cryst. (MeOH)

Melting Point: Mp 211-213°

Optical Rotation: [α]_D²⁶ -185.3 (c, 1.1 in MeOH)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O

Calculated Log P Data: Log P 3.08 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 230 (sh) (ϵ 48500); 258 (sh) (ϵ 17700); 266 (sh) (ϵ 14400); 278 (sh) (ϵ 10300); 310 (ϵ 4080); 322 (sh) (ϵ 3100) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 310 (ϵ 4075) (MeOH) (Berdy)

Other Data: Related to the Tryptoquivalines

>>Derivative: 1'-Hydroxy

Synonym(s): Asperlicin B

CAS Registry Number: 93413-08-2

Molecular Formula: C₃₁H₂₉N₅O₅

Molecular Weight: 551.601

Accurate Mass: 551.21687

Percentage Composition: C 67.50%; H 5.30%; N 12.70%; O 14.50%

Source/Synthesis: Minor metab. from *Aspergillus alliaceus*

Use/Importance: Cholecystikinin antagonist (7 times more potent than Asperlicin)

Physical Description: Powder

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O

Calculated Log P Data: Log P 2.93 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 230 (sh) (ϵ 48500); 258 (sh) (ϵ 17700); 266 (sh) (ϵ 14400); 278 (sh) (ϵ 10300); 310 (ϵ 4080); 322 (sh) (ϵ 3100) (MeOH) (Derep) [neutral] $\lambda_{\max}$ 310 (ϵ 4000) (MeOH) (Berdy)

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