

Certificate of Analysis

Print Date: Jan 14th 2016

www.tocris.com

Product Name: A 582941 Catalog No.: 4341 Batch No.: 1

CAS Number: 848591-90-2

IUPAC Name: Octahydro-2-methyl-5-(6-phenyl-3-pyridazinyl)-pyrrolo[3,4-c]pyrrole

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{17}H_{20}N_4$.1/2H₂O **Batch Molecular Formula:**

289.38 **Batch Molecular Weight:** White solid **Physical Appearance:**

Solubility: DMSO to 100 mM

1eq. HCl to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:

$$-N$$

2. ANALYTICAL DATA

 $R_f = 0.2$ (Dichloromethane:Methanol [95:5]) TLC:

HPLC: Shows 98% purity

¹H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> 7.31 Theoretical 70.56 19.36 Found 70.21 6.97 19.06



Product Information

Print Date: Jan 14th 2016

www.tocris.com

Product Name: A 582941 Catalog No.: 4341 Batch No.: 1

CAS Number: 848591-90-2

IUPAC Name: Octahydro-2-methyl-5-(6-phenyl-3-pyridazinyl)-pyrrolo[3,4-c]pyrrole

Description:

Selective $\alpha 7$ nAChR partial agonist; exhibits high affinity for both rat and human $\alpha 7$ receptors (K_i values are 10.8 and 16.7 nM respectively). Displays ~15-fold selectivity for $\alpha 7$ over 5-HT₃ receptors (K_i = 150 nM for 5-HT₃).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{20}N_4$. ½ H_2O Batch Molecular Weight: 289.38 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

$$-N$$
 $N=N$
 $N=N$

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM 1eg. HCl to 50 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:

Anderson et al (2008) [3 H]A-585539 [(1 5 A-585539 [(1 5 A-6-phenylpyridazin-3-yl)-5-aza-2-azoniabicyclo[2.2.1]heptane], a novel high-affinity α 7 neuronal nicotinic receptor agonist: radioligand binding characterization to rat and human brain. J.Pharmacol.Exp.Ther. **324** 179. PMID: 17959745.

Tel: +44 (0)1235 529449