

## Certificate of Analysis

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**Product Name:** MLI-2

**Catalog No.:** 5756

**Batch No.:** 1

CAS Number: 1627091-47-7

IUPAC Name: *rel*-3-[6-[(2*R*,6*S*)-2,6-Dimethyl-4-morpholinyl]-4-pyrimidyl]-5-[(1-methylcyclopropyl)oxy]-1*H*-indazole

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>25</sub>N<sub>5</sub>O<sub>2</sub>·¼H<sub>2</sub>O

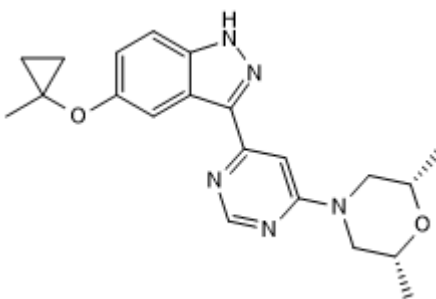
**Batch Molecular Weight:** 383.96

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.2 (Dichloromethane:Methanol [95:5])

**HPLC:** Shows 99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

Theoretical 65.69 6.69 18.24

Found 65.99 6.8 18.32

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**Description:**

Potent and selective LRRK2 inhibitor ( $IC_{50}$  = 0.76-3.4 nM depending on assay). Exhibits >295-fold selectivity for over 300 kinases and a diverse panel of receptors and ion channels. Centrally bioavailable and active in vivo.

**Physical and Chemical Properties:**

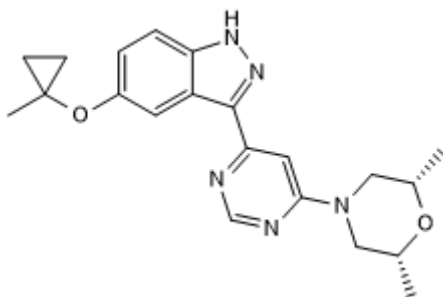
Batch Molecular Formula:  $C_{21}H_{25}N_5O_2 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 383.96

Physical Appearance: White 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.

**References:**

Fell *et al* (2015) MLI-2, a potent, selective, and centrally active compound for exploring the therapeutic potential and safety of LRRK2 kinase inhibition. *J.Pharmacol.Exp.Ther.* **355** 397. PMID: 26407721.

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