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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **R-96544 hydrochloride** **Catalog No.: 1742** **Batch No.: 1**

CAS Number: 167144-80-1

IUPAC Name: (2*R*,4*R*)-5-[2-[2-[2-(3-Methoxyphenyl)ethyl]phenoxy]ethyl]-1-methyl-3-pyrrolidinol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{29}NO_3.HCl$

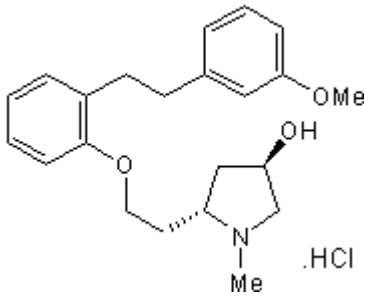
Batch Molecular Weight: 391.94

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.39 (Chloroform:Methanol:Ammonia soln. [9:0.8:0.2])

Melting Point: Between 95 - 98°C

HPLC: Shows >99.7% purity

^{1}H NMR: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -12 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.42	7.71	3.57
Found	67.46	7.81	3.56

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Description:

Potent, selective 5-HT_2 receptor antagonist; displays some selectivity for 5-HT_{2A} receptors (K_i = 1.6 nM). IC_{50} values are 2.2, 310, 2400, 3700, > 5000 and > 5000 nM for 5-HT_2, α_1-adrenergic, D_2 dopamine, 5-HT_1, 5-HT_3 and β-adrenergic receptors respectively. Inhibits 5-HT-induced platelet aggregation and pressor responses in vivo.

Physical and Chemical Properties:

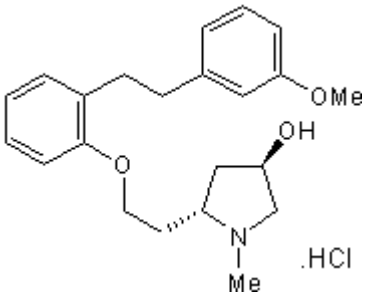
Batch Molecular Formula: $C_{22}H_{29}NO_3$.HCl

Batch Molecular Weight: 391.94

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

water to 100 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:

Tanaka *et al* (2000) [2-(ω-Phenylalkyl)phenoxy]alkylamines III: Synthesis and selective serotonin-2 receptor binding. Chem.Pharm.Bull. ***48*** 1729. PMID: 11086903.

Ogawa *et al* (2002) Pharmacological profiles of R-96544, the active form of a novel 5-HT_{2A} receptor antagonist R-102444. Eur.J.Pharmacol. ***457*** 107. PMID: 12464356.

Ogawa *et al* (2005) Effects of R-102444 and its active metabolite R-96544, selective 5-HT_{2A} receptor antagonists, on experimental acute and chronic pancreatitis: additional evidence for possible involvement of 5-HT_{2A} receptors in the development of experimental pancreatitis. Eur.J.Pharmacol. ***521*** 156. PMID: 16183055.

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