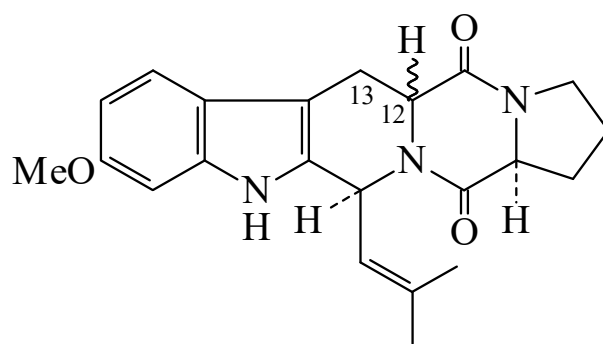




>>Entry Name: Fumitremorgin C



CAS Registry Number: 118974-02-0

Related CAS Registry Numbers(s): 118974-03-1 119066-67-0 119066-68-1 119066-69-2

Molecular Formula: C₂₂H₂₅N₃O₃

Molecular Weight: 379.458

Accurate Mass: 379.189592

Percentage Composition: C 69.64%; H 6.64%; N 11.07%; O 12.65%

General Statement: Config. at C-12 not specified. Of the two synthetic epimers the one with 12 α -H config. possessed spectroscopic characteristics identical with those reported for natural Fumitremorgin C. However, complete identification was not possible and the Mp's were widely different. Struct. revised in 1988

UV: [neutral] $\lambda_{\max}$ 224 (); 272 (); 294 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 225 (); 273 (); 299 () (EtOH) (Berdy)

>>Variant: Natural-form

Molecular Formula: C₂₂H₂₅N₃O₃

Molecular Weight: 379.458

Accurate Mass: 379.189592

Percentage Composition: C 69.64%; H 6.64%; N 11.07%; O 12.65%

Biological Source: Isol. from *Aspergillus fumigatus*

Use/Importance: Tremorgenic mycotoxin

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 125-130°

>>Derivative: 12,13-Epoxyde

Synonym(s): Epoxyfumitremorgin C

Biological Source: From *Aspergillus fumigatus*

>>Derivative: 12,13-Dihydroxy

Synonym(s): Dihydroxyfumitremorgin C

CAS Registry Number: 111427-99-7

Molecular Formula: C₂₂H₂₅N₃O₅

Molecular Weight: 411.457

Accurate Mass: 411.179422

Percentage Composition: C 64.22%; H 6.12%; N 10.21%; O 19.44%

Biological Source: From *Aspergillus fumigatus*

Physical Description: Yellow cryst.

Melting Point: Mp 197-198°

Optical Rotation: [α]_D +18.4

>>Derivative: Demethoxy

Synonym(s): Demethoxyfumitremosgin C

Molecular Formula: C₂₁H₂₃N₃O₂

Molecular Weight: 349.432

Accurate Mass: 349.179027

Percentage Composition: C 72.18%; H 6.63%; N 12.03%; O 9.16%

Biological Source: Prod. by *Aspergillus fumigatus*

Physical Description: Pale yellow needles

Melting Point: Mp 210-212°

Optical Rotation: [α]_D³⁰ +8 (c, 0.2 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH

UV: [neutral] $\lambda_{\max}$ 226 (ϵ 24950); 282 (ϵ 9000); 291 (sh) (ϵ 7450) (MeOH) [neutral] $\lambda_{\max}$ 226 (ϵ 24950); 282 (ϵ 9000); 291 () (MeOH) (Berdy)