

Certificate of Analysis

Print Date: Mar 7th 2019

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Product Name: LJI308 Catalog No.: 6754 Batch No.: 1

CAS Number: 1627709-94-7

IUPAC Name: 2,6-Difluoro-4-[4-[4-(4-morpholinyl)phenyl]-3-pyridinyl]phenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{18}F_2N_2O_2$

Batch Molecular Weight: 368.38

Physical Appearance: Off White solid
Solubility: DMSO to 50 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.47 4.93 7.6 Found 68.27 4.93 7.65

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

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Product Information

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Description:

Potent pan-ribosomal S6 protein kinase (RSK) inhibitor (IC_{50} values are 4 to 13 nM). Displays selectivity for RSK isoforms over other kinases. Inhibits RSK-dependent Y-box binding protein 1 (YB-1) phosphorylation in vitro. Suppresses growth of triple negative breast cancer cell lines.

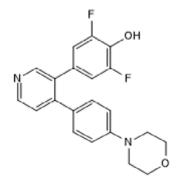
Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₁₈F₂N₂O₂

Batch Molecular Weight: 368.38 Physical Appearance: Off 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:

Davies *et al* (2015) Inhibition of RSK with the novel small-molecule inhibitor LJI308 overcomes chemoresistance by eliminating cancer stem cells. Oncotarget. *6* 20570. PMID: 26011941.

Jain et al (2015) Discovery of potent and selective RSK inhibitors as biological probes. J.Med.Chem. 58 6766. PMID: 26270416.

Aronchik *et al* (2014) Novel potent and selective inhibitors of p90 ribosomal S6 kinase reveal the heterogeneity of RSKfunction in MAPK-driven cancers. Mol.Cancer Res. *12* 803. PMID: 24554780.