

# Certificate of Analysis

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**Product Name:** LRRK2-IN-1

**Catalog No.:** 4273

**Batch No.:** 4

**CAS Number:** 1234480-84-2

**IUPAC Name:** 5,11-Dihydro-2-[[[2-methoxy-4-[[4-(4-methyl-1-piperazinyl)-1-piperidinyl]carbonyl]phenyl]amino]-5,11-dimethyl-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>31</sub>H<sub>38</sub>N<sub>8</sub>O<sub>3</sub>·2½H<sub>2</sub>O

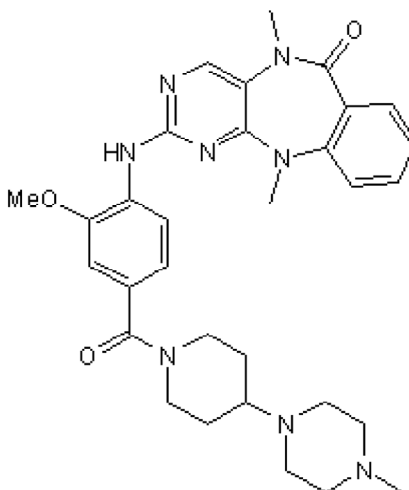
**Batch Molecular Weight:** 615.73

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.2% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

	Carbon	Hydrogen	Nitrogen
Theoretical	60.47	7.04	18.2
Found	59.78	6.83	18.21

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

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**Description:**

LRRK2-IN-1 is a potent and selective inhibitor of leucine-rich repeat kinase 2 (LRRK2). Inhibits both G2019S mutant and wild-type LRRK2 kinase activity (IC<sub>50</sub> values are 6 and 13 nM respectively). Causes dephosphorylation, ubiquitination and degradation of LRRK2. Inhibits IFN-γ-induced monocyte maturation in vitro.

**Physical and Chemical Properties:**

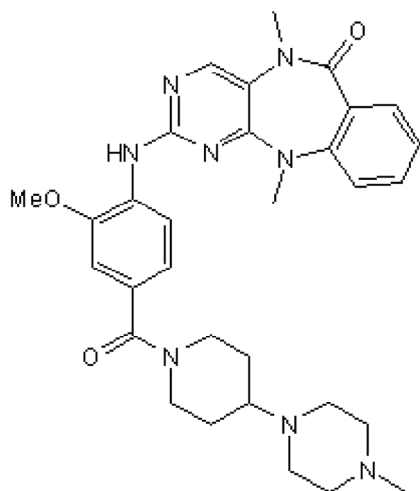
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Batch Molecular Weight: 615.73

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. \*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:**

Sold under license from the Dana-Farber Cancer Institute.

**References:**

**Zhao *et al*** (2015) LRRK2 Dephosphorylation increases its ubiquitination. *Biochem.J.* **469** 107. PMID: 25939886.

**Deng *et al*** (2011) Characterization of a selective inhibitor of the Parkinson's disease kinase LRRK2. *Nat.Chem.Biol.* **7** 203. PMID: 21378983.

**Thévenet *et al*** (2011) Regulation of LRRK2 expression points to a functional role in human monocyte maturation. *PLoS One* **6** e21519. PMID: 21738687.

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