

# **Certificate of Analysis**

Print Date: Jan 14th 2016

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Product Name: ML 228 Catalog No.: 4565 Batch No.: 1

CAS Number: 1357171-62-0

IUPAC Name: N-([1,1'Biphenyl]-4-ylmethyl)-6-phenyl-3-(2-pyridinyl)-1,2,4-triazin-5-amine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{21}N_5$ Batch Molecular Weight:415.49Physical Appearance:Brown solid

Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 78.05 5.09 16.86 Found 78.07 5.14 16.84



## **Product Information**

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## **Description:**

HIF pathway activator (EC $_{50}$  values are 1.23 and 1.4  $\mu$ M for HRE gene reporter assay and HIF-1 $\alpha$  nuclear translocation assay respectively); acts via chelation of iron, independently of PHD. Also exhibits > 80% inhibition of the human A $_3$  receptor, dopamine transporter,  $\mu$  receptor, hERG and 5-HT $_{2B}$  receptor, and rat sodium channel site 2, at a concentration of 10  $\mu$ M.

## **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{27}H_{21}N_5$ Batch Molecular Weight: 415.49 Physical Appearance: Brown solid

Minimum Purity: >98%

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

Storage: Store at -20°C

## Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

**Theriault** *et al* (2012) Discovery of a new molecular probe ML228: an activator of the hypoxia inducible factor (HIF) pathway. Bioorg.Med.Chem.Lett. **22** 76. PMID: 22172704.

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