

Certificate of Analysis

Print Date: May 4th 2020

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Product Name: Ispinesib Catalog No.: 5408 Batch No.: 1

CAS Number: 336113-53-2

IUPAC Name: N-(3-Aminopropyl)-N-[(1R)-1-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]-2-methylpropyl]-4-

methylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₃ClN₄O₂

Batch Molecular Weight: 517.06

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.69 6.43 10.84 Found 69.41 6.52 10.9

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



Product Information

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Description:

High affinity allosteric kinesin spindle protein (KSP) inhibitor (K_{i} app = 1.7 nM). Exhibits >10,000-fold selectivity for KSP over a range of other mitotic kinesins. Inhibits proliferation and induces apoptosis of prostate and breast cancer cells in vitro. Induces tumor regression of breast cancer cell xenografts in mice.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₀H₃₃ClN₄O₂

Batch Molecular Weight: 517.06 Physical Appearance: Beige 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.

References:

Purcell *et al* (2010) Activity of the kinesin spindle protein inhibitor ispinesib (SB-715992) in models of breast cancer. Clin.Cancer Res. **16** 566. PMID: 20068098.

Lad et al (2008) Mechanism of inhibition of human KSP by ispinesib. Biochemistry 47 3576. PMID: 18290633.

Davis et al (2006) Increased therapeutic potential of an experimental anti-mitotic inhibitor SB715992 by genistein in PC-3 human prostate cancer cell line. BMC Cancer 6 22. PMID: 16433906.

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