Print Date: Nov 11th 2016

Certificate of Analysis

www.tocris.com

Product Name: **Torin 1** **Catalog No.: 4247** **Batch No.: 5**

CAS Number: 1222998-36-8

IUPAC Name: 1-[4-[4-(1-Oxopropyl)-1-piperazinyl]-3-(trifluoromethyl)phenyl]-9-(3-quinolinyl)-benzo[*h*]-1,6-naphthyridin-2(1*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{35}H_{28}F_3N_5O_2 \cdot ¼H_2O$

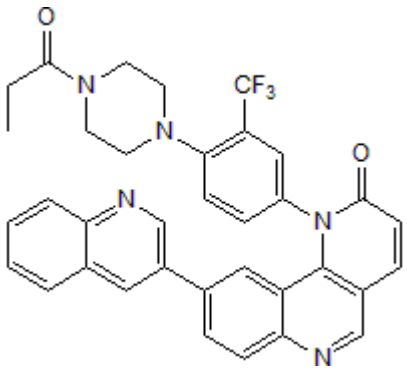
Batch Molecular Weight: 612.12

Physical Appearance: Beige solid

Solubility: DMSO to 1 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.67	4.69	11.44
Found	68.61	4.47	11.33

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Product Information

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Description:

Potent and selective mTOR inhibitor (IC_{50} = 2 - 10 nM for mTORC1 and mTORC2). Displays 200-fold selectivity for mTOR over DNA-PK, ATM and hVps34. Induces autophagy in HeLa cells.

Physical and Chemical Properties:

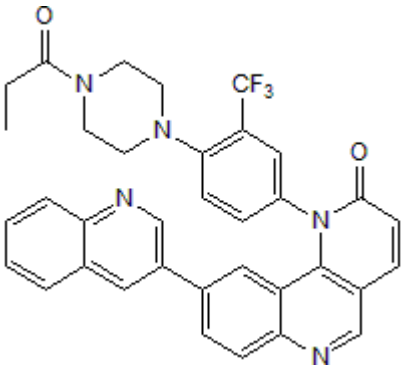
Batch Molecular Formula: $C_{35}H_{28}F_3N_5O_2.¼H_2O$

Batch Molecular Weight: 612.12

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 1 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.

Licensing Information:

Sold under license from Whitehead Institute for Biomedical Research.

References:

Peterson *et al* (2011) mTOR complex 1 regulates lipin 1 localization to control the SREBP pathway. Cell. ***146*** 408. PMID: 21816276.

Liu *et al* (2010) Discovery of 1-(4(-(4-propionylpiperazin-1-yl)-3-(trifluoromethyl)phenyl)-9-(quinolin-3-yl)benzo[*h*][1,6]naphthyridin-2(1*H*)-one as a highly potent, selective mammalian target of rapamycin (mTOR) inhibitor for the treatment of cancer. J.Med.Chem. ***53*** 7146. PMID: 20860370.

Guertin and Sabatini (2009) The pharmacology of mTOR inhibition. Sci.Signal. ***2*** pe24. PMID: 19383975.

Thoreen *et al* (2009) An ATP-competitive mammalian target of rapamycin inhibitor reveals rapamycin-resistant functions of mTORC1. J.Biol.Chem. ***284*** 8023. PMID: 19150980.