

**Product Name:** ML 315 hydrochloride

**Catalog No.:** 5700

**Batch No.:** 1

CAS Number: 1440251-53-5

IUPAC Name: 5-(1,3-Benzodioxol-5-yl)-N-[(3,5-dichlorophenyl)methyl]-4-pyrimidinamine hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub>.HCl

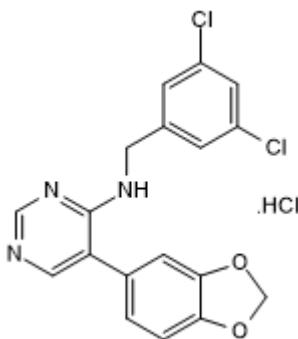
**Batch Molecular Weight:** 410.68

**Physical Appearance:** White solid

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

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.45 (Ethyl acetate:Petroleum ether [2:3])

**HPLC:** Shows 99.4% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	52.64	3.44	10.23
Found	52.58	3.37	10.11

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**Description:**

Inhibitor of cdc2-like kinases (Clk) and DYRK kinases (IC<sub>50</sub> values are 68, 68 and 231 nM for Clk1, Clk4 and Clk2, respectively, and 282 and 1156 nM for Dyrk1A and Dyrk1B). Shows 20-fold selectivity for Clk4 over Dyrk1A. Stable in both mouse and human plasma. Moderately cell permeable.

**Physical and Chemical Properties:**

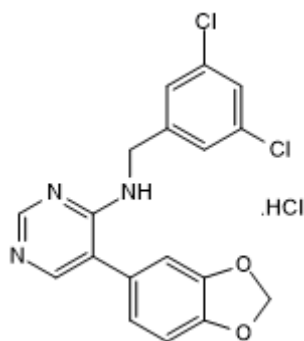
Batch Molecular Formula: C<sub>18</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub>.HCl

Batch Molecular Weight: 410.68

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°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:**

**Coombs et al** (2013) Small-molecule pyrimidine inhibitors of the cdc2-like (Clk) and dual specificity tyrosine phosphorylation-regulated (Dyrk) kinases: development of chemical probe ML315. *Bioorg.Med.Chem.Lett.* **23** 3654. PMID: 23642479.

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