

Certificate of Analysis

Print Date: Nov 18th 2017

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Product Name: RS 39604 hydrochloride Catalog No.: 0991 Batch No.: 3

CAS Number: 167710-87-4

IUPAC Name: 1-[4-Amino-5-chloro-2-(3,5-dimethoxyphenyl)methyloxy]-3-[1-[2-methylsulphonylamino]ethyl]piperidin-4-yl]propan-1-

one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₃₆ClN₃O₆S.HCl.½H₂O

Batch Molecular Weight: 595.06 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.48 6.35 7.06 Found 52.41 6.17 7.05



Product Information

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Description:

A potent and selective 5-HT₄ antagonist, with a pK_i of 9.1 at 5-HT₄ receptors in guinea pig striatal membranes and greater than 1000-fold selectivity over 5-HT_{1A, 2C, 3} and D₁, D₂, M₁, M₂, AT₁, B₁ and α_{1C} receptors. The ketone group gives RS 39604 a relatively long half life; it is also orally active and so suitable for in vivo studies.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₃₆CIN₃O₆S.HCI.¹/₄H₂O

Batch Molecular Weight: 595.06 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

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.: 0991

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.

Licensing Information:

Sold with the permission of Roche Bioscience

References:

Eglen et al (1995) Central 5-HT₄ receptors TiPS 16 391. PMID: 8578609.

Hegde (1995) RS 39604: a potent, selective and orally active 5-HT₄ receptor antagonist. Br.J.Pharmacol. 115 1087. PMID: 7582507.