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Print Date: Sep 23rd 2016

Certificate of Analysis

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Product Name: **LY 393558** **Catalog No.: 3350** **Batch No.: 1**

CAS Number: 271780-64-4

IUPAC Name: 1-[2-[4-(6-Fluoro-1*H*-indol-3-yl)-3,6-dihydro-1(2*H*)-pyridinyl]ethyl]-3,4-dihydro-3-(1-methylethyl)-6-(methylsulfonyl)-1*H*-2,1,3-benzothiadiazine-2,2-dioxide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{31}FN_4O_4S_2.½H_2O$

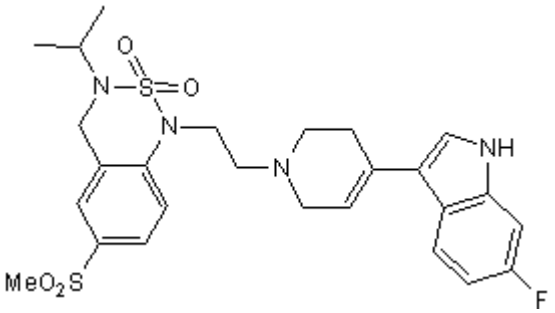
Batch Molecular Weight: 555.69

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Ethyl acetate)

HPLC: Shows 97.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.2	5.8	10.08
Found	56.01	5.72	9.74

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Description:

Dual 5-$HT_{1B/1D}$ receptor antagonist (pK_B values are 9.05 and 8.98 respectively) and 5-HT re-uptake inhibitor (pIC_{50} = 8.48). Potently antagonizes terminal autoreceptor activity in vitro and increases extracellular 5-HT levels above those evoked by fluoxetine (Cat. No. 0927) in vivo. Also acts as an antagonist at 5-HT_{2A} and 5-HT_{2B} receptors (pK_i values are 7.29 and 7.35 respectively).

Physical and Chemical Properties:

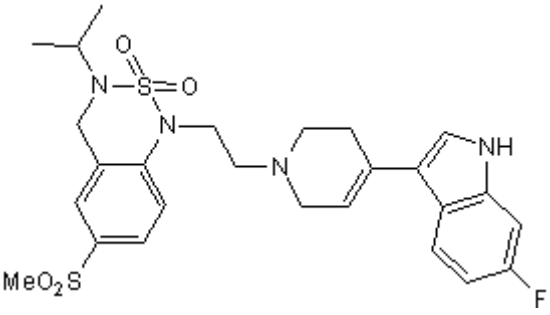
Batch Molecular Formula: $C_{26}H_{31}FN_4O_4S_2.½H_2O$

Batch Molecular Weight: 555.69

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Morecroft *et al* (2005) Functional interactions between 5-hydroxytryptamine receptors and the serotonin transporter in pulmonary arteries. J.Pharmacol.Exp.Ther. ***313*** 539. PMID: 15659538.

Mitchell *et al* (2001) LY393558, a 5-hydroxytryptamine reuptake inhibitor and 5-$HT_{1B/1D}$ receptor antagonist: effects on extracellular levels of 5-hydroxytryptamine in the guinea pig and rat. Eur.J.Pharmacol. ***432*** 19. PMID: 11734183.

Pullar *et al* (2001) In vitro activity of LY393558, an inhibitor of the 5-hydroxytryptamine transporter with 5-$HT_{1B/1D/2}$ receptor antagonist properties. Eur.J.Pharmacol. ***432*** 9. PMID: 11734182.

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