

Product Name: BIX 01294

Catalog No.: 3364

Batch No.: 1

CAS Number: 935693-62-2

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: C₂₈H₃₈N₆O₂·3HCl·6H₂O

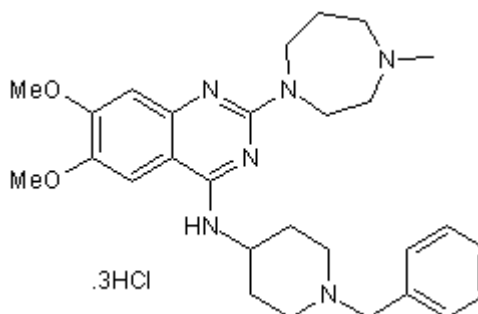
Batch Molecular Weight: 708.11

Physical Appearance: cream solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.13 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.49	7.54	11.87
Found	47.51	7.42	11.82

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

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Description:

G9a-like protein 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.

Physical and Chemical Properties:

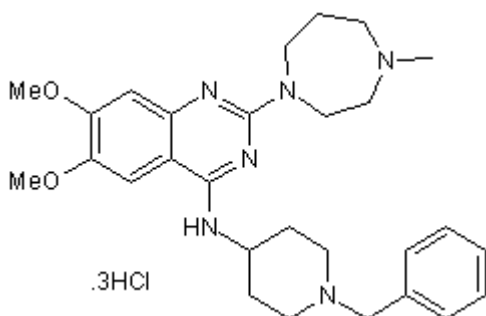
Batch Molecular Formula: C₂₈H₃₈N₆O₂·3HCl·6H₂O

Batch Molecular Weight: 708.11

Physical Appearance: cream 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:

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

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.

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

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