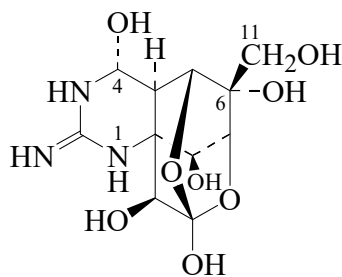




>>Entry Name: Tetrodotoxin

Synonym(s): Tarichatoxin. Spheroidine. Tetrodontoxin. Fugu poison. Maculotoxin. Araregai toxin



CAS Registry Number: 4368-28-9

Molecular Formula: $C_{11}H_{17}N_3O_8$

Molecular Weight: 319.271

Accurate Mass: 319.101567

Percentage Composition: C 41.38%; H 5.37%; N 13.16%; O 40.09%

Biological Source: Potent neurotoxin isol. from the ovaries and liver of Japanese puffer fish (*Sphoeroides rubripes*, *Sphoeroides vermicularis*, *Sphoeroides phyreus*) skin of Californian newt (*Taricha torosa*) from the Japanese ivory shell (*Babylonia japonica*) and *Tritus ensicauda* and believed to be a metabolic product of a *Pseudomonas* sp.

Use/Importance: Sodium channel (I, II, III, $\mu 1$, h1) blocker. Highly potent toxin. Of practical significance as a cause of accidental poisoning in Japan. Used in neurophysiological research

Physical Description: Cryst.

Optical Rotation: $[\alpha]_D^{25} -8.64$ (c, 8.55 in AcOH aq.)

Solubility: BERDY SOL: Sol. acids; fairly sol. H_2O ; poorly sol. EtOAc, hexane

pKa Value: pK_a 8.76

UV: [neutral] λ_{max} (H_2O) (Berdy)

Other Data: Darkens at 225° but does not melt

Hazard & Toxicity: LD_{50} (mus, orl) 435 $\mu g/kg$. LD_{50} (mus, ivn) 9 $\mu g/kg$. Highly toxic to mammals, birds, reptiles, amphibians and fish ; BERDY HAZD : LD_{50} (mus, ipr) .08 mg/kg , LD_{50} (mus, orl) .435 mg/kg , LD_{50} (mus, ivn) .009 mg/kg

Sigma: T5651

>>Derivative: Hydrobromide

Physical Description: Prisms (EtOH aq.)

Other Data: No definite Mp

>>Derivative: Picrate

Physical Description: Yellow needles + $1H_2O$ (H_2O)

Other Data: Darkens $>200^\circ$ without melting

>>Derivative: Penta-Ac

Molecular Formula: $C_{21}H_{27}N_3O_{13}$

Molecular Weight: 529.457

Accurate Mass: 529.154392

Percentage Composition: C 47.64%; H 5.14%; N 7.94%; O 39.28%

Melting Point: Mp $205.5-207^\circ$

>>Derivative: Hepta-Ac

Molecular Formula: $C_{23}H_{29}N_3O_{14}$

Molecular Weight: 571.494

Accurate Mass: 571.164957

Percentage Composition: C 48.34%; H 5.11%; N 7.35%; O 39.19%

Melting Point: Mp $188.5-191.5^\circ$

Optical Rotation: $[\alpha]_D^{30} +15.8$ (c, 0.39 in $CHCl_3$)