

Certificate of Analysis

Print Date: Jul 25th 2019

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Product Name: Cyclapolin 9 Catalog No.: 3116 Batch No.: 1

CAS Number: 40533-25-3

IUPAC Name: 7-Nitro-5-(trifluoromethyl)-2-benzothiazolecarboxamide-3-oxide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_9H_4F_3N_3O_4S$

Batch Molecular Weight: 307.21

Physical Appearance:Pale yellow solidSolubility:DMSO to 25 mM

ethanol to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point:Between 222 - 223°CHPLC:Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 35.19 1.31 13.68 Found 35.6 1.21 13.65

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



Product Information

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IUPAC Name: 7-Nitro-5-(trifluoromethyl)-2-benzothiazolecarboxamide-3-oxide

Description:

Selective, ATP-competitive polo-like kinase 1 (PLK1) inhibitor (IC_{50} = 500 nM).

Physical and Chemical Properties:

Batch Molecular Formula: $C_9H_4F_3N_3O_4S$

Batch Molecular Weight: 307.21

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 25 mM ethanol to 10 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:

Taylor *et al* (2008) Ligand discovery and virtual screening using the program LIDAEUS. Br.J.Pharmacol. *153* S55. PMID: 18037921. **McInnes** *et al* (2006) Inhibitors of polo-like kinase reveal roles in spindle pole maintenance. Nature Chem.Biol. *2* 608.

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