

# **Certificate of Analysis**

Print Date: May 3rd 2022

www.tocris.com

Product Name: LE 300 Catalog No.: 1674 Batch No.: 4

CAS Number: 274694-98-3

IUPAC Name: 6,7,8,9,14,15-Hexahydro-7-methyl-5*H*-indolo[3,2-*f*][3]benzazecine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{20}H_{22}N_2.^3/4H_2O$ 

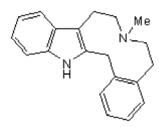
**Batch Molecular Weight:** 303.92 **Physical Appearance:** Beige solid

**Solubility:** 1eq. HCl to 50 mM

DMSO to 100 mM ethanol to 10 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 



#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.32$  (Chloroform:Methanol [9:1])

**HPLC:** Shows 98.5% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 79.04 7.79 9.22 Found 79.19 7.8 9.26

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



# **Product Information**

Print Date: May 3<sup>rd</sup> 2022

www.tocris.com

Product Name: LE 300 Catalog No.: 1674 Batch No.: 4

CAS Number: 274694-98-3

IUPAC Name: 6,7,8,9,14,15-Hexahydro-7-methyl-5*H*-indolo[3,2-*f*][3]benzazecine

## **Description:**

LE 300 is a potent and selective dopamine  $D_1$  receptor antagonist ( $K_i$  values are 0.08 - 1.9 nM and 6 - 45 nM for  $D_1$  and  $D_2$  receptors respectively). Also displays moderate affinity for the 5-HT<sub>2A</sub> receptor ( $K_i$  = 20 nM). Active in vivo.

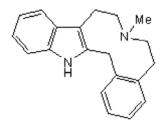
# **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>N<sub>2</sub>.<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 303.92 Physical Appearance: Beige solid

Minimum Purity: ≥98%

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



Storage: Store at -20°C

#### Solubility & Usage Info:

1eq. HCl to 50 mM DMSO to 100 mM ethanol to 10 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:

**El-Subbagh** *et al* (2002) DA/serotonin receptor ligands: Part IV [1]: Synthesis and pharmacology of novel 3-benzazecines and 3-benzazecines as potential 5-HT<sub>2A</sub> and DA receptor ligands. Arch.Pharm. (Weinheim). **9** 443. PMID: 12447918.

**Kassack** *et al* (2002) Pharmacological characterization of the benz[*d*]indolo[2,3-*g*]azecine LE300, a novel type of a nanomolar DA receptor antagonist. Naunyn Schmiedebergs Arch.Pharmacol. *366* 543. PMID: 12444495.

Witt et al (2000) 7-Methyl-6,7,8,9,14,15-hexahydro-5*H*-benz[d]indolo[2,3-g]azecine: a new heterocyclic system and a new lead compound for DA receptor antagonists. J.Med.Chem. **43** 2079. PMID: 10821720.

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