



# **Certificate of Analysis**

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Product Name: Anpirtoline hydrochloride Catalog No.: 0703 Batch No.: 6

CAS Number: 99201-87-3

IUPAC Name: 6-Chloro-2-[piperidinyl-4-thio]pyridine hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{10}H_{13}CIN_2S.HCI$ 

**Batch Molecular Weight:** 265.2 **Physical Appearance:** White solid

**Solubility:** water to 100 mM

DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

CI N S

.HCI

2. ANALYTICAL DATA

**TLC:**  $R_f = 0.2$  (Dichloromethane:Methanol:Acetic acid [9:1:0.1])

**HPLC:** Shows 99.9% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 45.29 5.32 10.56 Found 45.32 5.28 10.41



# **Product Information**

Print Date: Jan 8<sup>th</sup> 2016

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CAS Number: 99201-87-3

IUPAC Name: 6-Chloro-2-[piperidinyl-4-thio]pyridine hydrochloride

#### **Description:**

Highly potent 5-HT<sub>1B</sub> receptor agonist ( $K_i$  values are 28, 150 and 1490 nM at 5-HT<sub>1B</sub>, 5-HT<sub>1A</sub> and 5-HT<sub>2</sub> receptors respectively). Decreases central serotonin synthesis and attenuates aggressive behavior in vivo. Also acts as an antagonist at 5-HT<sub>3</sub> receptors ( $K_i$  = 29.5 nM) and is brain penetrant.

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

Batch Molecular Formula: C<sub>10</sub>H<sub>13</sub>CIN<sub>2</sub>S.HCI

Batch Molecular Weight: 265.2 Physical Appearance: White solid

**Minimum Purity:** >99%

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

Storage: Desiccate at +4°C

## 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:

**Swedberg** *et al* (1992) D-16949 (anpirtoline): a novel serotonergic (5-HT<sub>1B</sub>) psychotherapeutic agent assessed by its discriminative effect in the rat. J.Pharmacol.Exp.Ther. **263** 1015. PMID: 1335050.

**Göthert** *et al* (1995) 5HT<sub>3</sub> receptor antagonism by anpirtoline, a mixed 5HT<sub>1</sub> receptor agonist/5HT<sub>3</sub> receptor antagonist. Br.J.Pharmacol. *114* 269, PMID: 7881726.

**Almeida and Miczek** (2002) Aggression escalates by social instigation or by discontinuation of reinforcement ("frustration") in mice: inhibition by anpirtoline: a 5-HT<sub>1B</sub> receptor agonist. Neuropsychopharmacology **27** 171. PMID: 12093591.

**Watanabe** *et al* (2006) Effects of anpirtoline on regional serotonin synthesis in the rat brain: an autoradiographic study. Nucl.Med.Biol. **33** 325. PMID: 16631081.