

Product Information

Segetalin A

Cat. No.: X22-05-ZQ343

Size: 10 mg; 20 mg; 50 mg; 100 mg

CAS Number: 161875-97-4

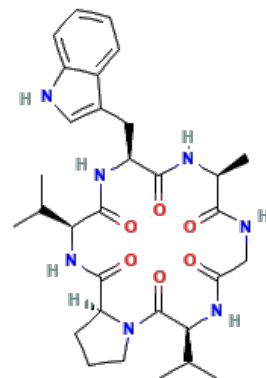
Compound CID: 10483858

Synonym: 161875-97-4; Segetalin a; Segetalin A trifluoroacetic acid salt;

(3S,9S,12S,15S,18S)-12-(1H

-Indol-3-ylmethyl)-9-methyl-3,15-di(propan-2-yl)-1,4,7,10,13,16-hexazabicyclo[16.3.0]

henicosane-2,5,8,11,14,17-hexone



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

Product Information

Description	Segetalin A is a trifluoroacetic acid fatty acid that has a macrocyclic structure and a unique chemical diversity. It is an antiangiogenic agent that inhibits endothelial cell proliferation and angiogenesis. Segetalin A has anti-cancer activity and is able to inhibit the growth of human cancer cells <i>in vitro</i> by suppressing angiogenesis. This product can be used for research in the fields of medicine and pharmacy.
Molecular Weight	609.72
Molecular Formula	C ₃₁ H ₄₃ N ₇ O ₆
IUPAC Name	(3S,9S,12S,15S,18S)-12-(1H -Indol-3-ylmethyl)-9-methyl-3,15-di(propan-2-yl)-1,4,7,10,13,16-hexazabicyclo[16.3.0]henicosane-2,5,8,11,14,17-hexone
InChI	InChI=1S/C31H43N7O6/c1-16(2)25-30(43)35-22(13-19-14-32-21-10-7-6-9-20(19)21)28(41)34-18(5)27(40)33-15-24(39)36-26(17(3)4)31(44)38-12-8-11-23(38)29(42)37-25/h6-7,9-10,14,16-18,22-23,25-26,32H,8,11-13,15H2,1-5H3,(H,33,40)(H,34,41)(H,35,43)(H,36,39)(H,37,42)/t18-,22-,23-,25-,26-/m0/s1
InChI Key	YVUZOKYOUUCVBV-WJTDBPPMSA-N
Canonical SMILES	CC1C(=O)NCC(=O)NC(C(=O)N2CCCC2C(=O)NC(C(=O)NC(C(=O)N1)CC3=CNC4=CC=CC=C43)C(C)C(C)C
Isomeric SMILES	C[C@H]1C(=O)NCC(=O)N[C@H](C(=O)N2CCC[C@H]2C(=O)N[C@H](C(=O)N[C@H](C(=O)N1)CC3=CNC4=CC=CC=C43)C(C)C(C)C
Source	<i>Semen vaccariae</i>



Form	White powder
Purity	≥98%, determined by HPLC.
Solubility	It is soluble in methanol and slightly soluble in ethyl acetate.
Identity	Confirmed by MS and NMR.
Stability	The product is stable for two years when stored at the recommended temperature.
Applications	Segetalin A can be used for research in the fields of medicine and pharmacy.
Storage	Store at 4°C. Protect from light.

Safety Information

Personal Protective Equipment	Gloves, eyeshields, N95 mask
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