

Certificate of Analysis

Product Name: CINPA 1

Catalog No.: 5605

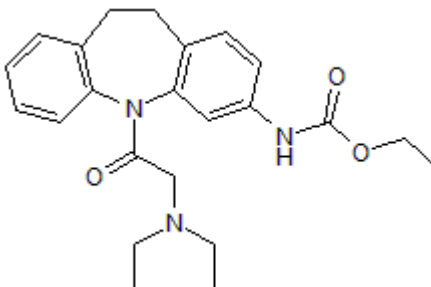
Batch No.: 1

CAS Number: 102636-74-8

IUPAC Name: Ethyl [5-[(diethylamino)acetyl]-10,11-dihydro-5H-dibenz[b,f]azepin-3-yl]carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₉N₃O₃
Batch Molecular Weight: 395.49
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 69.85 | 7.39 | 10.62 |
| Found | 69.8 | 7.39 | 10.64 |

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

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Description:

Potent CAR antagonist ($IC_{50} = 70$ nM). Exhibits >90-fold selectivity for CAR over pregnane X receptor (PXR). Also selective over a panel of other nuclear receptors including FXR, LXR, PPAR γ and RXR.

Physical and Chemical Properties:

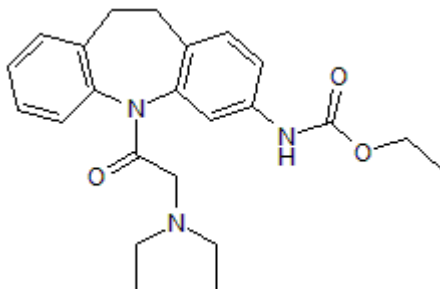
Batch Molecular Formula: C₂₃H₂₉N₃O₃

Batch Molecular Weight: 395.49

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Cherian et al (2015) CINPA1 is an inhibitor of constitutive androstane receptor that does not activate pregnane X receptor. *Mol.Pharmacol.* **87** 878. PMID: 25762023.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

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