

Certificate of Analysis

Product Name: PF 06447475

Catalog No.: 5716

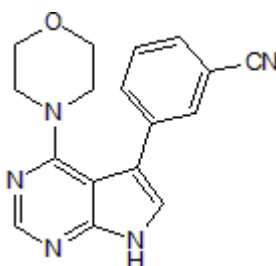
Batch No.: 1

CAS Number: 1527473-33-1

IUPAC Name: 3-[4-(4-Morpholinyl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₅N₅O
Batch Molecular Weight: 305.33
Physical Appearance: White solid
Solubility: DMSO to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Ethyl acetate)
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.87	4.95	22.94
Found	66.77	4.91	22.78

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

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CAS Number: 1527473-33-1

IUPAC Name: 3-[4-(4-Morpholinyl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile

Description:

Potent LRRK2 inhibitor (IC₅₀ = 3 nM). Attenuates α -synuclein-induced dopaminergic neurodegeneration and neuroinflammation in G2019S-LRRK2 expressing rats. Also neuroprotective in wild type rats. Brain penetrant.

Physical and Chemical Properties:

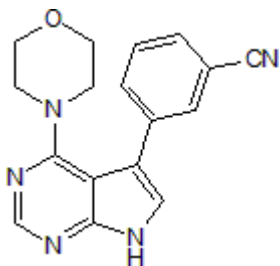
Batch Molecular Formula: C₁₇H₁₅N₅O

Batch Molecular Weight: 305.33

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Daher et al (2015) Leucine-rich repeat kinase 2 (LRRK2) pharmacological inhibition abates α -synuclein gene-induced neurodegeneration. *J.Biol.Chem.* **290** 19433. PMID: 26078453.

Henderson et al (2015) Discovery and preclinical profiling of 3-[4-(morpholin-4-yl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]benzotrile (PF-06447475), a highly potent, selective, brain penetrant, and *in vivo* active LRRK2 kinase inhibitor. *J.Med.Chem.* **58** 419. PMID: 25353650.

Storage: Store at +4°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.

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