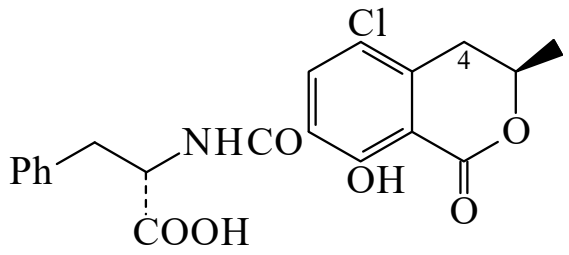
>>**Entry Name: Ochratoxin A**
ENTRY UNDER REVIEW
Synonym(s): *N*-[(5-Chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1*H*-2-benzopyran-7-yl)carbonyl]phenylalanine, 9Cl



CAS Registry Number: 303-47-9

Molecular Formula: $C_{20}H_{18}ClNO_6$
Molecular Weight: 403.818
Accurate Mass: 403.082266
Percentage Composition: C 59.49%; H 4.49%; Cl 8.78%; N 3.47%; O 23.77%
Biological Source: Prod. by *Aspergillus melleus, Aspergillus sulphureus* and *Penicillium viridicatum*
Use/Importance: Mycotoxin. Potential contaminant of foodstuffs, especially cereals
Physical Description: Cryst. (xylene)
Melting Point: Mp 169°
Optical Rotation: $[\alpha]_D^{20}$ –118 (c, 1.1 in $CHCl_3$)
Solubility: BERDY SOL: Sol. MeOH, $CHCl_3$; poorly sol. H_2O
UV: [neutral] λ_{max} 213 (ε 37600); 332 (ε 6500) (MeOH) (Derep) [neutral] λ_{max} 213 (ε 36800); 332 (ε 6400) (MeOH) (Berdy) [neutral] λ_{max} 215 (ε 34000); 333 (ε 2400) (EtOH) (Berdy)
Hazard & Toxicity: Possible human carcinogen. Exp. carcinogen and neoplastic agent. Nephrotoxic. Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 20 mg/kg, LD_{50} (pig, orl) 1 mg/kg. V. toxic if swallowed. Implicated in Balkan endemic nephropathy ; BERDY HAZD : LD_{50} (rats, orl) 22 mg/kg

Aldrich: 85628-2
Sigma: O1877
Supelco: R42-6010

>>**Derivative:** Et ester
Synonym(s): Ochratoxin C

CAS Registry Number: 4865-85-4

Molecular Formula: $C_{22}H_{22}ClNO_6$
Molecular Weight: 431.872
Accurate Mass: 431.113566
Percentage Composition: C 61.19%; H 5.13%; Cl 8.21%; N 3.24%; O 22.23%
Biological Source: Metab. of *Aspergillus ochraceus*
Physical Description: Amorph.
Optical Rotation: $[\alpha]_D$ –100 (c, 1.2 in EtOH)

>>**Derivative:** Dechloro
Synonym(s): Ochratoxin B

CAS Registry Number: 4825-86-9

Molecular Formula: $C_{20}H_{19}NO_6$
Molecular Weight: 369.373
Accurate Mass: 369.121239
Percentage Composition: C 65.03%; H 5.18%; N 3.79%; O 25.99%
Biological Source: Metab. of *Aspergillus ochraceus*
Physical Description: Cryst. (MeOH)
Melting Point: Mp 221°
Optical Rotation: $[\alpha]_D$ –35 (c, 0.15 in EtOH)
UV: [neutral] λ_{max} 218 (ε 33600); 318 (ε 6500) (MeOH) (Derep) [neutral] λ_{max} 218 (ε 37200); 318 (ε 6900) (EtOH) (Berdy)
Hazard & Toxicity: Highly toxic orally

Sigma: O1382
Supelco: R47-4465

>>**Derivative:** 4*S*-Hydroxy
Synonym(s): 4-Hydroxyochratoxin A