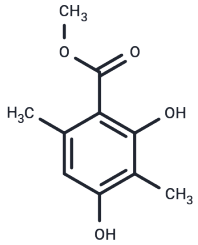
Data Sheet (Cat.No.TCS1372)

TargetMol

Atraric acid

Chemical Properties



CAS No. : 4707-47-5

Formula: C10H12O4

Molecular Weight: 196.2

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Atraric acid derivatives as a new chemical lead structure for novel therapeutic compounds as AR antagonists, that can be used for prophylaxis or treatment of prostatic diseases. It inhibits PTP1B activity in a dose-dependent manner with IC50 values of 51.5 uM, suggest that atraric acid has potential to treat diabetes.
Targets(IC50)	NF-κB,Androgen Receptor,NO Synthase,p38 MAPK,Phosphatase
In vitro	Androgen receptor (AR) antagonists are important compounds for the treatment of prostate cancer (PCa). The Atraric acid (AA), a natural compound, binds to the AR and acts as a specific AR antagonist. Interestingly, Atraric acid represents a novel chemical platform that could serve as a potential basis for new AR antagonists. METHODS AND RESULTS:Therefore, one objective of this study was to analyze the chemical/structural requirements for AR antagonism and to obtain predictions of where and how Atraric acid binds to the AR. Further, this study describes the chemical synthesis of 12 Atraric acid derivatives and their analysis using a combination of computational and functional assays. Functional analysis of Atraric acid derivatives indicated that none activated the AR. Both the para-hydroxyl group and the benzene ortho- and the meta-methyl groups of Atraric acid appeared to be essential to antagonize androgen-activated AR activity. Furthermore, extension of the hydrophobic side chain of Atraric acid led to slightly stronger AR antagonism. In silico data suggest that modifications to the basic Atraric acid structure change the hydrogen-bonding network with the AR ligand binding domain (LBD), so that the para-hydroxyl group of Atraric acid forms a hydrogen bond with the LBD, confirming the functional importance of this group for AR antagonism. Moreover, in silico modeling also suggested that the ortho- and meta- methyl groups of Atraric acid interact with hydrophobic residues of the ligand pocket of AR, which might explain their functional importance for antagonism. CONCLUSIONS:Thus, these studies identify the chemical groups of Atraric acid that play key roles in allowing the Atraric acid-based chemical platform to act as an AR antagonist.

Solubility Information

Solubility	DMSO: 13 mg/mL (66.26 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+90% Corn Oil: 1 mg/mL (5.1 mM),Sonication is recommended. *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.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	5.0968 mL	25.4842 mL	50.9684 mL
5 mM	1.0194 mL	5.0968 mL	10.1937 mL
10 mM	0.5097 mL	2.5484 mL	5.0968 mL
50 mM	0.1019 mL	0.5097 mL	1.0194 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

Computational and functional analysis of the androgen receptor antagonist atraric acid and its derivatives. Anticancer Agents Med Chem. 2013 Jun;13(5):801-10.

PTP1B inhibitory secondary metabolites from the Antarctic lichen Lecidella carpathica. Mycology An International Journal on Fungal Biology, 2011, 2(1):18-23.