



# **Certificate of Analysis**

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Product Name: M4K2163 dihydrochloride Catalog No.: 7754 Batch No.: 1

CAS Number: 2863635-04-3

IUPAC Name: 1-[4-[5-(4-Fluoro-3,5-dimethoxyphenyl)-4-methyl-3-pyridinyl]phenyl]piperazine dihydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>26</sub>FN<sub>3</sub>O<sub>2</sub>.2HCl.1½H<sub>2</sub>O

Batch Molecular Weight: 507.43

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 98.3% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.81 6.16 8.28 Found 55.55 6.06 8.16



## **Product Information**

Print Date: Mar 24th 2023

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IUPAC Name: 1-[4-[5-(4-Fluoro-3,5-dimethoxyphenyl)-4-methyl-3-pyridinyl]phenyl]piperazine dihydrochloride

### **Description:**

M4K2163 is a potent and selective activin receptor-like kinase 2 (ALK2) inhibitor ( $IC_{50}$  values are 19 nM in vivo and 98 nM in vitro). Orally bioavailable and brain penetrant.

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

Batch Molecular Formula: C<sub>24</sub>H<sub>26</sub>FN<sub>3</sub>O<sub>2</sub>.2HCl.1½H<sub>2</sub>O

Batch Molecular Weight: 507.43

Physical Appearance: Pale yellow solid

### Minimum Purity: ≥98%

### **Batch Molecular Structure:**

Storage: Store at -20°C

### Solubility & Usage Info:

water to 100 mM DMSO to 100 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.: 7754

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:

Rooney and Jones (2021) Recent advances in ALK2 inhibitors. ACS Omega 6 20729. PMID: 34423181.

**Smil** *et al* (2020) Leveraging an open science drug discovery model to develop CNS-penetrant ALK2 inhibitors for the treatment of diffuse intrinsic pontine glioma. J.Med.Chem. *63* 10061. PMID: 32787083.

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