

**Product Name:** TC-A 2317 hydrochloride

**Catalog No.:** 4066

**Batch No.:** 1

**CAS Number:** 1245907-03-2

**IUPAC Name:** 2-[(5-Hydroxy-1,5-dimethylhexyl)amino]-4-methyl-6-[(5-methyl-1*H*-pyrazol-3-yl)amino]-3-pyridinecarbonitrile hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>28</sub>N<sub>6</sub>O.HCl.¼H<sub>2</sub>O

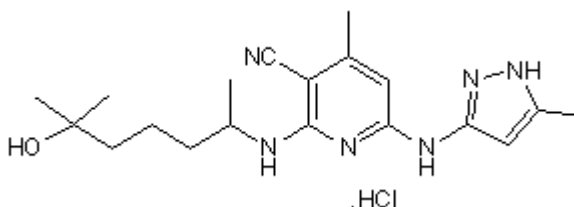
**Batch Molecular Weight:** 397.43

**Physical Appearance:** Pale yellow powder

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.33 (Ethyl acetate/1% NH<sub>3</sub>)

**HPLC:** Shows 98.6% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	57.42	7.48	21.15
Found	57.32	7.34	21.34

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**Description:**

Potent Aurora kinase A inhibitor ( $K_i = 1.2$  nM compared to 101 nM for inhibition of Aurora kinase B). Selective over 60 other kinases ( $IC_{50}$  values > 1000 nM). Exhibits good cell permeability and antitumor activity.

**Physical and Chemical Properties:**

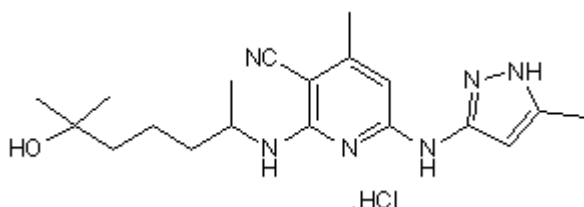
Batch Molecular Formula:  $C_{19}H_{28}N_6O \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 397.43

Physical Appearance: Pale yellow powder

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 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:**

**Ando et al** (2010) 3-Cyano-6-(5-methyl-3-pyrazoloamino)pyridines: Selective Aurora A kinase inhibitors. *Bioorg.Med.Chem.Lett.* **20** 4709. PMID: 20573509.

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