

Certificate of Analysis

Product Name: LY 344864 hydrochloride

Catalog No.: 2451

Batch No.: 3

CAS Number: 1217756-94-9

IUPAC Name: *N*-[(3*R*)-3-(Dimethylamino)-2,3,4,9-tetrahydro-1*H*-carbazol-6-yl]-4-fluorobenzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₂N₃OF.HCl.½H₂O

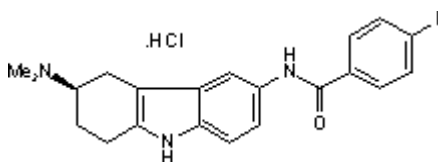
Batch Molecular Weight: 396.89

Physical Appearance: Off-white solid

Solubility:
water to 50 mM
DMSO to 100 mM
ethanol to 5 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.37 (Dichloromethane:Methanol:Ammonia soln. [90:10:2])

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = 58.28 (Concentration = 10, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.55	6.09	10.59
Found	63.27	6.03	10.53

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

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Description:

Potent, selective 5-HT_{1F} receptor agonist (EC₅₀ = 3 nM). Displays > 80-fold selectivity over other 5-HT receptors (K_i values are 0.006, 0.53, 0.55, 0.56, 1.42, 1.70, 3.50, 3.94 and 4.85 μM for 5-HT_{1F}, 5-HT_{1A}, 5-HT_{1B}, 5-HT_{1D}, 5-HT_{1E}, 5-HT_{2B}, 5-HT_{2C}, 5-HT_{2A} and 5-HT₇ receptors respectively). Inhibits neurogenic dural inflammation in vivo following i.v. and oral administration.

Physical and Chemical Properties:

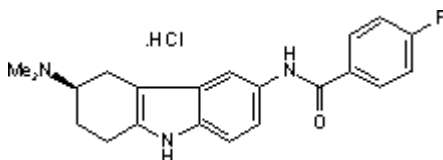
Batch Molecular Formula: C₂₁H₂₂N₃OF.HCl.½H₂O

Batch Molecular Weight: 396.89

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Lee et al (1997) Characterization of LY344864 as a pharmacological tool to study 5-HT_{1F} receptors: binding affinities, brain penetration and activity in the neurogenic dural inflammation model of migraine. *Life Science* **61** 2117.

Ramadan et al (2003) 5-HT_{1F} receptor agonists in acute migraine treatment: a hypothesis. *Cephalalgia* **23** 776. PMID: 14510923.

Goadsby and Classey (2003) Evidence for serotonin (5-HT)_{1B}, 5-HT_{1D} and 5-HT_{1F} receptor inhibitory effects on trigeminal neurons with craniovascular input. *Neuroscience* **122** 491. PMID: 14614913.

Storage: Store at +4°C

Solubility & Usage Info:

water to 50 mM
DMSO to 100 mM
ethanol to 5 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.

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