Certificate of Analysis

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Print Date: Mar 23rd 2021

Product Name: MLi-2

biotechne

Catalog No.: 5756 Batch No.: 2

CAS Number: IUPAC Name: 1627091-47-7

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure:

 $C_{21}H_{25}N_5O_2$ 379.46 White solid DMSO to 50 mM Store at -20°C

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.7% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 66.47 6.64 18.46 Found 66.03 6.71 18.66

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

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

Description:

IUPAC Name:

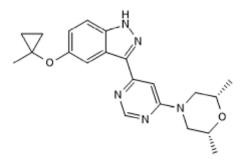
MLi-2 is a potent and selective LRRK2 inhibitor ($IC_{50} = 0.76-3.4$ nM depending on assay), which exhibits >295-fold selectivity for over 300 kinases and a diverse panel of receptors and ion channels. MLi-2 is centrally bioavailable and active in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{21}H_{25}N_5O_2$ Batch Molecular Weight: 379.46 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).

Catalog No.: 5756

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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