

Product Name: A 987306

Catalog No.: 3640

Batch No.: 2

CAS Number: 1082954-71-9

IUPAC Name: (±)-(7a*R**,11a*R**)-5,6,7a,8,9,10,11,11a-Octahydro-4-(1-piperaziny)-benzofuran[2,3-*h*]quinazolin-2-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₅N₅O.½H₂O

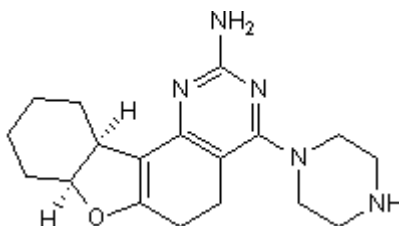
Batch Molecular Weight: 336.43

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

TLC: R_f = 0.33 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.26	7.79	20.82
Found	64.37	7.58	20.7

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

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Description:

Potent histamine H₄ receptor antagonist (pK_i values are 8.24 and 8.47 in human and rat H₄ receptors respectively). Displays 162-fold, 620-fold, and > 1600-fold selectivity over human H₃, H₁ and H₂ receptors. Blocks zymosan-induced neutrophil reflux and attenuates thermal hypersensitivity in vivo (ED₅₀ = 42 μmol/kg, ip).

Physical and Chemical Properties:

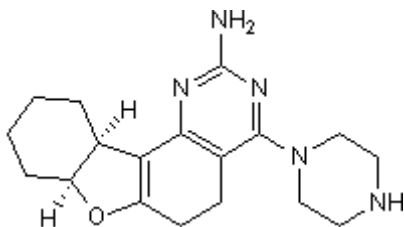
Batch Molecular Formula: C₁₈H₂₅N₅O · ½H₂O

Batch Molecular Weight: 336.43

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Liu *et al* (2008) *cis*-4-(Piperazin-1-yl)-5,6,7a,8,9,10,11,11a-octahydrobenzofuro[2,3-*h*]quinazolin-2-amine (A-987306), a new histamine H₄R antagonist that blocks pain responses against carrageenan-induced hyperalgesia. *J.Med.Chem.* **51** 7094. PMID: 18983139.

Leurs *et al* (2009) Molecular and biochemical pharmacology of the histamine H₄ receptor. *Br.J.Pharmacol.* **157** 14. PMID: 19413568.

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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