

**Certificate of Analysis** 

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Print Date: Jan 14th 2016

Product Name: A 844606 Catalog No.: 4477 Batch No.: 1

CAS Number: 861119-08-6

IUPAC Name: 2-(Hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-9H-xanthen-9-one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Solubility:** ethanol to 5 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.43$  (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99.6% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 74.98 6.29 8.74 Found 75.23 6.29 8.89



# **Product Information**

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**IUPAC Name:** 2-(Hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-9H-xanthen-9-one

## **Description:**

Selective  $\alpha 7$  nicotinic acetylcholine receptor (nAChR) partial agonist (EC50 values are 1.4 and 2.2 µM at human and rat receptors respectively). Displays no measurable effect on  $\alpha 4\beta 2$ Stimulates α7 nAChR-induced phosphorylation in PC12 cells.

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

Batch Molecular Formula: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub> Batch Molecular Weight: 320.38 Physical Appearance: Yellow solid

Minimum Purity: >99%

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

Storage: Store at -20°C

## Solubility & Usage Info:

ethanol to 5 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:

Briggs et al (2008) Alpha7 nicotinic acetylcholine receptor agonist properties of tilorone and related tricyclic analogues. Br.J.Pharmacol. 153 1054. PMID: 18157163.

Tel: +44 (0)1235 529449 www.tocris.com/distributors Tel:+1 612 379 2956