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Print Date: Oct 12th 2017

Certificate of Analysis

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Product Name: **SR 49059** **Catalog No.: 2310** **Batch No.: 2**

CAS Number: 150375-75-0

IUPAC Name: (2*S*)-1-[[(2*R*,3*S*)-5-Chloro-3-(2-chlorophenyl)-1-[(3,4-dimethoxyphenyl)sulfonyl]-2,3-dihydro-3-hydroxy-1*H*-indol-2-yl] carbonyl]-2-pyrrolidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{27}Cl_2N_3O_7S.½H_2O$

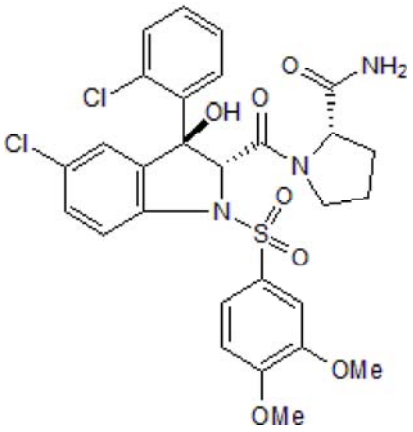
Batch Molecular Weight: 629.51

Physical Appearance: White solid

Solubility: DMSO to 30 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.27 (Ethyl acetate)

HPLC: Shows 99.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -195.3 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.42	4.48	6.68
Found	53.65	4.32	6.64

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Description:

Potent and selective non-peptide vasopressin V_{1A} receptor antagonist; devoid of agonist activity. Displays high affinity and efficacy at both rat (K_i = 1.6 nM) and human (K_i = 1.1 - 6.3 nM) V_{1A} receptors. Potently antagonizes arginine vasopressin-induced effects in vitro (IC_{50} = 3.7 nM for inhibition of human platelet aggregation) and is orally active in vivo.

Physical and Chemical Properties:

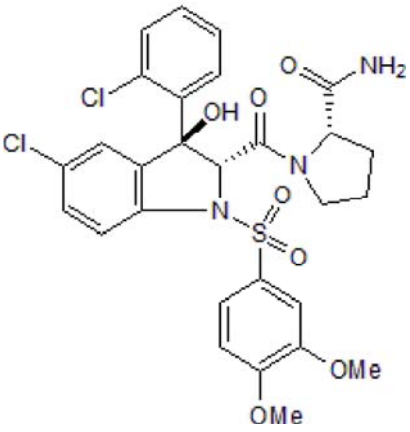
Batch Molecular Formula: $C_{28}H_{27}Cl_2N_3O_7S.½H_2O$

Batch Molecular Weight: 629.51

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 30 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:

Tahtaoui *et al* (2003) Identification of the binding sites of the SR 49059 nonpeptide antagonist into the V_{1a} vasopressin receptor using sulfydryl-reactive ligands and cysteine mutants as chemical sensors. J.Biol.Chem. ***278*** 40010. PMID: 12869559.

Serradeil-Le Gal *et al* (1994) Binding of [^{3}H]SR 49059, a potent nonpeptide vasopressin V_{1a} antagonist, to rat and human liver membranes. Biochem.Biophys.Res.Comm. ***199*** 353.

Serradeil-Le Gal *et al* (1993) Biochemical and pharmacological properties of SR 49059, a new, potent, nonpeptide antagonist of rat and human vasopressin V_{1a} receptors. J.Clin.Invest. ***92*** 224. PMID: 8392086.