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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **A 331440 dihydrochloride** **Catalog No.: 4697** **Batch No.: 1**

CAS Number: 1049740-32-0

IUPAC Name: 4'-[3-[(3*R*)-3-(Dimethylamino)-1-pyrrolidinyl]propoxy]-[1,1'-biphenyl]-4-carbonitrile dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{27}N_3O.2HCl.½H_2O$

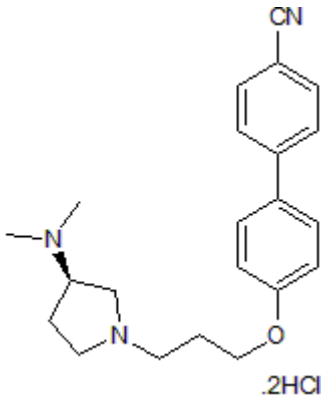
Batch Molecular Weight: 431.4

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol:NH4OH [85:14:1])

HPLC: Shows 99.6% purity

Chiral HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +9.1 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.25	7.01	9.74
Found	61.21	6.84	9.75

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Description:

High affinity histamine H_3 receptor antagonist (K_i values are 21.7 and 22.7 nM for rat and human H_3 receptors, respectively). Exhibits selectivity for human H_3 over H_1, H_2 and H_4 receptors (K_i values are 2940, 14400 and >10000 nM respectively). Shown to reduce weight in a diet-induced obesity model.

Physical and Chemical Properties:

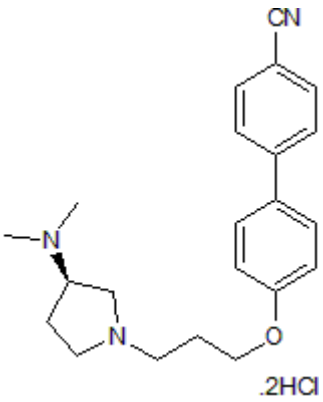
Batch Molecular Formula: $C_{22}H_{27}N_3O.2HCl.½H_2O$

Batch Molecular Weight: 431.4

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
DMSO to 20 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:

Hancock *et al* (2004) Antiobesity effects of A-331440, a novel non-imidazole histamine H_3 receptor antagonist. Eur.J.Pharmacol. ***487*** 183. PMID: 15033391.

Hancock *et al* (2004) *In vitro* optimization of structure activity relationships by analogues of A-331440 combining radioligand receptor binding assays and micronucleus assays of potential antiobesity histamine H_3 receptor antagonists. Basic Clin.Pharmacol.Toxicol. ***95*** 144. PMID: 15447739.