

**Product Name:** BIX 01294

**Catalog No.:** 3364

**Batch No.:** 2

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-piperidiny]-4-quinazolinamine trihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>28</sub>H<sub>38</sub>N<sub>6</sub>O<sub>2</sub>·3HCl·1<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

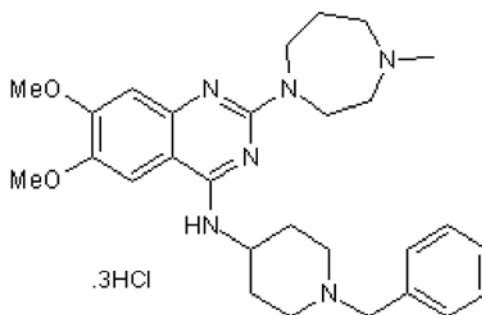
**Batch Molecular Weight:** 631.54

**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

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	53.25	7.1	13.31
Found	52.95	7.2	13.14

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**Description:**

GLP and G9a histone lysine methyltransferase inhibitor (IC<sub>50</sub> 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<sub>50</sub> values are 40 - 112 μM).

**Physical and Chemical Properties:**

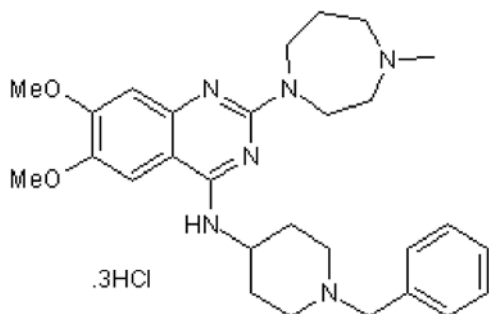
Batch Molecular Formula: C<sub>28</sub>H<sub>38</sub>N<sub>6</sub>O<sub>2</sub>·3HCl·1½H<sub>2</sub>O

Batch Molecular Weight: 631.54

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:**

**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.

**Chang et al** (2009) Structural basis for G9a-like protein lysine methyltransferase inhibition by BIX-01294. *Nat.Struct.Mol.Biol.* **16** 312. PMID: 19219047.

**Shi et al** (2008) Induction of pluripotent stem cells from mouse embryonic fibroblasts by Oct4 and Klf4 with small-molecule compounds. *Cell Stem Cell* **3** 568. PMID: 18983970.

**Kubicek et al** (2007) Reversal of H3K9me2 by a small-molecule inhibitor for the G9a histone methyltransferase. *Mol.Cell* **25** 473. PMID: 17289593.

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