

# **Certificate of Analysis**

Print Date: Nov 15th 2018

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**Product Name: TM N1324** Catalog No.: 6325 Batch No.: 1

CAS Number: 1144477-35-9

**IUPAC Name:** 4-(2-Chloro-4-fluorophenyl)-1,4,5,7-tetrahydro-3-methyl-1-(9H-purin-6-yl)-6H-pyrazolo[3,4-b]pyridin-6-one

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

C<sub>18</sub>H<sub>13</sub>CIFN<sub>7</sub>O.1/<sub>4</sub>H<sub>2</sub>O **Batch Molecular Formula:** 

**Batch Molecular Weight:** 402.29

**Physical Appearance:** Off White solid

DMSO to 10 mM with gentle warming Solubility:

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.7% purity

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

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 53.74 3.38 24.37 53.55 Found 3.28 23.97

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## **Product Information**

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IUPAC Name: 4-(2-Chloro-4-fluorophenyl)-1,4,5,7-tetrahydro-3-methyl-1-(9*H*-purin-6-yl)-6*H*-pyrazolo[3,4-*b*]pyridin-6-one

#### **Description:**

Potent and selective GPR39 agonist ( $IC_{50}$  values are 280 and 9 nM in the absence and presence of  $Zn^{2+}$ , respectively). Exhibits no significant activity against a panel of 165 other GPCRs. Inhibits the release of ghrelin and somatostatin from primary gastric mucosa cells in vitro. Cell permeable and orally bioavailable.

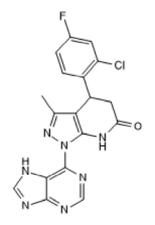
#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>18</sub>H<sub>13</sub>CIFN<sub>7</sub>O.1/4H<sub>2</sub>O

Batch Molecular Weight: 402.29 Physical Appearance: Off White solid

Minimum Purity: >98%

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



Storage: Store at -20°C

#### Solubility & Usage Info:

DMSO to 10 mM with gentle warming

#### 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:

**Frimurer** *et al* (2017) Model-based discovery of synthetic agonists for the Zn<sup>2+</sup>-sensing G-protein-coupled receptor 39 (GPR39) reveals novel biological functions. J.Med.Chem. *60* 886. PMID: 28045522.