



Certificate of Analysis

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Product Name: Qc 1 Catalog No.: 5055 Batch No.: 1

CAS Number: 403718-45-6

IUPAC Name: 1,2,3,4-Tetrahydro-4-oxo-*N*-(phenylmethyl)-2-thioxo-3-[3-(trifluoromethyl)phenyl]-7-quinazolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{16}F_3N_3O_2S$

Batch Molecular Weight: 455.45 **Physical Appearance:** White solid

Solubility: DMSO to 50 mM

ethanol to 5 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 99.4% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen
Theoretical 60.65 3.54 9.23
Found 60.26 3.54 9.24

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





Product Information

Print Date: Dec 5th 2013

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IUPAC Name: 1,2,3,4-Tetrahydro-4-oxo-*N*-(phenylmethyl)-2-thioxo-3-[3-(trifluoromethyl)phenyl]-7-quinazolinecarboxamide

Description:

Reversible, non-competitive inhibitor of threonine dehydrogenase (TDH) (IC $_{50}$ ~500 nM). Induces autophagy and inhibits cell proliferation in mouse embryonic stem (ES) cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₁₆F₃N₃O₂S Batch Molecular Weight: 455.45

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol to 5 mM with gentle warming

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:

Alexander et al (2011) Targeted killing of a mammalian cell based upon its specialized metabolic state. Proc.Natl.Acad.Sci.USA 108 15828. PMID: 21896756.

