Product Name: **DIPPA hydrochloride** **Catalog No.: 0794** **Batch No.: 3**

CAS Number: 155512-52-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{23}Cl_2N_3OS.HCl$

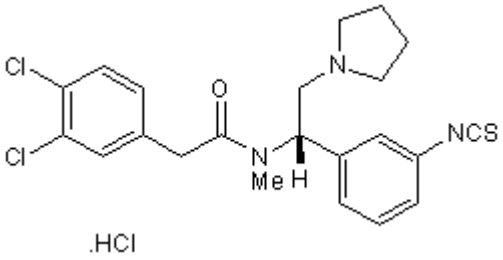
Batch Molecular Weight: 484.87

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 (Chloroform:Methanol:Ammonia soln. [20:0.2:0.4])

Melting Point: Between 208 - 209°C

HPLC: Shows >99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +159 (Concentration = 0.48, Solvent = Acetonitrile)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.5	4.99	8.67
Found	54.27	5.01	8.42

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Description:

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

Physical and Chemical Properties:

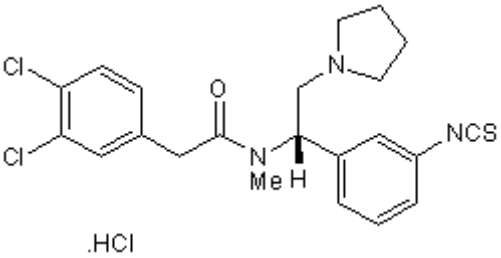
Batch Molecular Formula: $C_{22}H_{23}Cl_2N_3OS.HCl$

Batch Molecular Weight: 484.87

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

ethanol to 30 mM
DMSO to 50 mM

CAUTION - This product has been shwon 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°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:

Chang *et al* (1994) 2-(3,4-Dichlorophenyl)-*N*-methyl-*N*-[(1*S*)-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.