# **Certificate of Analysis**

# www.tocris.com

Print Date: Oct 11th 2018

#### E 2012 Product Name:

Catalog No.: 5550

Batch No.: 1

CAS Number: 870843-42-8

**IUPAC Name:** (3E)-1-[(1S)-1-(4-Fluorophenyl)ethyl]-3-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-2-piperidone

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula: Batch Molecular Weight: Physical Appearance:** Solubility:

C<sub>25</sub>H<sub>26</sub>FN<sub>3</sub>O<sub>2</sub> 419.49 White solid 1eq. HCl to 100 mM DMSO to 100 mM ethanol to 100 mM Store at -20°C

Storage: **Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

TLC: HPLC: **Chiral HPLC:** <sup>1</sup>H NMR: Mass Spectrum: **Microanalysis:** 

R<sub>f</sub> = 0.25 (Dichloromethane:Methanol [95:5]) Shows 99.4% purity Shows 99.6% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen

	Carbon H	yarogen r	vitrogen
Theoretical	71.58	6.25	10.02
Found	71.61	6.28	9.77

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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(3E)-1-[(1S)-1-(4-Fluorophenyl)ethyl]-3-[[3-methoxy-4-(4-methyl-1H-imidazol-1-yl)phenyl]methylene]-2-piperidone

### **Description:**

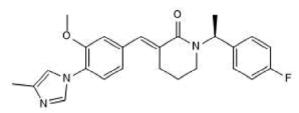
 $\gamma$ -secretase modulator. Lowers A $\beta$ 40 and A $\beta$ 42 levels and increases A $\beta$ 37 levels, in vitro and in vivo. Displays no effect on  $\gamma$ -secretase processing of Notch, EphA4 and EphB2.

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

Batch Molecular Formula:  $C_{25}H_{26}FN_3O_2$ Batch Molecular Weight: 419.49 Physical Appearance: White solid

Minimum Purity: >98%

**Batch Molecular Structure:** 



Storage: Store at -20°C

#### Solubility & Usage Info:

1eq. HCl to 100 mM DMSO to 100 mM ethanol to 100 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  $45-60^{\circ}C$  water bath).

Catalog No.: 5550

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:**

**Borgegard** *et al* (2012) First and second generation  $\gamma$ -secretase modulators (GSMs) modulate amyloid- $\beta$  (A $\beta$ ) peptide production through different mechanisms. J.Biol.Chem. **287** 15. PMID: 22334705.

**Portelius** *et al* (2010) Acute effect on the A $\beta$  isoform pattern in CSF in response to  $\gamma$ -secretase modulator and inhibitor treatment in dogs. J.Alzheimers Dis. **21** 1005. PMID: 20634579.

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