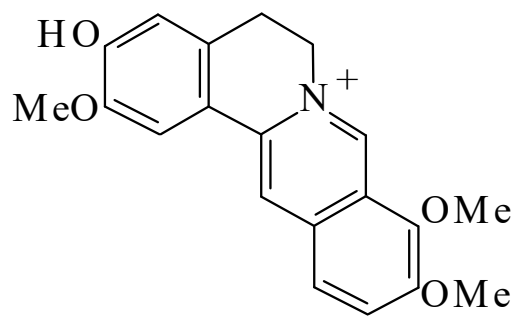




>>Entry Name: Jatrorrhizine

Synonym(s): Jateorhizine. Neprotine. Yatrorzine



CAS Registry Number: 3621-38-3

Molecular Formula: $C_{20}H_{20}NO_4^{(+)}$

Molecular Weight: 338.382

Accurate Mass: 338.139234

Percentage Composition: C 70.99%; H 5.96%; N 4.14%; O 18.91%

Biological Source: Quaternary alkaloid from the root of *Jateorhiza palmata*, many *Berberis* and *Mahonia* spp. and many other spp. in several families (Menispermaceae, Berberidaceae)

Use/Importance: Butyrylcholinesterinase inhibitor. Shows antibacterial activity vs. *Mycobacterium smegmatis*. Antiinflammatory, antihypertensive agent. Shows CNS stimulant props.

Calculated Log P Data: Log P -0.57 (uncertain value) (calc)

Rare Chemicals Library: S42536-2

>>Derivative: Chloride

Molecular Formula: $C_{20}H_{20}ClNO_4$

Molecular Weight: 373.835

Accurate Mass: 373.108086

Percentage Composition: C 64.26%; H 5.39%; Cl 9.48%; N 3.75%; O 17.12%

Physical Description: Copper-coloured needles

Melting Point: Mp 206°

>>Derivative: Iodide

Molecular Formula: $C_{20}H_{20}INO_4$

Molecular Weight: 465.287

Accurate Mass: 465.043707

Percentage Composition: C 51.63%; H 4.33%; I 27.27%; N 3.01%; O 13.75%

Physical Description: Orange-yellow needles

Melting Point: Mp 210°

>>Derivative: Me ether

References:

Späth, E. *et al.*, *Ber.*, 1925, **58**, 1939, (*struct*)

Cava, M.P. *et al.*, *J. Nat. Prod.*, 1965, **28**, 73, (*isol, uv, ir*)

Jewers, K. *et al.*, *J.C.S. Perkin 2*, 1972, 1393, (*cmr*)

Pavelka, S. *et al.*, *Coll. Czech. Chem. Comm.*, 1976, **41**, 3157, (*uv*)

Hussain, R.A. *et al.*, *Heterocycles*, 1989, **29**, 2257, (*pmr, cmr*)

Ghosh, R. *et al.*, *Acta Cryst. C*, 1993, **49**, 1665, (*cryst struct*)