

Batch No.: 1



# **Certificate of Analysis**

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Catalog No.: 2777

Product Name: Nefazodone hydrochloride

CAS Number: 82752-99-6

IUPAC Name: 2-[3-[4-(3-Chlorophenyl)-1-piperazinyl]propyl]-5-ethyl-2,4-dihydro-4-(2-phenoxyethyl)-3*H*-1,2,4-triazol-3-one

hydrochloride

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C<sub>25</sub>H<sub>32</sub>CIN<sub>5</sub>O<sub>2</sub>.HCI

Batch Molecular Weight: 506.47

Physical Appearance: White crystalline solid
Solubility: 1eq. HCl to 10 mM
DMSQ to 25 mM

DMSO to 25 mM ethanol to 10 mM

Storage: Desiccate at RT

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

Microanalysis:

Melting Point:Between 186 - 188°CHPLC:Shows >99.9% purity¹H NMR:Consistent with structureMass Spectrum:Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 59.28 6.57 13.83 Found 59.18 6.63 13.83



# **Product Information**

Print Date: Jan 15<sup>th</sup> 2016 **WWW.tocris.com** 

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hydrochloride

#### **Description:**

Serotonin 5-HT $_{2A}$  receptor antagonist ( $K_i = 5.8$  nM) and inhibitor of serotonin and noradrenalin uptake (IC $_{50}$  values are 290 and 300 nM respectively). Displays no activity at 5-HT $_{1B}$  and 5-HT $_{1D}$  receptors. Active in models predictive of antidepressant potential.

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

Batch Molecular Formula: C<sub>25</sub>H<sub>32</sub>ClN<sub>5</sub>O<sub>2</sub>.HCl

Batch Molecular Weight: 506.47

Physical Appearance: White crystalline solid

#### Minimum Purity: >99%

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

Storage: Desiccate at RT

## Solubility & Usage Info:

1eq. HCl to 10 mM DMSO to 25 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:

Eison et al (1990) Nefazodone: preclinical pharmacology of a new antidepressant. Psychopharmacol.Bull. 26 311. PMID: 2274630.

Davis et al (1997) Nefazodone. A review of its pharmacology and clinical efficacy in the management of major depression. Drugs 53 608. PMID: 9098663.

**Pullar** *et al* (2000) LY367265, an inhibitor of the 5-hydroxytryptamine transporter and 5-hydroxytryptamine<sub>2A</sub> receptor antagonist: a comparison with the antidepressant, nefazodone. Eur.J.Pharmacol. *407* 39. PMID: 11050288.