TOCRIS a biotechne brand

Batch No.: 4

Certificate of Analysis

www.tocris.com

Catalog No.: 1661

Product Name: SB 206553 hydrochloride

CAS Number: IUPAC Name: 1197334-04-5

3,5-Dihydro-5-methyl-N-3-pyridinylbenzo[1,2-b:4,5-b']dipyrrole-1(2H)-carboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: $C_{17}H_{16}N_4O.HCI.$ ^{1/4}H₂O 333.3 Yellow solid DMSO to 100 mM Desiccate at RT

.HCI Me

2. ANALYTICAL DATA

TLC:Rf = 0.3 (Dichloromethane:Methanol [95:5])HPLC:Shows 99.3% purity¹H NMR:Consistent with structureMass Spectrum:Consistent with structureMicroanalysis:Carbon Hydrogen NitrogenTheoretical 61.265.2916.81

Theoretical61.265.2916.81Found61.444.9716.73

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

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Print Date: Jan 11th 2016

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IUPAC Name: 3,5-Dihydro-5-methyl-N-3-pyridinylbenzo[1,2-b:4,5-b']dipyrrole-1(2H)-carboxamide hydrochloride

Description:

Potent and selective 5-HT_{2B}/5-HT_{2C} receptor antagonist (rat 5-HT_{2B} pA₂ = 8.89, human 5-HT_{2C} pK_i = 7.92). Displays > 80-fold selectivity over all other 5-HT receptor subtypes and a variety of other receptors (pK_i < 6). Centrally active following oral administration in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{16}N_4O.HCI.$ ^{1/4}H₂O Batch Molecular Weight: 333.3 Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

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).

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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:

Forbes *et al* (1995) 5-Methyl-1-(3-pyridylcarbamoyl)-1,2,3,5-tetrahydropyrrolo[2,3-f]indole: a novel 5-HT_{2C}/5-HT_{2B} receptor antagonist with improved affinity, selectivity and oral activity. J.Med.Chem. **38** 2524. PMID: 7629791.

Kennett *et al* (1996) *In vitro* and *in vivo* profile of SB 206553, a potent 5-HT_{2C}/5-HT_{2B} receptor antagonist with anxiolytic-like properties. Br.J.Pharmacol. **117** 427. PMID: 8821530.

Porras *et al* (2002) 5-HT_{2A} and 5-HT_{2C/2B} receptor subtypes modulate dopamine release induced in vivo by amphetamine and morphine in both the rat nucleus accumbens and striatum. Neuropsychopharmacology **26** 311. PMID: 11850146.

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