

## Certificate of Analysis

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**Product Name:** L-741,742 hydrochloride

**Catalog No.:** 1004

**Batch No.:** 2

CAS Number: 874882-93-6

IUPAC Name: 5-(4-Chlorophenyl)-4-methyl-3-(1-(2-phenylethyl)piperidin-4-yl)isoxazole hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>25</sub>N<sub>2</sub>ClO.HCl

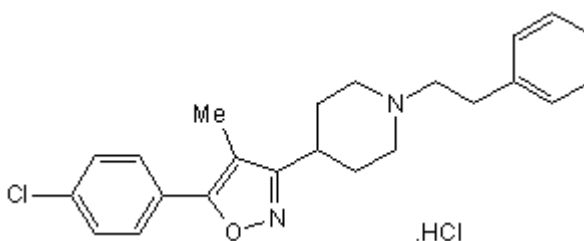
**Batch Molecular Weight:** 417.38

**Physical Appearance:** White solid

**Solubility:** DMSO to 10 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.35 (Dichloromethane:Methanol [95:5])

**HPLC:** Shows 99.3% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 66.19  | 6.28     | 6.71     |
| Found       | 66.05  | 6.29     | 6.83     |

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

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**Description:**

A potent and highly selective D<sub>4</sub> dopamine receptor antagonist, with K<sub>i</sub> values of > 1700, 770 and 3.5 nM at cloned human D<sub>2</sub>, D<sub>3</sub> and D<sub>4</sub> receptors.

**Physical and Chemical Properties:**

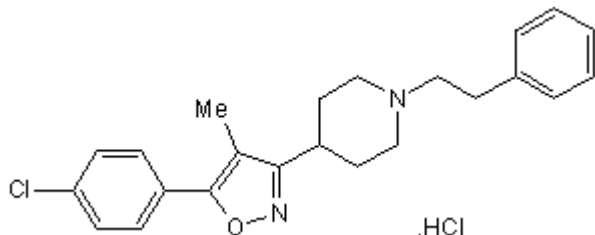
Batch Molecular Formula: C<sub>23</sub>H<sub>25</sub>N<sub>2</sub>ClO.HCl

Batch Molecular Weight: 417.38

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

DMSO 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.

**Licensing Information:**

Sold with the permission of Merck Sharp and Dohme Ltd.

**References:**

**Rowley et al** (1997) 4-Heterocyclypiperidines as selective high-affinity ligands at the human dopamine D<sub>4</sub> receptor. *J.Med.Chem.* **40** 2374. PMID: 9240352.

**Rowley et al** (1996) 5-(4-Chlorophenyl)-4-methyl-3-(1-(2-phenylethyl)piperidin-4-yl)isoxazole: a potent, selective antagonist at human cloned dopamine D<sub>4</sub> receptors. *J. Med. Chem.* **39** 1943. PMID: 8642551.

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