

Product Name: ML 145

Catalog No.: 4172

Batch No.: 2

CAS Number: 1164500-72-4

IUPAC Name: 2-Hydroxy-4-[4-(5Z)-5-[(E)-2-methyl-3-phenylprop-2-enylidene]-4-oxo-2-sulfanylidene-1,3-thiazolidin-3-yl]butanoylamino]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₂N₂O₅S₂·H₂O

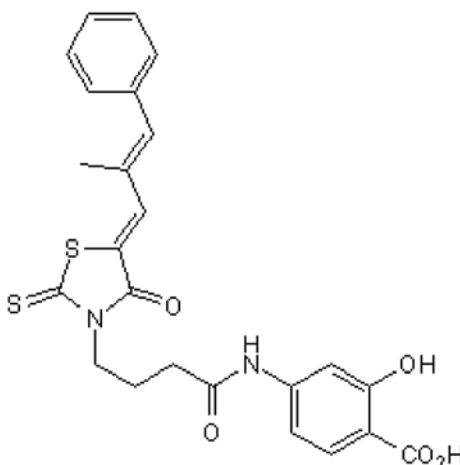
Batch Molecular Weight: 500.59

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.59	4.83	5.6
Found	57.62	4.69	5.65

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Description:

Selective antagonist for the GPR35 orphan receptor GPCR (IC₅₀ = 20.1 nM). Over 1000-fold more selective for GPR35 compared to GPR55 antagonists.

Physical and Chemical Properties:

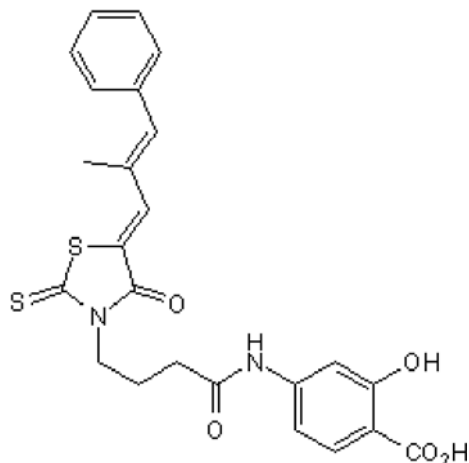
Batch Molecular Formula: C₂₄H₂₂N₂O₅S₂.H₂O

Batch Molecular Weight: 500.59

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Jenkins *et al* (2012) Antagonists of GPR35 display high species ortholog selectivity and varying modes of action. *J.Pharmacol.Exp.Ther.* **343** 683. PMID: 22967846.

Heynen-Genel *et al* (2010) Antagonists for the orphan receptor GPR35. Probe Reports from the Molecular Libraries Program NBK5070.

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