

Certificate of Analysis

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Product Name:	BIX 01294	Catalog No.:	3364	Batch No.:	3
CAS Number:	1392399-03-9				
IUPAC Name:	2-(Hexahydro-4-methyl-1 <i>H</i> -1,4-diazepin-1-yl)-6,7-dimethoxy- <i>N</i> -[1-(phenylmethyl)-4-piperidinyl]-4-quinazolinamine trihydrochloride				

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₈N₆O₂·3HCl·4¹/₄H₂O

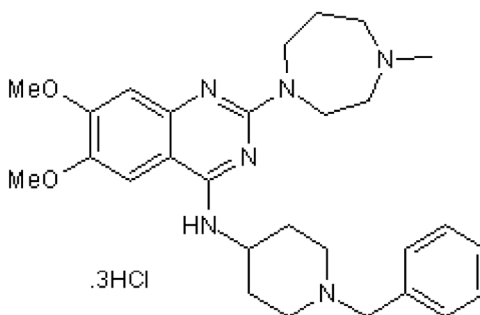
Batch Molecular Weight: 676.57

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

¹H 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

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

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Description:

BIX 01294 is a GLP and G9a histone lysine methyltransferase inhibitor (IC₅₀ 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 (IC₅₀ values are 40 - 112 μM). Restores metabolic and antiviral function in exhausted CD8⁺ T cells from patients with chronic HCV infection. Promotes conversion of fibroblasts to cardiomyocytes as part of 9C cocktail (see our protocol below). For m... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

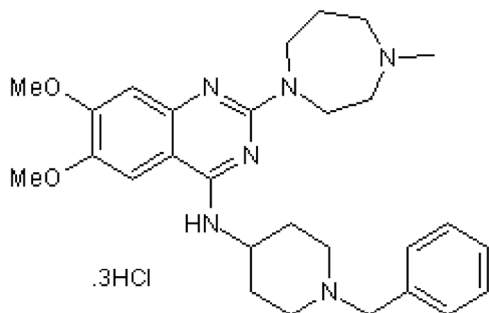
Batch Molecular Formula: C₂₈H₃₈N₆O₂·3HCl·4½H₂O

Batch Molecular Weight: 676.57

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



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.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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