

Certificate of Analysis

Print Date: Dec 12th 2017

www.tocris.com

Product Name: (+)-U-50488 hydrochloride Catalog No.: 0471 Batch No.: 2

CAS Number: 114528-81-3

IUPAC Name: trans-(+)-3,4-Dichloro-N-methyl-N-[2-(1-pyrrolidinyl)-cyclohexyl]benzeneacetamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{26}CI_2N_2O.HCI.H_2O$

Batch Molecular Weight: 423.81 **Physical Appearance:** White solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

.HCI

2. ANALYTICAL DATA

TLC: $R_f = 0.48$ (Chloroform:Methanol:Ammonia soln. [92:7:0.3])

HPLC: Shows 98.9% purity **Chiral HPLC:** Shows 100% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.85 6.9 6.61 Found 53.98 6.73 6.52



Product Information

Print Date: Dec 12th 2017

www.tocris.com

Batch No.: 2

Product Name: (+)-U-50488 hydrochloride

CAS Number: 114528-81-3

IUPAC Name: trans-(+)-3,4-Dichloro-N-methyl-N-[2-(1-pyrrolidinyl)-cyclohexyl]benzeneacetamide hydrochloride

Description:

Less active enantiomer of (±)-U-50488. Racemate and (-)-enantiomer also available.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₆Cl₂N₂O.HCl.H₂O

Batch Molecular Weight: 423.81 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 100 mM DMSO to 100 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).

Catalog No.: 0471

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:

De Costa *et al* (1987) Synthesis and absolute configuration of optically pure enantiomers of a κ-opioid receptor selective antagonist. FEBS Lett. *223* 335. PMID: 2822490.

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