

# **Certificate of Analysis**

Print Date: Nov 18th 2019

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Product Name: NVS-CECR2-1 Catalog No.: 5744 Batch No.: 2

CAS Number: 1992047-61-6

IUPAC Name: N-Cyclopropyl-2-(propylsulfonyl)-6-(1-(2,2,6,6-tetramethylpiperidin-4-yl)-1H-indol-5-yl)pyrimidin-4-amine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{27}H_{37}N_5O_2S.\frac{1}{2}H_2O$ 

**Batch Molecular Weight:** 504.69 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.3$  (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.5% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.26 7.59 13.88 Found 64.14 7.88 13.79

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## **Product Information**

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#### **Description:**

Potent and selective CECR2 (cat eye syndrome chromosome region, candidate 2) inhibitor ( $IC_{50}$  = 47 nM). Selective for CECR2 over a panel of bromodomains. A concentration of 1  $\mu$ M is recommended for use in cellular assays.

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

Batch Molecular Formula:  $C_{27}H_{37}N_5O_2S.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 504.69 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at -20°C

#### 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.

#### **Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the NVS-CECR2-1 probe summary on the SGC website.