

# **Certificate of Analysis**

Print Date: Sep 25th 2018

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Product Name: AS 2444697 Catalog No.: 5430 Batch No.: 2

CAS Number: 1287665-60-4

IUPAC Name: N-[3-Aminocarbonyl)-1-(tetrahydro-2*H*-pyran-4-yl)-1*H*-pyrazol-4-yl]-2-(2-methyl-4-pyridinyl)-4-oxazolecarboxamide

hydrochloride

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{19}H_{20}N_6O_4.HCI.H_2O$ 

Batch Molecular Weight: 450.88

Physical Appearance: Off White solid

**Solubility:** DMSO to 20 mM with gentle warming

Storage: Desiccate at RT

**Batch Molecular Structure:** 

HCI

# 2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.61 5.14 18.64 Found 50.33 5.22 18.51



# **Product Information**

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### **Description:**

Potent and selective interleukin-1 receptor-associated kinase 4 (IRAK4) inhibitor (IC $_{50}$  = 21 nM). Displays 30-fold selectivity for IRAK4 over IRAK1. Inhibits LPS-induced TNF- $\alpha$  and IL-6 production in PBMCs in vitro. Renoprotective and anti-inflammatory in a rodent model of chronic kidney disease.

# **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>19</sub>H<sub>20</sub>N<sub>6</sub>O<sub>4</sub>.HCl.H<sub>2</sub>O

Batch Molecular Weight: 450.88 Physical Appearance: Off White solid

**Minimum Purity:** >98%

# **Batch Molecular Structure:**

HCI

Storage: Desiccate at RT

# Solubility & Usage Info:

DMSO to 20 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:

**Chaudhary** (2015) Recent advances in the discovery of small molecule inhibitors of interleukin-1 receptor-associated kinase 4 (IRAK4) as a therapeutic target for inflammation and oncology disorders. J.Med.Chem. **58** 96. PMID: 25479567.

**Kondo** *et al* (2014) Renoprotective effects of novel interleukin-1 receptor-associated kinase 4 inhibitor AS2444697 through anti-inflammatory action in 5/6 nephrectomized rats. Naunyn Schmiedebergs Arch.Pharmacol. **387** 909. PMID: 25052043.

**Schmaderer and Heemann** (2014) Blocking innate immunity to slow the progression of chronic kidney disease. Naunyn Schmiedebergs Arch.Pharmacol. **387** 905. PMID: 25107563.

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