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Print Date: Apr 12th 2022

Certificate of Analysis

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Batch No.: 5

Catalog No.: 0794

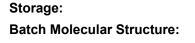
Product Name: DIPPA hydrochloride

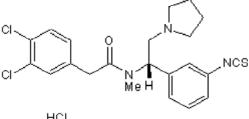
CAS Number: IUPAC Name: 155512-52-0

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: Batch Molecular Weight: Physical Appearance: Solubility: C₂₂H₂₃Cl₂N₃OS.HCl.¼H₂O 489.37 Yellow solid ethanol to 30 mM DMSO to 50 mM Desiccate at -20°C





.HCI

Found

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Optical Rotation: Microanalysis:
$$\begin{split} &\mathsf{R_{f}} = 0.8 \text{ (Dichloromethane:Methanol [98:2])} \\ &\mathsf{Shows } 99.7\% \text{ purity} \\ &\mathsf{Consistent with structure} \\ &\mathsf{Consistent with structure} \\ &\mathsf{[\alpha]_{D}} = +158.1 \text{ (Concentration = 0.48, Solvent = Acetonitrile)} \\ &\mathsf{Carbon Hydrogen Nitrogen} \\ &\mathsf{Theoretical } 54 \qquad 5.05 \qquad 8.59 \end{split}$$

8.53

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

53.97

4.87

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Product Name: DIPPA hydrochloride

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

Description:

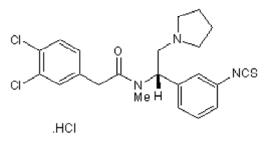
DIPPA hydrochloride is an an irreversible and selective antagonist at the κ receptor, with persistent effect in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₂H₂₃Cl₂N₃OS.HCI.¼H₂O Batch Molecular Weight: 489.37 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 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.

Catalog No.: 0794

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

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.

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