

Product Name: DIPPA hydrochloride

Catalog No.: 0794

Batch No.: 5

CAS Number: 155512-52-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₃Cl₂N₃OS.HCl.¼H₂O

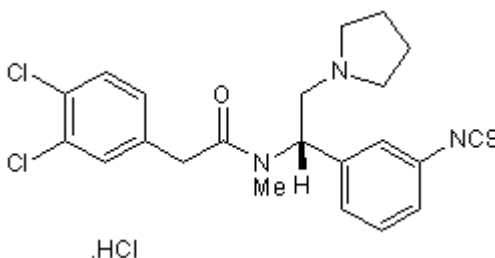
Batch Molecular Weight: 489.37

Physical Appearance: Yellow solid

Solubility: ethanol to 30 mM
DMSO to 50 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.8 (Dichloromethane:Methanol [98:2])

HPLC: Shows >99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +158.1 (Concentration = 0.48, Solvent = Acetonitrile)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54	5.05	8.59
Found	53.97	4.87	8.53

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Description:

An irreversible and selective antagonist at the κ receptor, with persistent effect in vivo.

Physical and Chemical Properties:

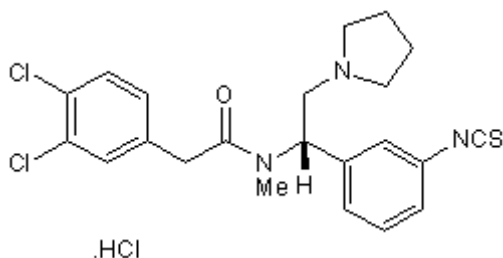
Batch Molecular Formula: $C_{22}H_{23}Cl_2N_3OS \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 489.37

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at $-20^{\circ}C$

Solubility & Usage Info:

ethanol to 30 mM

DMSO to 50 mM

CAUTION - This product has been shown to undergo decomposition in aqueous solution. We estimate that at room temperature up to 20% decomposition occurs after 2 hours. We therefore recommend that solutions of this product be made up and used as rapidly as possible.

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ 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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Chang et al (1994) 2-(3,4-Dichlorophenyl)-N-methyl-N-[(1S)-1-(3-isothiocyanatophenyl)-2-(1-pyrrolidinyl)ethyl]acetamide: an opioid receptor affinity label that produces selective and long lasting κ antagonism in mice. *J.Med.Chem.* **37** 1547. PMID: 8201586.

Chang et al (1994) κ opioid receptor selective affinity labels: Electrophilic benzeneacetamides as κ -selective opioid antagonists. *J.Med.Chem.* **37** 4490. PMID: 7799399.

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