Print Date: Jul 31st 2018

Certificate of Analysis

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Product Name: **Autophinib** **Catalog No.: 6324** **Batch No.: 1**

CAS Number: 1644443-47-9

IUPAC Name: 6-Chloro-*N*-(5-methyl-1*H*-pyrazol-3-yl)-2-(4-nitrophenoxy)-pyrimidinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{11}ClN_6O_3$

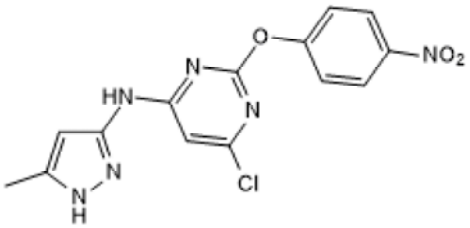
Batch Molecular Weight: 346.73

Physical Appearance: White solid

Solubility: DMSO to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.5	3.2	24.24
Found	48.49	3.31	24.31

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Product Information

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IUPAC Name: 6-Chloro-*N*-(5-methyl-1*H*-pyrazol-3-yl)-2-(4-nitrophenoxy)-pyrimidinamine

Description:

Potent VPS34 inhibitor (IC_{50} = 19 nM). Inhibits starvation- and Rapamycin-induced autophagy (IC_{50} values = 40 and 90 nM, respectively).

Physical and Chemical Properties:

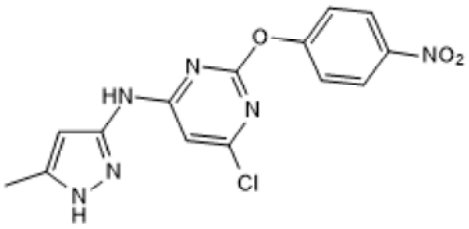
Batch Molecular Formula: $C_{14}H_{11}ClN_6O_3$

Batch Molecular Weight: 346.73

Physical Appearance: White 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.

References:

Robke *et al* (2017) Phenotypic identification of a novel autophagy inhibitor chemotype targeting lipid kinase VPS34. Angew.Chem.Int.Ed.Engl. ***56*** 8153. PMID: 28544137.

Richters *et al* (2015) Identification and further development of potent TBK1 inhibitors. ACS Chem Biol. ***10*** 289. PMID: 25540906.