Print Date: Feb 18th 2019

Certificate of Analysis

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Product Name: **Ro 5-3335** **Catalog No.: 4694** **Batch No.: 3**

CAS Number: 30195-30-3

IUPAC Name: 7-Chloro-1,3-dihydro-5-(1*H*-pyrrol-2-yl)-2*H*-1,4-benzodiazepin-2-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{10}ClN_3O$

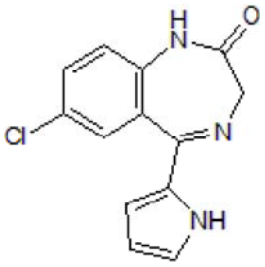
Batch Molecular Weight: 259.69

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.67 (Ethyl acetate:Petroleum ether [1:2])

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.13	3.88	16.17
Found	60.11	3.86	16.03

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Description:

Core binding factor (CBF) inhibitor; preferentially kills human leukemia cell lines with CBF fusion proteins (IC_{50} = 1.1 μM). Represses RUNX1/CBFβ-dependent transactivation in reporter assays and inhibits transcriptional regulation by RUNX1 and CBFβ. Reduces leukemia burden in a mouse model. Attenuates RUNX1-dependent hematopoiesis in zebrafish embryos. Also a Tat antagonist; inhibits HIV-1 replication in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{13}H_{10}ClN_3O$

Batch Molecular Weight: 259.69

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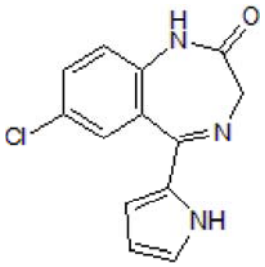
Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

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:

Cunningham *et al* (2012) Identification of benzodiazepine Ro5-3335 as an inhibitor of CBF leukemia through quantitative high throughput screen against RUNX1-CBFß interaction. Proc.Natl.Acad.Sci.USA ***109*** 14592. PMID: 22912405.

Okuda *et al* (2001) RUNX1/AML1: a central player in hematopoiesis. Int. J. Hematol. ***74*** 252. PMID: 11721959.

Cupelli *et al* (1995) The human immunodeficiency virus type 1 Tat antagonist, Ro 5-3335, predominantly inhibits transcription initiation from the viral promoter. J.Virol. ***69*** 2640. PMID: 7884917.