

**Certificate of Analysis** 

www.tocris.com

Print Date: Oct 11th 2016

Product Name: BRD 4354 Catalog No.: 6010 Batch No.: 1

CAS Number: 315698-07-8

IUPAC Name: 5-Chloro-7-[(4-ethyl-1-piperazinyl)-3-pyridinylmethyl]-8-quinolinol

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{21}H_{23}CIN_4O$ .

Batch Molecular Weight: 382.89

Physical Appearance: Off White solid

Solubility: DMSO to 20 mM ethanol to 50 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 99.1% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen
Theoretical 65.88 6.05 14.63
Found 65.82 5.9 14.54



# **Product Information**

Print Date: Oct 11<sup>th</sup> 2016

www.tocris.com

Product Name: BRD 4354 Catalog No.: 6010 Batch No.: 1

CAS Number: 315698-07-8

IUPAC Name: 5-Chloro-7-[(4-ethyl-1-piperazinyl)-3-pyridinylmethyl]-8-quinolinol

## **Description:**

HDAC5 and HDAC9 inhibitor (IC $_{50}$  values are 0.85 and 1.88  $\mu$ M, respectively). Also weakly inhibits HDAC4, HDAC6, HDAC7 and HDAC8 (IC $_{50}$  values are 3.88 - 13.8  $\mu$ M). Exhibits >20-fold selectivity for HDAC5/9 over HDAC1/2/3.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>21</sub>H<sub>23</sub>CIN<sub>4</sub>O. Batch Molecular Weight: 382.89 Physical Appearance: Off White solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

### Solubility & Usage Info:

DMSO to 20 mM ethanol to 50 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:

Boskovic et al (2016) Inhibition of zinc-dependent histone deacetylases with a chemically triggered electrophile. ACS Chem.Biol. 11 1844. PMID: 27064299.