

# Certificate of Analysis

**Product Name:** ML 352 hydrochloride

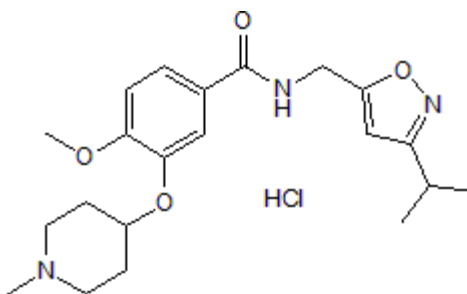
**Catalog No.:** 5725

**Batch No.:** 1

**IUPAC Name:** 4-Methoxy-N-[[3-(1-methylethyl)-5-isoxazolyl]methyl]-3-[(1-methyl-4-piperidyl)oxy]benzamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	$C_{21}H_{29}N_3O_4 \cdot HCl \cdot \frac{1}{2}H_2O$
<b>Batch Molecular Weight:</b>	432.94
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	water to 10 mM with gentle warming DMSO to 100 mM ethanol to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>TLC:</b>	$R_f = 0.2$ (Dichloromethane:Methanol [95:5])
<b>HPLC:</b>	Shows 99.2% purity
<b><math>^1H</math> NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	58.26	7.22	9.71
Found	58.31	7.14	9.72

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**Description:**

High affinity and selective presynaptic choline transporter (CHT) inhibitor ( $K_i = 92$  nM). Exhibits selectivity for CHT over dopamine, serotonin and noradrenalin transporters; acetylcholinesterase and cholineacetyltransferase; and a panel of 65 other GPCRs, ion channels and transporters.

**Physical and Chemical Properties:**

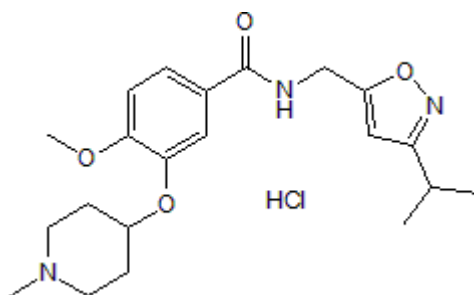
Batch Molecular Formula:  $C_{21}H_{29}N_3O_4 \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 432.94

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 10 mM with gentle warming

DMSO to 100 mM

ethanol 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:**

**Bollinger et al** (2015) Synthesis and structure-activity relationships of a series of 4-methoxy-3-(piperidin-4-yl)oxy benzamides as novel inhibitors of the presynaptic choline transporter. *Bioorg.Med.Chem.Lett.* **25** 1757. PMID: 25801932.

**Ennis et al** (2015) Identification and characterization of ML352: a novel, noncompetitive inhibitor of the presynaptic choline transporter. *ACS Chem.Neurosci.* **6** 417. PMID: 25560927.

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel: +1 612 379 2956