

# **Certificate of Analysis**

Print Date: Sep 6th 2021

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Product Name: Centrinone B Catalog No.: 5690 Batch No.: 3

CAS Number: 1798871-31-4

IUPAC Name: 2-[[2-Fluoro-4-[[(2-fluoro-3-nitrophenyl)methyl]sulfonyl]phenyl]thio]-5-methoxy-*N*-(5-methyl-1*H*-pyrazol-3-yl)

-6-(1-piperidinyl)-4-pyrimidinamine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{27}H_{27}F_2N_7O_5S_2$ .

Batch Molecular Weight: 631.67

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**HPLC:** Shows 99.9% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 51.34 4.31 15.52 Found 51.36 4.31 15.5

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

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## **Product Information**

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IUPAC Name: 2-[[2-Fluoro-4-[[(2-fluoro-3-nitrophenyl)methyl]sulfonyl]phenyl]thio]-5-methoxy-N-(5-methyl-1H-pyrazol-3-yl)

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#### **Description:**

Centrinone B is a high affinity and selective PLK4 inhibitor ( $K_i = 0.6 \text{ nM}$ ). Exhibits >2000-fold selectivity for PLK4 over Aurora A and Aurora B. Depletes centriole and centrosome levels in vitro. Induces cell cycle arrest in normal human cell lines in a p53-dependent manner.

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

Batch Molecular Formula: C<sub>27</sub>H<sub>27</sub>F<sub>2</sub>N<sub>7</sub>O<sub>5</sub>S<sub>2</sub>.

Batch Molecular Weight: 631.67 Physical Appearance: Yellow solid

Minimum Purity: ≥98%

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

Storage: Store at -20°C

## Solubility & Usage Info:

DMSO to 50 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:**

Sold with the permission of the Ludwig Institute for Cancer Research Ltd

#### References:

Wong et al (2015) Reversible centriole depletion with an inhibitor of Polo-like kinase 4. Science 348 1155. PMID: 25931445.