

Product Name: 6'-GNTI dihydrochloride

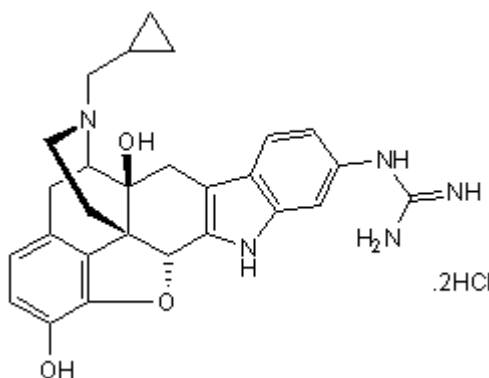
Catalog No.: 2962

Batch No.: 2

IUPAC Name: 6''-Guanidiny-17-(cyclopropylmethyl)-6,7-dehydro-4,5a-epoxy-3,14-dihydroxy-6,7-2',3'-indolomorphinan dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₉N₅O₃.2HCl.3H₂O
Batch Molecular Weight: 598.53
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Dichloromethane:Methanol:Ammonia soln. [70:27:3])
HPLC: Shows 97.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.18	6.23	11.7
Found	53.97	6.07	11.54

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

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Description:

Selective κ/δ -opioid heterodimer receptor agonist (EC_{50} = 39.8, 112.5 and > 1000 nM for κ/δ , κ/μ and δ/μ respectively) that has no effect on opioid receptor homodimers (EC_{50} > 1000 nM). Displays tissue-specific analgesic effects in vitro.

Physical and Chemical Properties:

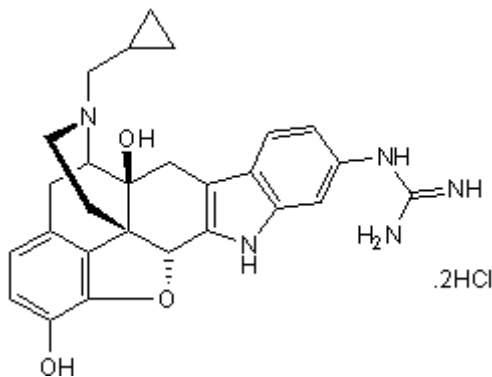
Batch Molecular Formula: $C_{27}H_{29}N_5O_3 \cdot 2HCl \cdot 3H_2O$

Batch Molecular Weight: 598.53

Physical Appearance: Off-white solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°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:

Sharma et al (2001) Transformation of a κ -opioid receptor antagonist to a κ -agonist by transfer of a guanidinium group from the 5' to 6' position of naltrindole. *J.Med.Chem.* **44** 2073. PMID: 11405645.

Waldhoer et al (2005) A heterodimer-selective agonist shows *in vivo* relevance of G protein-coupled receptor dimers. *Proc.Natl.Acad.Sci.USA* **102** 9050.

Rozenfeld et al (2006) Heterodimers of G protein-coupled receptors as novel and distinct drug targets. *Drug Discov.Today Ther.Strateg.* **3** 437.

Rives et al (2012) 6'-guanidinaltrindole (6'-GNTI) is a G protein-biased κ -opioid receptor agonist that inhibits arrestin recruitment. *J.Biol.Chem.* **287** 27050. PMID: 22736766.

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