

# **Certificate of Analysis**

Print Date: Jan 14th 2016

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Catalog No.: 5248 Batch No.: 1

Product Name: XAP 044 CAS Number: 196928-50-4

**IUPAC Name:** 7-Hydroxy-3-(4-iodophenoxy)-4H-1-benzopyran-4-one

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

C<sub>15</sub>H<sub>9</sub>IO<sub>4</sub> **Batch Molecular Formula:** 380.13 **Batch Molecular Weight:** Beige solid **Physical Appearance:** 

Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC**: Shows 99.4% purity <sup>1</sup>H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 47.39 2.39 Found 47.31 2.33



# **Product Information**

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IUPAC Name: 7-Hydroxy-3-(4-iodophenoxy)-4*H*-1-benzopyran-4-one

### **Description:**

Potent and selective  $mGlu_7$  antagonist ( $IC_{50} = 88$  nM); inhibits lateral amygdala long term potentiation (LTP) in brain slices from wild type mice. Displays no effects on the LTP of  $mGlu_7$  deficient mice. Exhibits novel activity by binding to the  $mGlu_7$  Venus flytrap domain (VFTD). Exhibits anti-anxiety effects in rodent models. Brain penetrant.

## **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{15}H_9IO_4$ Batch Molecular Weight: 380.13 Physical Appearance: Beige 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 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:

Gee et al (2014) Blocking metabotropic glutamate receptor subtype 7 (mGlu $_7$ ) via the Venus flytrap domain (VFTD) inhibits amygdala plasticity, stress, and anxiety-related behavior. J.Biol.Chem. **289** 10975. PMID: 24596089.

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