TOCRIS
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# Certificate of Analysis

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**Product Name:** **3-pyr-Cytisine** **Catalog No.: 4125** **Batch No.: 1**

CAS Number: 948027-43-8

IUPAC Name: (1*R*,5*S*)-1,2,3,4,5,6-Hexahydro-9-(3-pyridinyl)-1,5-methano-8*H*-pyrido[1,2-*a*][1,5]diazocin-8-one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{16}H_{17}N_3O.¼H_2O$

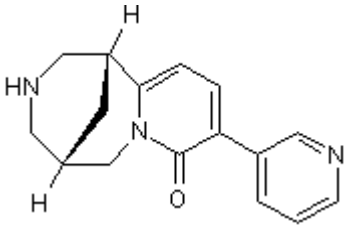
**Batch Molecular Weight:** 271.83

**Physical Appearance:** White solid

**Solubility:** water to 100 mM
DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.2 (Chloroform:Methanol [4:1])

**HPLC:** Shows >99.8% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** $[\alpha]_D$ = -88.1 (Concentration = 1.13, Solvent = Water)

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 70.7 | 6.49 | 15.46 |
| Found | 70.86 | 6.3 | 15.3 |



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**Description:**

High affinity α4β2 partial agonist ($K_i$ values are 0.91, 119 and 1100 nM for α4β2, α3β4 and α7 receptors respectively). Shows little activity at α3β4 and α7 receptors. Exhibits antidepressant-like effects in mouse models of antidepressant efficacy.

**Physical and Chemical Properties:**

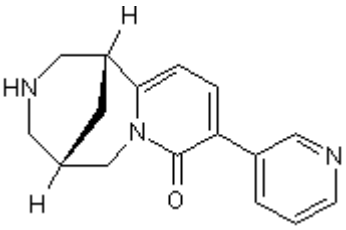
Batch Molecular Formula: $C_{16}H_{17}N_3O.¼H_2O$

Batch Molecular Weight: 271.83

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:**

water to 100 mM
DMSO 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°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:**

**Mineur** *et al* (2009) Cytisine-based nicotinic partial agonists as novel antidepressant compounds. J.Pharmacol.Exp.Ther. ***329*** 377. PMID: 19164465.

**Papke** *et al* (2010) Activation and inhibition of mouse muscle and neuronal nicotinic acetylcholine receptors expressed in *Xenopus* oocytes. J.Pharmacol.Exp.Ther. ***333*** 501. PMID: 20100906.

**Papke** *et al* (2011) Electrophysiological perspectives on the therapeutic use of nicotinic acetylcholine receptor partial agonists. J.Pharmacol.Exp.Ther. ***337*** 1.



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