

# **Certificate of Analysis**

# www.tocris.com

### Product Name: A 419259 trihydrochloride

Catalog No.: 3914 Batch No.: 3

CAS Number: 1435934-25-0

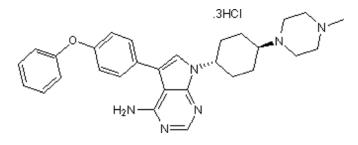
IUPAC Name: 7-[*trans*-4-(4-Methyl-1-piperazinyl)cyclohexyl]-5-(4-phenoxyphenyl)-7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine trihydrochloride

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>29</sub>H<sub>34</sub>N<sub>6</sub>O.3HCI.2<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O 641.55 White solid water to 100 mM DMSO to 20 mM Desiccate at RT

# Storage:

**Batch Molecular Structure:** 



## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis:

Shows 99.5% purity Consistent with structure Consistent with structure

	Carbon Hy	ydrogen N	litrogen	Chlorine
Theoretical	54.29	6.68	13.1	16.58
Found	54.06	6.45	13.26	16.78

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

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#### **Description:**

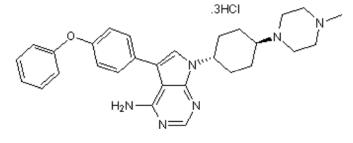
Potent Hck inhibitor ( $IC_{50} = 0.43$  nM). Also inhibits other Src family kinases (SFKs). Suppresses proliferation and induces apoptosis in CML cell lines including CD34<sup>+</sup>. Also inhibits acute myeloid leukemia (AML) stem cell proliferation in vitro and in vivo.

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

Batch Molecular Formula: C<sub>29</sub>H<sub>34</sub>N<sub>6</sub>O.3HCl.2<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O Batch Molecular Weight: 641.55 Physical Appearance: White solid

#### Minimum Purity: ≥98%

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



#### Storage: Desiccate at RT

#### Solubility & Usage Info:

water to 100 mM 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).

Catalog No.: 3914

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:**

**Saito** *et al* (2013) A pyrrolo-pyrimidine derivative targets human primary AML stem cells *in vivo*. Sci.Transl.Med. **5**. PMID: 23596204. **Pene-Dumitrescu** *et al* (2008) An inhibitor-resistant mutant of Hck protects CML cells against the antiproliferative and apoptotic effects of the broad spectrum Src family kinase inhibitor A-419259. Oncogene **27** 7055. PMID: 18794796.

Wilson et al (2002) Selective pyrrolo-pyrimidine inhibitors reveal a necessary role for Src family kinases in Bcr-Abl signal transduction and oncogenesis. Oncogene 21 8075. PMID: 12444544.

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