

# **Certificate of Analysis**

Print Date: Oct 18th 2014

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Product Name: OXF BD 02 Catalog No.: 4928 Batch No.: 1

CAS Number: 1429129-68-9

IUPAC Name: 3-(3,5-Dimethyl-4-isoxazolyl)-5-hydroxy-α-phenylbenzenemethanol

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{17}NO_3$ Batch Molecular Weight:295.33Physical Appearance:White solid

**Solubility:** DMSO to 100 mM

ethanol to 10 mM with gentle warming

Storage: Store at +4°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 73.2 5.8 4.74 Found 73.16 5.75 4.87



# **Product Information**

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#### **Description:**

Selective inhibitor of the first bromodomain of BRD4 (BRD4(1)) ( $IC_{50}$  = 382 nM). Exhibits 2-3-fold selectivity for BRD4(1) over the CBP bromodomain and has little affinity for a range of other bromodomains. Reduces viability of lung adenocarcinoma cell lines and attenuates proliferation of MV-4-11 leukemia cells. Cell permeable.

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

Batch Molecular Formula: C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub> Batch Molecular Weight: 295.33 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at +4°C

#### Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

#### 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:

**Hewings** et al (2011) 3,5-dimethylisoxazoles act as acetyl-lysine-mimetic bromodomain ligands. J.Med.Chem. **54** 6761. PMID: 21851057.

**Hewings** *et al* (2013) Optimization of 3,5-dimethylisoxazole derivatives as potent bromodomain ligands. J.Med.Chem. *56* 3217. PMID: 23517011.

