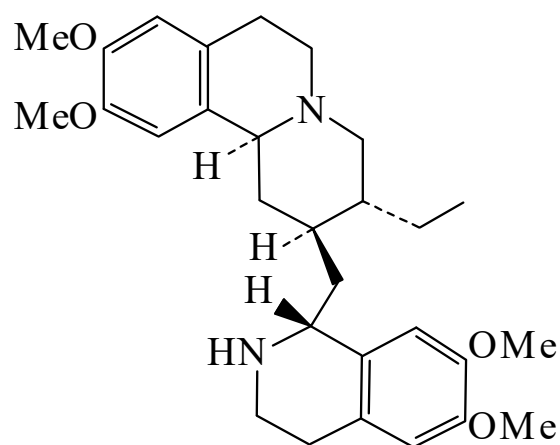




>>Entry Name: Emetine, BAN

Synonym(s): 6',7',10,11-Tetramethoxyemetan, 9Cl. Ipecine. Methylcephaeline. NSC 33669



Absolute
configuration

Type of Compound Code(s): XA4050 XA1150 XA2400 XA1950 VX3690

Molecular Formula: C₂₉H₄₀N₂O₄

Molecular Weight: 480.646

Accurate Mass: 480.298808

Percentage Composition: C 72.47%; H 8.39%; N 5.83%; O 13.31%

Use/Importance: Inhibitor of RNA, DNA and protein synthesis. Orally-active emetic. Amoebicide, general parasiticide, shows antiviral, antineoplastic and antibacterial activity. Also shows neuromuscular and cardiovascular effects. *A. lamarckii* has been extensively used in Indian medicine and the biochemistry of Emetine has been comprehensively studied. 2,3-Didehydroemetine is a v. active amoebicide

Calculated Log P Data: Log P 4.55 (calc)

>>Variant: (-)-form

CAS Registry Number: 483-18-1

Type of Compound Code(s): XA0960

Molecular Formula: C₂₉H₄₀N₂O₄

Molecular Weight: 480.646

Accurate Mass: 480.298808

Percentage Composition: C 72.47%; H 8.39%; N 5.83%; O 13.31%

Source/Synthesis: Alkaloid from *Alangium lamarckii*, *Cephaelis acuminata* (biosynthesis), *Psychotria granadensis* and *Psychotria ipecacuanha* (Alangiaceae, Rubiaceae). The occurrence of emetine in the common ivy, *Hedera helix* (Araliaceae) and in the roots of *Borreria verticillata* (Rubiaceae) remains unconfirmed

Physical Description: Amorph.

Melting Point: Mp 74° (efferv.) (sinters at 70°)

Optical Rotation: [α]_D -46.55 (c, 1.16 in CHCl₃). [α]_D -22 (EtOH). [α]_D -26 (CHCl₃). [α]_D -50 (CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; fairly sol. H₂O, hexane

Calculated Log P Data: Log P 4.55 (calc)

Other Data: Pharmacol. active isomer

Hazard & Toxicity: Severe skin and eye irritant. Adverse systemic effects by ingestion and intravenous routes. Cumulative poison. Cardiotoxic. Reported fatal dose approx. 2 g. LD₅₀ (rat, orl) 68 mg/kg

>>Derivative: Hydrochloride (1:2)

Synonym(s): Emetine hydrochloride, USAN. Emetinal. Encol. Erketin. Hemometina

CAS Registry Number: 316-42-7

Physical Description: Needles + 7H₂O

Melting Point: Mp 255 dec.° (sinters at 235°)

Hazard & Toxicity: Skin, eye and respiratory tract irritant. Local and cumulative systemic effects when used therapeutically. Cardiotoxic, nephrotoxic, hepatotoxic. LD₅₀ (rat, orl) 0.012 mg/kg. LD₅₀ (rat, ipr) 17 mg/kg

Fluka: 45160

Sigma: E2375

>>Derivative: Hydrobromide (1:2)

Physical Description: Needles + 4H₂O

Melting Point: Mp 250-260° (sinters at 245°)

>>Derivative: Hydroiodide (1:2)

Physical Description: Needles + 3H₂O (EtOH)

Melting Point: Mp 235-238° (sinters at 230°)