

Product Name: LRRK2-IN-1

Catalog No.: 4273

Batch No.: 1

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: C₃₁H₃₈N₈O₃·½H₂O

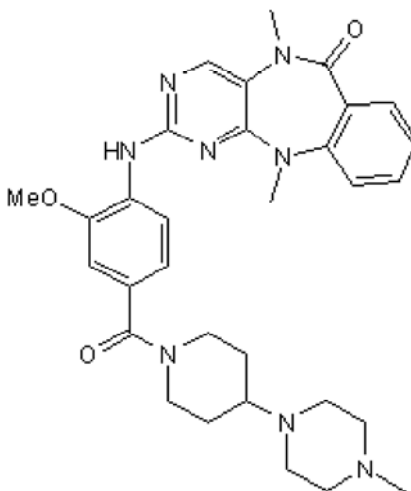
Batch Molecular Weight: 579.1

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.16 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.23	6.78	19.33
Found	64.19	6.45	19.32

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

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Description:

Potent and selective inhibitor of leucine-rich repeat kinase 2 (LRRK2). Inhibits both G2019S mutant and wild-type LRRK2 kinase activity (IC₅₀ 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:

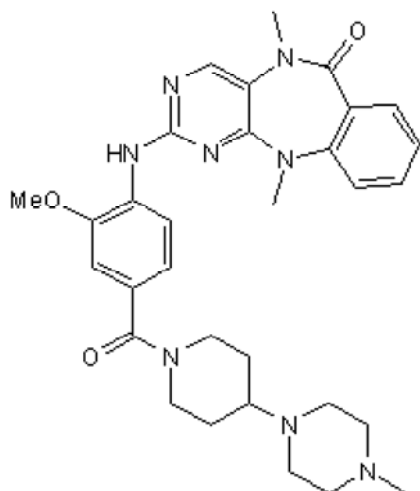
Batch Molecular Formula: C₃₁H₃₈N₈O₃·½H₂O

Batch Molecular Weight: 579.1

Physical Appearance: Off-white 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).

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 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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