

# **Certificate of Analysis**

Print Date: Mar 23rd 2021

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Product Name: BAY 293 Negative Control Catalog No.: 6906 Batch No.: 1

CAS Number: 2244904-69-4

IUPAC Name: (S)-6,7-Dimethoxy-2-methyl-N-[1-[4-[2-[(methylamino)methyl]phenyl]thiophene-2-yl]ethyl]quinazolin-4-amine

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{25}H_{28}N_4O_2S.\frac{1}{4}H_2O$ 

Batch Molecular Weight: 453.09

Physical Appearance: Light Beige solid
Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.5$  (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

**HPLC:** Shows 99.5% purity **Chiral HPLC:** Shows 99.8% purity

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

**Optical Rotation:**  $[\alpha]_D = +111.1$  (Concentration = 1, Solvent = DMSO)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 66.27 6.34 12.37 Found 66.49 6.45 12.01

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



## **Product Information**

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## **Description:**

Negative control for BAY 293 (Cat. No. 6857)

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>25</sub>H<sub>28</sub>N<sub>4</sub>O<sub>2</sub>S.½H<sub>2</sub>O

Batch Molecular Weight: 453.09

Physical Appearance: Light Beige solid

## **Minimum Purity:** ≥98%

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

Storage: Store at -20°C

## Solubility & Usage Info:

DMSO to 100 mM ethanol 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).

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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.

#### **Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 293 probe summary on the SGC website.

#### References:

**Hillig** *et al* (2019) Discovery of potent SOS1 inhibitors that block RAS activation via disruption of the RAS-SOS1 interaction. Proc.Natl.Acad.Sci.USA. *116* 2551. PMID: 30683722.

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