Batch No.: 1



Certificate of Analysis

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Product Name: ML 00253764 hydrochloride Catalog No.: 4854

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₈BrFN₂O.HCl.¼H₂O

Batch Molecular Weight: 418.21

Physical Appearance: Off-white solid

Solubility: water to 10 mM

DMSO to 100 mM

Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Storage:

TLC: $R_f = 0.04$ (Chloroform:Methanol [9:1])

HPLC: Shows >98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 51.7 4.7 6.7 Found 51.48 4.54 6.65



Product Information

Print Date: May 29th 2014

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

Description:

Non-peptide, melanocortin MC $_4$ receptor antagonist (IC $_{50}$ values are 0.32, 0.81 and 2.12 μ M 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.¼H₂O

Batch Molecular Weight: 418.21 Physical Appearance: Off-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).

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:

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.

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

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

