

Certificate of Analysis

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Print Date: Jan 15th 2016

Product Name: SGS 518 oxalate Catalog No.: 3688 Batch No.: 1

CAS Number: 445441-27-0

IUPAC Name: 1-Methyl-3-(1-methyl-4-piperindin-4-yl)-5-hydroxy-1*H*-indole 2,6-difluorobenzenesulfonic acid ester oxalate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{22}F_2N_2O_3S.C_2H_2O_4$

Batch Molecular Weight: 510.51

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.52 \text{ (Propan-2-o1/Ammonia(aq)/Water 10:2:1)}$

HPLC: Shows 98.6% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.11 4.74 5.49 Found 54.04 4.72 5.43



Product Information

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IUPAC Name: 1-Methyl-3-(1-methyl-4-piperindin-4-yl)-5-hydroxy-1H-indole 2,6-difluorobenzenesulfonic acid ester oxalate

Description:

Selective antagonist of the 5-HT₆ subtype of the serotonin receptor. Useful for the treatment of cognitive impairment that is associated with schizophrenia and Alzheimer's disease.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₂₂F₂N₂O₃S.C₂H₂O₄

Batch Molecular Weight: 510.51 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

/ ---N.

Storage: Desiccate 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).

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:

Romero et al (2006) Efficacy of selective 5-HT₆ receptor ligands determined by monitoring 5-HT₆ receptor-mediated cAMP signaling pathways. Br.J.Pharmocol. **148** 1133. PMID: 16865095.

Kim et al (2008) New serotonin 5-HT₆ ligands from common feature pharmacophore hypotheses. J.Chem.Inf.Model. **48** 197. PMID: 18044950.