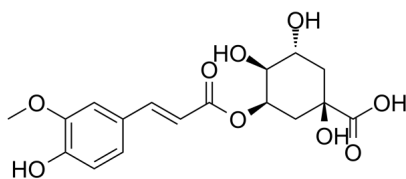


Data Sheet

Product Information

Catalog Number	BP13646
Product Name	5-Feruloylquinic acid
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.
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.
Synonyms	5-FQA, 5-O-Feruloylquinic acid
CAS No.	40242-06-6
Chemical Formula	C ₁₇ H ₂₀ O ₉
Molecular Weight	368.338
Solubility	
Storage	Powder: -20°C for 2 years In solvent: -80°C for 1 year

Chemical Structure
OR
Tested Image



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