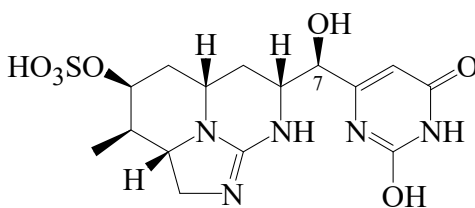




>>Entry Name: Cyindrospermopsin



CAS Registry Number: 143545-90-8

Molecular Formula: C₁₅H₂₁N₅O₇S

Molecular Weight: 415.426

Accurate Mass: 415.11617

Percentage Composition: C 43.37%; H 5.09%; N 16.86%; O 26.96%; S 7.72%

General Statement: Exists as prototropic zwitterion. C-7 config. revised in 2001

Biological Source: Alkaloid from the cyanobacteria *Aphanizomenon ovalisporum*, *Cylindrospermopsis raciborskii* and *Umezikia natans*

Biological Use/Importance: Potent hepatotoxin

Physical Description: Off-white microcryst.

Optical Rotation: [α]_D -31 (c, 0.1 in H₂O)

UV: [neutral] $\lambda_{\max}$ 262 (ϵ 5800); 290 (sh) (ϵ 2100) (H₂O) (Derep) [neutral] $\lambda_{\max}$ 262 (ϵ 5800); 290 (ϵ 2100) (H₂O) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) .2 mg/kg , LD₅₀ (mus, ipr) 2.1 mg/kg

>>Derivative: 7-Epimer

Synonym(s): 7-Epicyindrospermopsin

CAS Registry Number: 265652-18-4

Molecular Formula: C₁₅H₂₁N₅O₇S

Molecular Weight: 415.426

Accurate Mass: 415.11617

Percentage Composition: C 43.37%; H 5.09%; N 16.86%; O 26.96%; S 7.72%

Biological Source: Alkaloid from *Aphanizomenon ovalisporum*

Biological Use/Importance: Hepatotoxin

Physical Description: Amorph. solid

Optical Rotation: [α]_D²⁵ -20.5 (c, 0.06 in H₂O)

>>Derivative: 7-Deoxy

Synonym(s): 7-Deoxycylindrospermopsin

CAS Registry Number: 221554-69-4

Molecular Formula: C₁₅H₂₁N₅O₆S

Molecular Weight: 399.427

Accurate Mass: 399.121255

Percentage Composition: C 45.11%; H 5.30%; N 17.53%; O 24.03%; S 8.03%

Biological Source: Alkaloid from *Cylindrospermopsis raciborskii*

References:

- Ohtani, I. *et al.*, *J.A.C.S.*, 1992, **114**, 7941-7942, (*isol, uv, pmr, cmr, ms, struct*)
Norris, R.L. *et al.*, *Environ. Toxicol.*, 1999, **14**, 163-165, (*7-Deoxycylindrospermopsin*)
Banker, R. *et al.*, *J. Nat. Prod.*, 2000, **63**, 387-389, (*7-epimer*)
Xie, C. *et al.*, *J.A.C.S.*, 2000, **122**, 5018-5024, (*synth*)
Burgoyne, D.L. *et al.*, *J.O.C.*, 2000, **65**, 152-156, (*biosynth*)
Heintzelman, G.R. *et al.*, *J.A.C.S.*, 2001, **123**, 8851-8853, (*synth, stereochem*)