

Product Information

Bruceine D

Cat. No.: X23-04-XQ314

Size: 20 mg; 50 mg; 100 mg; 200 mg; 500 mg; 1 g

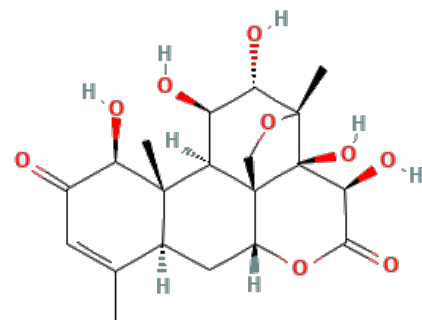
CAS Number: 21499-66-1

Compound CID: 441788

Synonym: 21499-66-1; Bruceine D; Brucein D; (1beta,11beta,12alpha,15beta)-1,11,1

2,14,15-Pentahydroxy-13,20-epoxypicras-3-ene-2,16-dione

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	Bruceine D is an effective botanical insect antifeedant with outstanding systemic properties, causing potent pest growth inhibitory activity.
Molecular Weight	410.419
Molecular Formula	C ₂₀ H ₂₆ O ₉
IUPAC Name	(1 <i>R</i> ,2 <i>R</i> ,3 <i>R</i> ,6 <i>R</i> ,8 <i>S</i> ,12 <i>S</i> ,13 <i>S</i> ,14 <i>R</i> ,15 <i>R</i> ,16 <i>S</i> ,17 <i>R</i>))-2,3,12,15,16-Pentahydroxy-9,13,17-trimethyl-5,18-dioxapentacyclo[12.5.0.01,6.02,17.08,13]nonadec-9-ene-4,11-dione
InChI	InChI=1S/C20H26O9/c1-7-4-9(21)13(23)17(2)8(7)5-10-19-6-28-18(3,14(24)11(22)12(17)19)20(19,27)15(25)16(26)29-10/h4,8,10-15,22-25,27H,5-6H2,1-3H3/t8-,10+,11+,12+,13+,14-,15-,17-,18+,19+,20+/m0/s1
InChI Key	JBDMZGKDLMGOFR-KQSRGDCESA-N
Canonical SMILES	CC1=CC(=O)C(C2(C1CC3C45C2C(C(C(C4(C(C(=O)O ₃)O)O)(OC5)C)O)O)C)O
Isomeric SMILES	CC1=CC(=O)[C@H]([C@]2([C@H]1C[C@@H]3[C@]45[C@@H]2[C@H]([C@@H]([C@]([C@@]4([C@H](C(=O)O ₃)O)O)(OC5)C)O)O)C)O
Form	White crystal or powder
Purity	>98%, determined by HPLC.
Identity	Confirmed by NMR and MS.
Stability	The product is stable for two years when stored at the recommended temperature.
Applications	Bruceine D can be used for anti-cancer activity experiments, etc.
Storage	Store at 4°C. Protect from light.



Safety Information

Personal Protective Equipment Gloves, eyeshields, N95 mask
