

# **Certificate of Analysis**

Print Date: Jun 16<sup>th</sup> 2016 **WWW.tocris.com** 

Product Name: PF 05089771 Catalog No.: 5931 Batch No.: 1

CAS Number: 1430806-04-4

IUPAC Name: 4-[2-(3-Amino-1*H*-pyrazol-4-yl)-4-chlorophenoxy]-5-chloro-2-fluoro-*N*-4-thiazolylbenzenesulfonamide tosylate

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{18}H_{12}CI_2FN_5O_3S_2.C_7H_8O_3S$ 

**Batch Molecular Weight:** 672.56 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Desiccate at RT

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC:** Shows 100% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 44.65 3 10.41 Found 44.84 2.98 10.39



# **Product Information**

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## **Description:**

Potent and selective  $Na_v1.7$  channel blocker (IC<sub>50</sub> = 8, 11 and 171 nM for mouse, human and rat Na<sub>v</sub>1.7, respectively). Exhibits selectivity for  $Na_v 1.7$  over other  $Na_v 1$  channels ( $IC_{50}$  values are 0.11, 0.16, 0.85, 10, 11 and 25  $\mu$ M for Na<sub>v</sub>1.2, Na<sub>v</sub>1.6, Na<sub>v</sub>1.1, Na<sub>v</sub>1.4, Na<sub>v</sub>1.3 and Na<sub>v</sub>1.5, respectively). Also exhibits selectivity over a panel of 81 other ion channels, receptors, enzymes and transporters. Blocks spontaneous firing of inherited erythromelalgia (IEM)-derived iPSC sensory neurons in vitro.

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

Batch Molecular Formula: C<sub>18</sub>H<sub>12</sub>Cl<sub>2</sub>FN<sub>5</sub>O<sub>3</sub>S<sub>2</sub>.C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>S

Batch Molecular Weight: 672.56 Physical Appearance: White solid

Minimum Purity: >98%

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

NH.

Storage: Desiccate at RT

#### Solubility & Usage Info:

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).

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:

Alexandrou et al (2016) Subtype-selective small molecule inhibitors reveal a fundamental role for Na, 1.7 in nociceptor electrogenesis, axonal conduction and presynaptic release. PLoS One 11 e0152405. PMID: 27050761.

Cao et al (2016) Pharmacological reversal of a pain phenotype in iPSC-derived sensory neurons and patients with inherited erythromelalgia. Sci. Transl. Med. 8 335ra56. PMID: 27099175.