

# **Certificate of Analysis**

Print Date: Jan 15th 2016

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Product Name: T2AA Catalog No.: 4723 Batch No.: 1

CAS Number: 1380782-27-3

IUPAC Name:  $(\beta S)$ - $\beta$ -Amino-4-(4-hydroxyphenoxy)-3,5-diiodobenzenpropanol

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{15}I_2NO_3$ Batch Molecular Weight:511.09Physical Appearance:White solid

Solubility: DMSO to 100 mM

1eq. HCl to 10 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

HO NH<sub>2</sub> OH

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.67$  (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

HPLC: Shows 99.2% purity

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

Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -15.3$  (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 35.35 2.96 2.74 Found 35.63 3.02 2.68



## **Product Information**

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### **Description:**

Proliferating cell nuclear antigen (PCNA) inhibitor; inhibits PCNA/PIP-box peptide interaction (IC $_{50}$  ~1  $\mu$ M). Causes DNA replication stress by stalling DNA replication forks. Inhibits PCNA interaction with DNA polymerase  $\delta$  and arrests cell growth in S-phase. Suppresses cancer cell growth.

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

Batch Molecular Formula: C<sub>15</sub>H<sub>15</sub>l<sub>2</sub>NO<sub>3</sub> Batch Molecular Weight: 511.09 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

#### Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl 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:

**Punchihewa** *et al* (2012) Identification of small molecule proliferating cell nuclear antigen (PCNA) inhibitor that disrupts interactions with PIP-box proteins and inhibits DNA replication. J.Biol.Chem. **287** 14289. PMID: 22383522.