

# **Certificate of Analysis**

Print Date: May 22<sup>nd</sup> 2025

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Product Name: BAY 6096 Catalog No.: 8006 Batch No.: 1

CAS Number: 2313483-41-7

IUPAC Name: 1-[2-[[[3-(3,5-Dimethyl-4-isoxazolyl)imidazo[1,2-a]pyridin-7-yl]carbonyl]amino]ethyl]-4-(methylamino)pyridinium

chloride

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{21}H_{23}CIN_6O_2.21/4H_2O$ 

Batch Molecular Weight: 467.44

Physical Appearance: Off White solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

# 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 Chlorine

Theoretical 53.96 5.93 17.98 7.58 Found 53.14 5.72 17.62 7.63



# **Product Information**

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#### **Description:**

BAY 6096 is a potent (IC $_{50}$  = 14 nM), and selective adrenergic  $\alpha_{2B}$  receptor antagonist that displays 394, 725, >845-fold selectivity over  $\alpha_{1A}$ ,  $\alpha_{2A}$ , and  $\alpha_{2C}$ , respectively. BAY 6096 reduces  $\alpha_{2B}$  receptor agonist-induced vasoconstriction and has a high clearance and low mean residence times in rats. BAY 6096 is highly water-soluble.

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

Batch Molecular Formula: C<sub>21</sub>H<sub>23</sub>ClN<sub>6</sub>O<sub>2</sub>.2½H<sub>2</sub>O

Batch Molecular Weight: 467.44 Physical Appearance: Off White 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).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

# **Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 6096 probe summary on the SGC website.

# References:

**Meibom** et al (2023) BAY-6096: A potent, selective, and highly water-soluble adrenergic a2B antagonist. J Med Chem **66** 4659. PMID: 36932954.

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