Certificate of Analysis

Product Name: **BIX 01294** **Catalog No.: 3364** **Batch No.: 3**

CAS Number: 1392399-03-9

IUPAC Name: 2-(Hexahydro-4-methyl-1*H*-1,4-diazepin-1-yl)-6,7-dimethoxy-*N*-[1-(phenylmethyl)-4-piperidinyl]-4-quinazolinamine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{38}N_6O_2.3HCl.4¼H_2O$

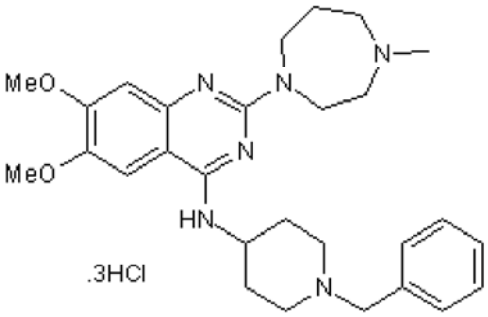
Batch Molecular Weight: 676.57

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	49.71	7.37	12.42	15.72
Found	49.34	7.17	12.2	15.71

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Description:

BIX 01294 is a GLP and G9a histone lysine methyltransferase inhibitor (IC_{50} values are 0.7 and 1.7 μM respectively) that displays no activity at other histone methyltransferases up to 37 μM. Modulates H3K9me2 levels in mammalian cells and potentiates induction of pluripotent stem cells from somatic cells in vitro. Also inhibits H3K36 methylation by oncoproteins NSD1, NSD2 and NSD3 (IC_{50} values are 40 - 112 μM). Restores metabolic and antiviral function in exhausted $CD8^+$ T cells from patients with chronic HCV infection.

Physical and Chemical Properties:

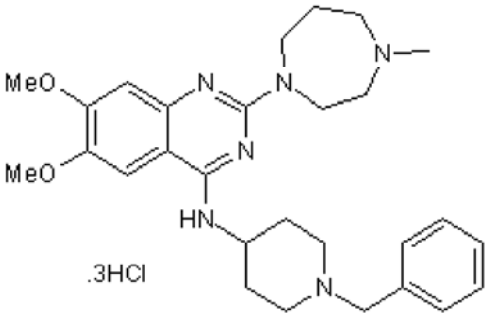
Batch Molecular Formula: $C_{28}H_{38}N_6O_2.3HCl.4¼H_2O$

Batch Molecular Weight: 676.57

Physical Appearance: White 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.

References:

Barili *et al* (2020) Targeting p53 and histone methyltransferases restores exhausted CD8+ T cells in HCV infection. Nat.Commun. ***11*** 604. PMID: 32001678.

Morishita *et al* (2017) BIX-01294 inhibits oncoproteins NSD1, NSD2, and NSD3. Med.Chem.Res. ***26*** 2038.

Malmquist *et al* (2012) Small-molecule histone methyltransferase inhibitors display rapid antimalarial activity against all blood stage forms in *Plasmodium falciparum*. Proc.Natl.Acad.Sci.U.S.A. ***109*** 16708. PMID: 23011794.