

Product Data Sheet

Product Name: 12-Deoxywithastramonolide

Cat. No.: GC18531

Chemical Properties

Cas. No. 60124-17-6

Chemical Name 6 α ,7 α -epoxy-5 α ,22R,27-trihydroxy-1-oxo-ergosta-2,24-dien-26-oic acid δ -lactone

SMILES CC(C1)=C(CO)C(O[C@@]1([H])[C@@H](C)[C@@]2([H])CC[C@@]3([H])[C@]4([H])[C@H]5[C@H](O5)[C@@]([C@@]6(C)[C@@]4([H])CC[C@@]32C)(O)CC=CC6=O)=O

Formula C₂₈H₃₈O₆

M.Wt 470.6

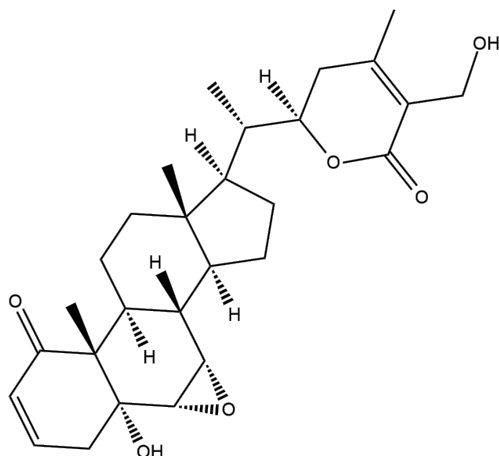
Solubility DMF: 2 mg/ml, DMSO: 0.1 mg/ml, Ethanol: 20 mg/ml, Ethanol: PBS (pH 7.2) (1:2): 0.3 mg/ml

Storage Store at -20°C, protect from light

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Caution: Product has not been fully validated for medical applications. For research use only.

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Protocol

Cell experiment [1]:

Cell lines J774A.1 mouse BALB/c macrophages

Preparation Method Following 24h incubation, macrophages were incubated for 2h with 100ng/mL LPS, preceded by 12-Deoxywithastramonolide (10 μ M) treatment at 37°C in 5% CO₂. Diclofenac (10 μ M) was used as positive control. After 2, 12 and 24h of lactone treatment, supernatant was collected and kept at -80°C for the quantification of nitric oxide (NO) using the Griess reaction with slight modifications.

Reaction Conditions 10 μ M; 24h

Applications 12-Deoxywithastramonolide significantly inhibited NO production in LPS-activated macrophages.

Animal experiment [1]:

Animal models Mice

Preparation Method Tail-flick assay: The mouse tail (3-5cm) was kept on the analgesimeter nichrome wire after that the reaction time was measured in terms of tail removal. A reaction time was recorded as the interval between tail exposure to the hot beam and the tail withdrawal reflex. Reaction times to analyze pain were recorded at 0-4h at different intervals after the oral administration of 12-Deoxywithastramonolide (20mg/kg). A cut-off time of 20s was enacted as a protection against skin damage. Diclofenac at a dose of 50 mg/kg was used as a reference drug.

Dosage form 20mg/kg; p.o.; once

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Applications 12-Deoxywithastramonolide significantly decreased the acute thermal nociception in mice (0.5-2h) and extended the animal's response time to the temperature incitement when compared to the vehicle-treated control.

References:

[1] Chandan G, Kumar C, Chibber P, et al. Evaluation of analgesic and anti-inflammatory activities and molecular docking analysis of steroidal lactones from *Datura stramonium* L. *Phytomedicine*. 2021;89:153621.

Background

12-Deoxywithastramonolide is a natural lactone found in ashwagandha (*W.somnifera*)^[1].

In vitro, 12-Deoxywithastramonolide (0-200µM; 24 or 48h) exhibited low cytotoxicity in J774A.1 macrophages^[2]. 12-Deoxywithastramonolide (10µM; 24h) significantly inhibited NO production in LPS-activated J774A.1 macrophages^[2]. 12-Deoxywithastramonolide (1.25-10µM; 24h) dose-dependently increased erythrocyte membrane stability and inhibited protein denaturation, with an IC₅₀ of 8.16µM^[2].

In vivo, a single oral dose of 12-Deoxywithastramonolide (20mg/kg) significantly attenuated acute thermal nociception in mice, as evidenced by prolonged withdrawal latency to thermal stimulus^[2]. A single oral dose of 12-Deoxywithastramonolide (20mg/kg) reduced acetic acid-induced abdominal constrictions in mice (writhing response), exhibiting a 32% inhibition^[2]. A single oral dose of 12-Deoxywithastramonolide (20mg/kg) inhibited rat paw edema with a rate of approximately 38%^[2].

References:

[1] Nile SH, Nile A, Gansukh E, Baskar V, Kai G. Subcritical water extraction of withanosides and withanolides from ashwagandha (*Withania somnifera* L) and their biological activities. *Food Chem Toxicol*. 2019;132:110659.

[2] Chandan G, Kumar C, Chibber P, et al. Evaluation of analgesic and anti-inflammatory activities and molecular docking analysis of steroidal lactones from *Datura stramonium* L. *Phytomedicine*. 2021;89:153621.

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