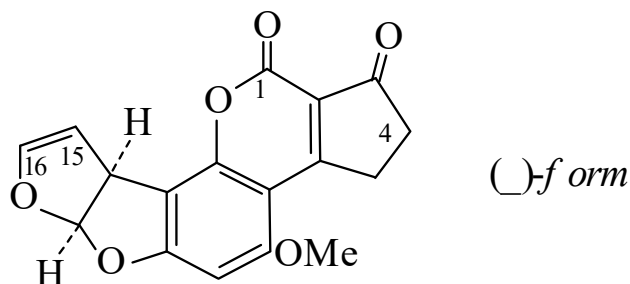




>>Entry Name: Aflatoxin B₁

ENTRY UNDER REVIEW

Synonym(s): 2,3,6a,9a-Tetrahydro-4-methoxycyclopenta[*c*]furo[3,2':4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 9Cl. Aflatoxin FB₁. Aflatoxin B



CAS Registry Number: 1162-65-8

Related CAS Registry Numbers(s): 42583-46-0

Molecular Formula: C₁₇H₁₂O₆

Molecular Weight: 312.278

Accurate Mass: 312.06339

Percentage Composition: C 65.39%; H 3.87%; O 30.74%

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

UV: [neutral] λ_{max} 220 (ε 25600); 265 (ε 13400); 362 (ε 21800) (MeOH) (Berdy) [neutral] λ_{max} 223 (ε 25100); 265 (ε 13400); 362 (ε 21800) (EtOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, orl) 1 mg/kg

Aldrich: 85620-7

Sigma: A6636

Supelco: R42-6050

>>Variant: (–)-form

Molecular Formula: C₁₇H₁₂O₆

Molecular Weight: 312.278

Accurate Mass: 312.06339

Percentage Composition: C 65.39%; H 3.87%; O 30.74%

Biological Source: Isol. from *Aspergillus flavus* and *Aspergillus parasiticus*

Use/Importance: Toxin causing Turkey X disease. One of the most potent carcinogens known in animals. Potential food containment esp. grains and nuts

Physical Description: Cryst. exhibiting blue fluor.

Melting Point: Mp 268-269 dec.°

Optical Rotation: [α]_D²⁵ –562 (c, 0.115 in CHCl₃)

Hazard & Toxicity: Human and exp. carcinogen; LD₅₀ (rat, orl) 5 mg/kg. Exp. reprod. and teratogenic effects. Hepatotoxic. Crystalline material, e.g. from preparative tlc plates, presents an inhalation hazard because the crystals develop electrostatic charge and cling to dust particles

>>Derivative: 15,16-Dihydro

Synonym(s): Aflatoxin B₂

CAS Registry Number: 7220-81-7

Molecular Formula: C₁₇H₁₄O₆

Molecular Weight: 314.294

Accurate Mass: 314.07904

Percentage Composition: C 64.97%; H 4.49%; O 30.54%

Biological Source: Metab. of *Aspergillus flavus*

Use/Importance: Mycotoxin

Physical Description: Yellow cryst. with blue fluor. (MeOH)

Melting Point: Mp 310 dec.°

Optical Rotation: [α]_D²³ –492 (c, 0.1 in CHCl₃)

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

UV: [neutral] λ_{max} 222 (ε 19600); 265 (ε 9200); 363 (ε 14700) (MeOH) (Berdy) [neutral] λ_{max} 220 (ε 20800); 265 (ε 12700); 363 (ε 24000) (EtOH) (Berdy)

Hazard & Toxicity: Human and exp. carcinogen. LD₅₀ (dck, orl) 1.7 mg/kg. Hepatotoxic

Aldrich: 85621-5

Sigma: A9887

Supelco: R42-6040