

Product Name: Gedunin

Catalog No.: 3387

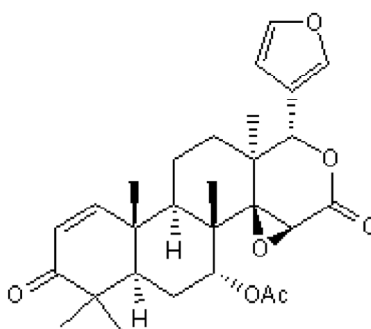
Batch No.: 4

CAS Number: 2753-30-2

IUPAC Name: (1*S*,3*aS*,4*aR*,4*bS*,5*R*,6*aR*,10*aR*,10*bR*,12*aS*)-5-(Acetyloxy)-1-(3-furanyl)-1,5,6,6*a*,7,10*a*,10*b*,11,12,12*a*,decahydro-4*b*,7,7,10*a*,12*a*,pentamethyloxireno[*c*]phenanthro[1,2-*d*]pyran-3,8(3*aH*,4*bH*)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₈ H ₃₄ O ₇
Batch Molecular Weight:	482.57
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 10 mM with gentle warming
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.5 (5:3:2 petrol:DCM:EtOAc)
HPLC:	Shows 98.9% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Optical Rotation:	[α] _D = +67.1 (Concentration = 1, Solvent = Methanol)
Microanalysis:	
	Carbon Hydrogen Nitrogen
	Theoretical 69.69 7.1
	Found 69.75 7.15 0.1

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Gedunin is a naturally occurring Hsp90 inhibitor. Induces Hsp90-dependent client protein degradation and displays antiproliferative activity in vitro (IC₅₀ values are 3.22, 8.84 and 16.8 μM in SKBr3, MCF-7 and CaCo-2 cancer cell lines respectively). Decreases ovarian cancer cell proliferation in vitro and may enhance cisplatin-induced reduction in proliferation (CAT.No 3387). Also exhibits antimalarial activity against Plasmodium falciparum (IC₅₀ values are 0.14 and 3.1 μM in parasite development and [³H]-hypoxanthine uptake assays respectively).

Physical and Chemical Properties:

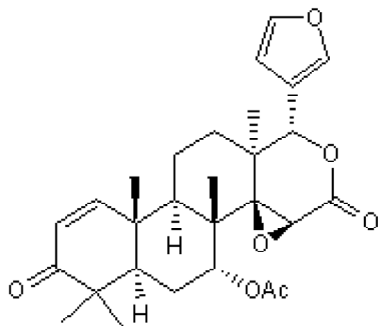
Batch Molecular Formula: C₂₈H₃₄O₇

Batch Molecular Weight: 482.57

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Kamath et al (2009) Gedunin, a novel natural substance, inhibits ovarian cancer cell proliferation. *Int J Gynecol Cancer*. **19** 1564. PMID: 19955938.

Brandt et al (2008) Gedunin, a novel Hsp90 inhibitor: semisynthesis of derivatives and preliminary structure-activity relationships. *J.Med.Chem.* **51** 6495. PMID: 18816111.

Lee et al (2008) Antimalarial activity of anthothocol derived from *Khaya anthotheca* (Meliaceae). *Phytomedicine* **15** 533. PMID: 17913482.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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