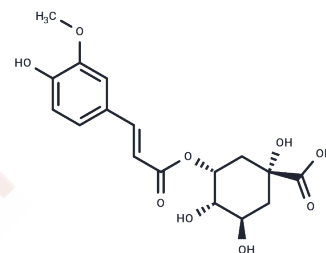


5-Feruloylquinic acid

Chemical Properties

CAS No. :	40242-06-6
Formula:	C ₁₇ H ₂₀ O ₉
Molecular Weight:	368.34
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	5-Feruloylquinic acid (5-FQA) is a potent Sirt1 agonist and a potential lead compound for further testing in the drug development process for aging-associated diseases.
Targets(IC50)	Sirtuin, Tyrosinase
In vitro	Traditional Chinese Medicine (TCM) compounds were employed for screening potent Sirt1 agonists, and molecular dynamics (MD) simulation was implemented to simulate ligand optimum docking poses and protein structure under dynamic conditions. TCM compounds such as (S)-tryptophan-betaxanthin, 5-O-Feruloylquinic acid, and RosA exhibited good binding affinity across different computational methods, and their drug-like potential were validated by MD simulation. Docking poses indicate that the carboxylic group of the three candidates generated H-bonds with residues in the protein chain from Ser441 to Lys444 and formed H-bond, π -cation interactions, or hydrophobic contacts with Phe297 and key active residue, His363. During MD, stable π -cation interactions with residues Phe273 or Arg274 were formed by (S)-tryptophan-betaxanthin and RosA[1].

Solubility Information

Solubility	DMSO: 33.33 mg/mL (90.49 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.7149 mL	13.5744 mL	27.1488 mL
5 mM	0.543 mL	2.7149 mL	5.4298 mL
10 mM	0.2715 mL	1.3574 mL	2.7149 mL
50 mM	0.0543 mL	0.2715 mL	0.543 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

Investigation of silent information regulator 1 (Sirt1) agonists from Traditional Chinese Medicine. Journal of Biomolecular Structure and Dynamics, 2013, 31(11):1207-1218.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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