Certificate of Analysis

Product Name: **BI 9321** **Catalog No.: 6665** **Batch No.: 1**

IUPAC Name: (4-(5-(7-Fluoroquinolin-4-yl)-1-methyl-1*H*-imidazol-4-yl)-3,5-dimethylphenyl)methanamine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{21}FN_4.3HCl.1½H_2O$

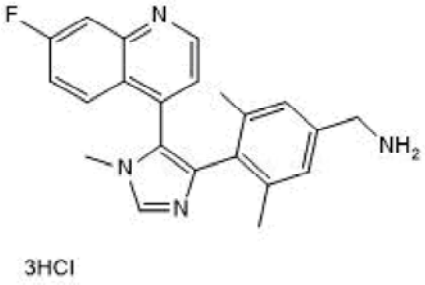
Batch Molecular Weight: 496.83

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (5% 1M NH3 in MeOH in DCM)

HPLC: Shows 97.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.18	5.48	11.28
Found	52.91	5.55	11.1

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Description:

Nuclear receptor-binding SET domain (NSD) 3 antagonist (IC_{50} = 1.2 µM). Selectively binds the PWWP1 domain of NSD3 (K_d = 166 nM). Antagonizes the interaction of H3 with NSD3-PWWP1 in U2OS cells.

Physical and Chemical Properties:

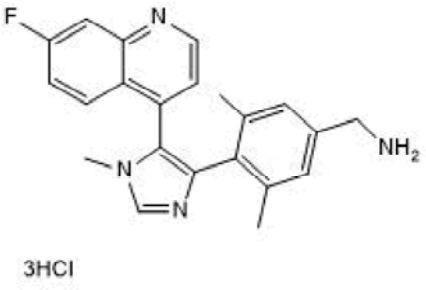
Batch Molecular Formula: $C_{22}H_{21}FN_4.3HCl.1½H_2O$

Batch Molecular Weight: 496.83

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BI 9321 probe summary on the SGC website.