

# **Certificate of Analysis**

www.tocris.com

Product Name: ML 145 Catalog No.: 4172 Batch No.: 1

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:  $C_{24}H_{22}N_2O_5S_2$ 

Batch Molecular Weight: 482.57

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

HPLC: Shows 98.0% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.73 4.6 5.81 Found 59.63 4.55 5.95

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use







# **Product Information**

www.tocris.com

Product Name: ML 145 Catalog No.: 4172 Batch No.: 1

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

#### **Description:**

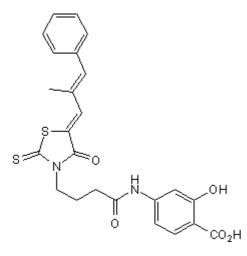
Selective antagonist for the GPR35 orphan receptor GPCR ( $IC_{50} = 20.1$  nM). Over 1000-fold more selective for GPR35 compared to GPR55 antagonists.

### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O<sub>5</sub>S<sub>2</sub> Batch Molecular Weight: 482.57 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:

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

**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.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

