

# Certificate of Analysis

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**Product Name:** ICI 199,441 hydrochloride

**Catalog No.:** 0778

**Batch No.:** 2

CAS Number: 115199-84-3

IUPAC Name: 2-(3,4-Dichlorophenyl)-N-methyl-N-[(1S)-1-phenyl-2-(1-pyrrolidiny)ethyl]acetamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>24</sub>Cl<sub>2</sub>N<sub>2</sub>O.HCl

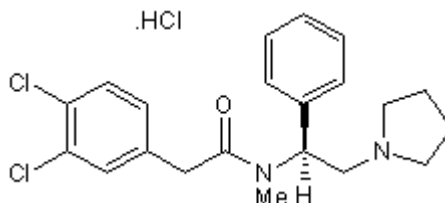
**Batch Molecular Weight:** 427.8

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.55 (Dichloromethane:Methanol:Ammonia soln. [95:5:0.1])

**Melting Point:** Between 227 - 234°C(Dec)

**HPLC:** Shows 100% purity

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

**Optical Rotation:** [α]<sub>D</sub> = +146.7 (Concentration = 1, Solvent = Ethanol)

**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |   |   |
|-------------|--------|----------|----------|---|---|
| Theoretical | 58.96  | 5.89     | 6.55     | 0 | 0 |
| Found       | 58.96  | 5.82     | 6.5      | 0 | 0 |

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**Description:**

Highly potent  $\kappa$  agonist, 146-fold more active than U-50488 (Cat. No. 0495) in vitro.

**Physical and Chemical Properties:**

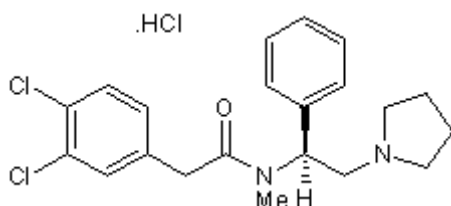
Batch Molecular Formula:  $C_{21}H_{24}Cl_2N_2O \cdot HCl$

Batch Molecular Weight: 427.8

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 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:**

**Barlow et al** (1991) Structure/activity studies related to 2-(3,4-dichlorophenyl)-N-methyl-N-[2-(1-pyrrolidinyl)-1-substituted-ethyl]acetamides: a novel series of potent and selective  $\kappa$ -opioid agonists. *J.Med.Chem.* **34** 3149. PMID: 1659636.

**Costello et al** (1991) 2-(3,4-Dichlorophenyl)-N-methyl-N-[2-(1-pyrrolidinyl)-1-substituted-ethyl]-acetamides: the use of conformational analysis in the development of a novel series of potent opioid  $\kappa$  agonists. *J.Med.Chem.* **34** 181. PMID: 1846918.

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