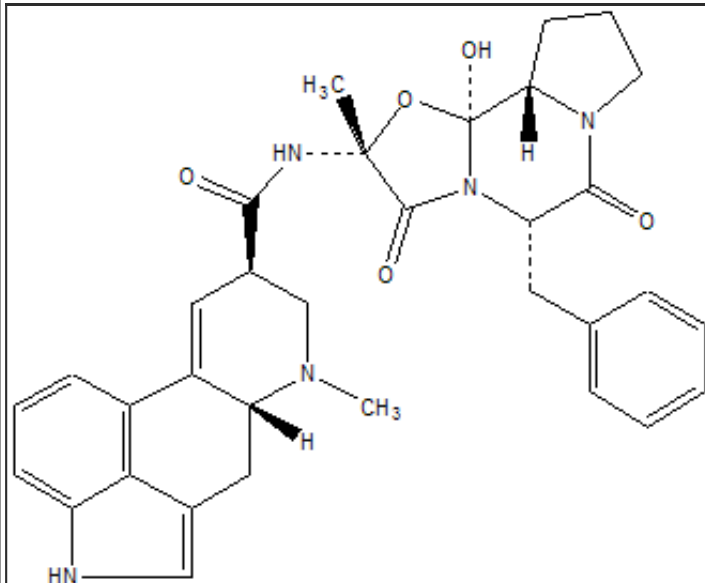


Records found: 1

Compound: Ergotamine



CAS:	113-15-5						
Category:	Central Nervous System Agents						
Subcategory:	Antimigraine Agents						
Formula:	C33 H35 N5 O5						
Molecular Weight:	581.66						
SMILES:	[H][C@@]12CCCN1C(=O)[C@H](CC1=CC=CC=C1)N1C(=O)[C@](C)(NC(=O)[C@H]3CN(C)[C@]4([H])CC5=CNC6=CC=CC(=C56)C4=C3)O[C@@]21O>						
pKa:	6.4						
Low est Solubility (mg/ml):	0.313						
Human Permeability (x 10 ⁴ cm/s):	N/A						
cLogP (BioLoom 5.0):	4.66	HIGH Permeability					
logP:	2.0	HIGH Permeability					
Country List:	Minimum Dose (mg)	Maximum Dose (mg)	Do (min)**	Do (max)**	Solubility	BCS Class (cLogP)	BCS Class (logP)
WHO	1.0	1.0	0.012779553	0.012779553	HIGH	Class I	Class I

** A volume of 250 mL is used for the drugs on the US, UK, SP, KOR, and WHO lists, and a volume of 150 mL is used for drugs on the JP list.