

Certificate of Analysis

Print Date: Jan 18th 2016

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Product Name: S 14506 hydrochloride Catalog No.: 1771 Batch No.: 2

CAS Number: 286369-38-8

IUPAC Name: 4-Fluoro-N-[2-[4-(7-methoxy-1-naphthalenyl)-1-piperazinyl]ethyl]benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{26}FN_3O_2.HCI$

Batch Molecular Weight: 443.94 **Physical Appearance:** White solid

Solubility: ethanol to 10 mM

DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.71 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])

Melting Point: At 228°C

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.93 6.13 9.46 Found 64.84 6.19 9.42



Product Information

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IUPAC Name: 4-Fluoro-*N*-[2-[4-(7-methoxy-1-naphthalenyl)-1-piperazinyl]ethyl]benzamide hydrochloride

Description:

Highly potent selective 5-HT $_{1A}$ receptor full agonist (pK $_{i}$ values are 9.0, 6.6, 7.5, 6.6 and < 6.0 for 5-HT $_{1A}$, 5-HT $_{1B}$, 5-HT $_{1C}$, 5-HT $_{2}$ and 5-HT $_{3}$ receptors respectively). Possibly binds between the agonist binding site and the G protein interaction switch site, affecting the activation mechanism, and may display positive cooperativity. Anxiolytic following central administration in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₂₆FN₃O₂.HCl

Batch Molecular Weight: 443.94 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at RT

Solubility & Usage Info:

ethanol 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:

Colpaert *et al* (1992) S 14506: a novel, potent, high-efficacy 5-HT_{1A} agonist and potential anxiolytic agent. Drug Dev.Res. **26** 21. **Lima** *et al* (1997) Atypical in vitro and in vivo binding of [³H]S-14506 to brain 5-HT_{1A} receptors. J.Neural Transm. **104** 1059. PMID: 9503258

Milligan et al (2001) S 14506: novel receptor coupling at 5-HT_{1A} receptors. Neuropharmacology 40 334. PMID: 11166326.