

Certificate of Analysis

Print Date: Mar 17th 2022

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Product Name: BS 181 dihydrochloride Catalog No.: 5608 Batch No.: 1

CAS Number: 1883548-83-1

IUPAC Name: N^5 -(6-Aminohexyl)-3-(1-methylethyl)- N^7 -(phenylmethyl)pyrazolo[1,5-a]pyrimidine-5,7-diamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₃₂N₆.2HCl

Batch Molecular Weight: 453.45 **Physical Appearance:** White solid

Solubility: water to 100 mM

DMSO to 100 mM ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

Theoretical 58.27 7.56 18.53 15.64 Found 57.92 7.32 18.36 15.65

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Product Information

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Description:

BS 181 dihydrochloride is a selective cdk7 inhibitor ($IC_{50} = 21$ nM). Displays >40-fold selectivity for cdk7 over other cdks. Promotes cell cycle arrest and apoptosis in a range of cancer cells in vitro and inhibits MCF-7 tumor xenograft growth in mice.

Physical and Chemical Properties:

Batch Molecular Formula: C22H32N6.2HCl

Batch Molecular Weight: 453.45 Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM ethanol 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.: 5608

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:

Ali et al (2009) The development of a selective cyclin-dependent kinase inhibitor that shows antitumor activity. Cancer Res. **69** 6208. PMID: 19638587.