



# **Certificate of Analysis**

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Product Name: Torin 2 Catalog No.: 4248 Batch No.: 3

CAS Number: 1223001-51-1

IUPAC Name: 9-(6-Amino-3-pyridinyl)-1-[3-(trifluoromethyl)phenyl]-benzo[h]-1,6-naphthyridin-2(1H)-one

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{24}H_{15}F_3N_4O.72H_2O$ 

Batch Molecular Weight:441.41Physical Appearance:Yellow solidSolubility:DMSO to 20 mMStorage:Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 98.8% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 65.31 3.65 12.69 Found 65.2 3.48 12.61



# **Product Information**

Print Date: Jun 2<sup>nd</sup> 2017

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## **Description:**

Potent and selective mTOR inhibitor ( $IC_{50} = 2.1$  nM). Displays 800-fold cellular selectivity for mTOR over PI3K (cellular EC<sub>50</sub> values are 0.25 and 200 nM for mTOR and PI3K respectively). Activates autophagy. Orally available.

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

Batch Molecular Formula: C<sub>24</sub>H<sub>15</sub>F<sub>3</sub>N<sub>4</sub>O.½H<sub>2</sub>O

Batch Molecular Weight: 441.41 Physical Appearance: Yellow solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at +4°C

#### Solubility & Usage Info:

DMSO to 20 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.

#### Licensing Information:

Sold under license from Whitehead Institute for Biomedical Research.

#### References:

**Galluzzi** *et al* (2017) Pharmacological modulation of autophagy: therapeutic potential and persisting obstacles. Nat.Rev.Drug.Discov.. PMID: 28529316.

Simioni et al (2014) Activity of the novel mTOR inhibitor Torin-2 in B-precursor acute lymphoblastic leukemia and its therapeutic potential to prevent Akt reactivation. Oncotarget 30 10034. PMID: 25296981.

**Liu** *et al* (2011) Discovery of 9-(6-aminopyridin-3-yl)-1-(3-(trifluoromethyl)phenyl)benzo[*h*][1,6]naphthyridin-2(1*H*)-one (Torin2) as a potent, selective, and orally available mammalian target of rapamycin (mTOR) inhibitor for treatment of cancer. J.Med.Chem. *54* 1473. PMID: 21322566.

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