Certificate of Analysis

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Product Name: ML 00253764 hydrochloride

Catalog No.: 4854 Batch No.: 2

CAS Number: IUPAC Name:

TOCRIS

a biotechne brand

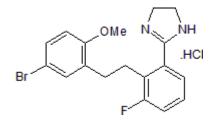
1706524-94-8

2-[2-[2-(5-Bromo-2-methoxyphenyl)ethyl]-3-fluorophenyl]-4,5-dihydro-2-1H-imidazole hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Storage: Batch Molecular Structure: C₁₈H₁₈BrFN₂O.HCl 413.71 White solid water to 10 mM DMSO to 100 mM Store at +4°C



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis: R_f = 0.55 (Dichloromethane:Methanol:Ammonia soln. [190:9:1]) Shows 99.7% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen

| Theoretical | 52.26 | 4.63 | 6.77 |
|-------------|-------|------|------|
| Found | 52.18 | 4.53 | 6.73 |

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

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Print Date: Jul 8th 2016

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Description:

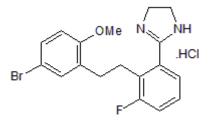
Non-peptide, melanocortin MC_4 receptor antagonist (IC_{50} values are 320, 810 and 2120 nM for MC_4 , MC_3 and MC_5 receptors respectively). Decreases cAMP accumulation in HEK-293 cells expressing the MC_4 receptor. Increases food intake and reduces loss of lean body mass in tumor bearing mice. Brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₈BrFN₂O.HCl Batch Molecular Weight: 413.71 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info: water to 10 mM 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).

Catalog No.: 4854

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:

Nicholson et al (2006) Peripheral administration of a melanocortin 4-receptor inverse agonist prevents loss of lean body mass in tumorbearing mice. J.Pharmacol.Exp.Ther. **317** 771. PMID: 16436498.

Tucci *et al* (2005) Potent and orally active non-peptide antagonists of the human melanocortin-4 receptor based on a series of trans-2disubstituted cyclohexylpiperazines. Bioorg.Med.Chem.Lett. **15** 4389. PMID: 16098742.

Vos *et al* (2004) Identification of 2-[2-[2-(5-bromo-2- methoxyphenyl)-ethyl]-3-fluorophenyl]-4,5-dihydro-1H-imidazole (ML00253764), a small molecule melanocortin 4 receptor antagonist that effectively reduces tumor-induced weight loss in a mouse model. J.Med.Chem. **47** 1602. PMID: 15027849.

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