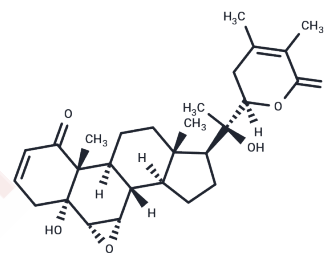


Withanolide A

Chemical Properties

CAS No. :	32911-62-9
Formula:	C ₂₈ H ₃₈ O ₆
Molecular Weight:	470.60
Storage:	Store at low temperature Powder: -20°C for 3 years In solvent: -80°C for 1 year <i>Actual storage temperature shall be subject to the COA.</i>



Biological Description

Description	Withanolide A extends the lifespan in human EGFR-driven cancerous Caenorhabditis elegans.
Targets(IC50)	Apoptosis,EGFR,NF-κB,Gamma-secretase,TNF
In vitro	A quantitative structure activity relationship (QSAR) model was developed by a forward stepwise multiple linear regression method to predict the activity of Withanolide Analogs against human breast cancer. The most effective QSAR model for anticancer activity against the SK-Br-3 cell showed the best correlation with activity ($r_2=0.93$ and $r_{CV2}=0.90$). Similarly, cross-validation regression coefficient ($r_{CV2}=0.85$) of the best QSAR model against the MCF7/BUS cells showed a high correlation ($r_2=0.91$). In particular, compounds CID 73621, CID 435144, CID 301751 and CID 3372729 have a marked antiproliferative activity against the MCF7/BUS cells, while 2,3-dihydrowithaferin A-3-beta-O-sulfate, withanolide 5, Withanolide A, withaferin A, CID 10413139, CID 11294368, CID 53477765, CID 135887, CID 301751 and CID 3372729 have a high activity against the Sk-Br-3 cells compared to standard drugs 5-fluorouracil (5-FU) and camptothecin[1]

Solubility Information

Solubility	DMSO: 55.00 mg/mL (116.87 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 1.67 mg/mL (3.55 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1249 mL	10.6247 mL	21.2495 mL
5 mM	0.425 mL	2.1249 mL	4.2499 mL
10 mM	0.2125 mL	1.0625 mL	2.1249 mL
50 mM	0.0425 mL	0.2125 mL	0.425 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Molecular docking, QSAR and ADMET studies of withanolide analogs against breast cancer. Drug Des Devel Ther. 2017 Jun 22;11:1859-1870.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel: 781-999-4286 E_mail: info@targetmol.com Address: 34 Washington Street, Wellesley Hills, MA 02481