

Certificate of Analysis

Catalog Number	BP13646
Product Name	5-Feruloylquinic acid

Physical and Chemical Properties

Synonyms	5-FQA, 5-O-Feruloylquinic acid
CAS No.	40242-06-6
Chemical Formula	C17H20O9
Molecular Weight	368.338
Solubility	
Storage	Powder: -20°C for 2 years In solvent: -80°C for 1 year
Chemical Structure OR Tested Image	OHOOHOOHOOHOOHOOHOOHOOHOOHOOHOOHOOHOOHO

Product Information

Description	5-O-Feruloylquinic acid is a potent Sirt1 agonist, it is a potential lead compound that can be further tested in drug development process for diseases associated with aging.
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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.
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Analytical Data

HPLC	Shows Min >99% purity
H-NMR	Consistent with structure
Stability and Solubility Advice	Information on product stability, especially in solution, has rarely been reported and in most cases we can only provide a general guideline. We recommend that once the stock solution has been prepared, it be stored in equal quantities in sealed vials and used within 1 month. Avoid repeated freezing and thawing cycles. Storage conditions for some special products should be referred to their storage details.

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