

## Certificate of Analysis

**Product Name:** JNJ 777120

**Catalog No.:** 4021

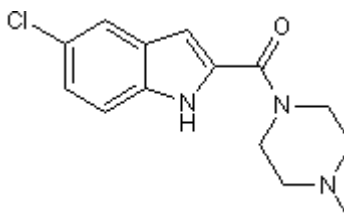
**Batch No.:** 3

CAS Number: 459168-41-3

IUPAC Name: 1-[(5-Chloro-1*H*-indol-2-yl)carbonyl]-4-methylpiperazine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>14</sub>H<sub>16</sub>ClN<sub>3</sub>O  
**Batch Molecular Weight:** 277.75  
**Physical Appearance:** White solid  
**Solubility:** 1eq. HCl to 100 mM  
DMSO to 50 mM  
ethanol to 50 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.32 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.54	5.81	15.13
Found	60.15	5.75	14.96

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

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**Description:**

Histamine H<sub>4</sub> receptor antagonist; displays high affinity (K<sub>i</sub> = 4.5 nM) and is >1000-fold selective for H<sub>4</sub> over other histamine receptors.

**Physical and Chemical Properties:**

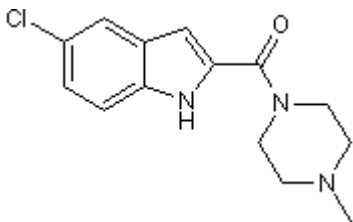
Batch Molecular Formula: C<sub>14</sub>H<sub>16</sub>ClN<sub>3</sub>O

Batch Molecular Weight: 277.75

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

1eq. HCl to 100 mM

DMSO to 50 mM

ethanol to 50 mM

USE WITH CARE; NOT FULLY TESTED - YOUR SUBLICENSE UNDER CERTAIN PATENT RIGHTS OF ORTHO-MCNEIL-JANSSEN PHARMACEUTICAL, INC. RESTRICTS USE TO INTERNAL RESEARCH ONLY - MAY NOT BE USED IN HUMANS - MAY NOT BE SOLD, TRANSFERRED, OR USED IN COMMERCIAL SERVICES

**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 Ortho-McNeil-Janssen Pharmaceuticals, Inc.

**References:**

**Strakhova et al** (2009) *In vitro* and *in vivo* characterization of A-940894: a potent histamine H<sub>4</sub> receptor antagonist with anti-inflammatory properties. *Br.J.Pharmacol.* **157** 44. PMID: 19413570.

**Thurmond et al** (2004) A potent and selective histamine H<sub>4</sub> receptor antagonist with anti-inflammatory properties. *J.Pharmacol.Exp.Ther.* **309** 404. PMID: 14722321.

**Jablanowski et al** (2003) The first potent and selective non-imidazole human histamine H<sub>4</sub> receptor antagonists. *J.Med.Chem.* **46** 3957. PMID: 12954048.

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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