

Certificate of Analysis

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Product Name: MRT 10

Catalog No.: 4585

Batch No.: 1

CAS Number: 330829-30-6

IUPAC Name: *N*-[[[3-Benzoylamino)phenyl]amino]thioxomethyl]-3,4,5-trimethoxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{23}N_3O_5S \cdot \frac{1}{4}H_2O$

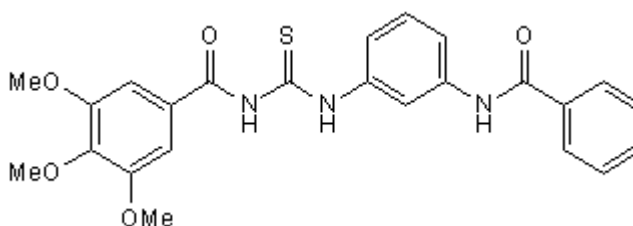
Batch Molecular Weight: 470.02

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

GC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical	61.33	5.04	8.94
Found	61.3	4.94	9.04

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

Product Information

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IUPAC Name: *N*-[[[3-Benzoylamino)phenyl]amino]thioxomethyl]-3,4,5-trimethoxybenzamide

Description:

Smoothened (Smo) receptor antagonist (IC_{50} = 0.5 μ M in HEK293 cells transiently expressing mouse Smo). Inhibits ShhN-induced Gli luciferase reporter activity in Shh-light 2 cells (IC_{50} = 2.5 μ M); acts as an inverse agonist during nontranscriptional Hedgehog pathway activation (IC_{50} = 2.5 μ M in HEK293 cells).

Physical and Chemical Properties:

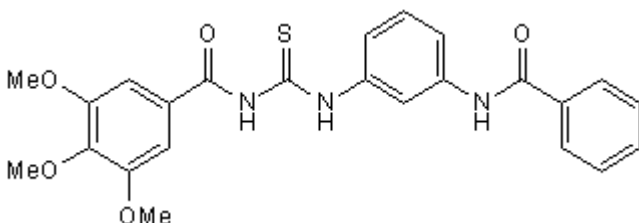
Batch Molecular Formula: $C_{24}H_{23}N_3O_5S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 470.02

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Manetti et al (2010) Virtual screening-based discovery and mechanistic characterization of the acylthiourea MRT-10 family as smoothened antagonists. *Mol.Pharmacol.* **78** 658. PMID: 20664000.

Solinas et al (2012) Acylthiourea, acylurea, and acylguanidine derivatives with potent hedgehog inhibiting activity. *J.Med.Chem.* **55** 1559. PMID: 22268551.

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