

# **Certificate of Analysis**

Print Date: Aug 4th 2017

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Product Name: JH-II-127 Catalog No.: 6289 Batch No.: 1

CAS Number: 1700693-08-8

IUPAC Name: [4-[[5-Chloro-4-(methylamino)-7*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl]amino]-3-methoxyphenyl]-4-morpholinyl-methanone

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{19}H_{21}CIN_6O_3$ 

**Batch Molecular Weight:** 416.87

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

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

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 54.74 5.08 20.16 Found 54.67 5.09 20.12



## **Product Information**

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#### **Description:**

Potent and selective LRRK2 inhibitor ( $IC_{50}$  values are 2.2, 6.6 and 47.7 nM for G2019S-mutant, wild-type and A2016T-mutant LRRK2, respectively). Selective for LRRK2 over a panel of 138 kinases. Brain penetrant and orally bioavailable.

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

Batch Molecular Formula: C<sub>19</sub>H<sub>21</sub>CIN<sub>6</sub>O<sub>3</sub> Batch Molecular Weight: 416.87 Physical Appearance: Off 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:

Sold under license from Dana-Farber Cancer Institute.

#### References:

Hatcher et al (2015) Discovery of a pyrrolopyrimidine (JH-II-127), a highly potent, selective, and brain penetrant LRRK2 inhibitor. ACS Med.Chem.Lett. 6 584. PMID: 26005538.

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