

Certificate of Analysis

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Print Date: Jan 15th 2016

Product Name: CI 988 Catalog No.: 2607 Batch No.: 1

CAS Number: 130332-27-3

IUPAC Name: 4-[[(1R)-2-[[(2R)-3-(1H-indol-3-yl)-2-methyl-1-oxo-2-[[(tricyclo[3.3.1.13,7]dec-2-yloxy)carbonyl]amino]propyl]amino]-

1-phenylethyl]amino]-4-oxobutanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{35}H_{42}N_4O_6$. $^{1/2}H_2O$

Batch Molecular Weight: 623.74 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.31$ (Dichloromethane:Methanol [90:10])

HPLC: Shows 100% purity

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

Optical Rotation: $[\alpha]_D = -9.1$ (Concentration = 0.22, Solvent = Acetone)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.4 6.95 8.98 Found 67.58 7.06 8.59



Product Information

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1-phenylethyl]amino]-4-oxobutanoic acid

Description:

Potent and selective CCK $_2$ (CCK-B) receptor antagonist that displays \sim 1600-fold selectivity over CCK $_1$ receptors (IC $_{50}$ values are 1.7 and 2717 nM for CCK $_2$ and CCK $_1$ respectively). Has negligible affinity at a range of other binding sites (IC $_{50}$ > 10 μ M). Exhibits anxiolytic activity following oral administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₅H₄₂N₄O₆. ½H₂O

Batch Molecular Weight: 623.74 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

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).

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:

Hughes *et al* (1990) Development of a class of selective cholecystokinin type B receptor antagonists having potent anxiolytic activity. Proc.Natl.Acad.Sci.USA *87* 6728.

Moody et al (2001) CI-988 inhibits growth of small cell lung cancer cells. J.Pharmacol.Exp.Ther. 299 1154. PMID: 11714907.

Andre et al (2005) Involvement of cholecystokininergic systems in anxiety-induced hyperalgesia in male rats: behavioral and biochemical studies. J.Neurosci. 25 7896. PMID: 16135746.