

Certificate of Analysis

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Product Name: SR 12813

Catalog No.: 2969

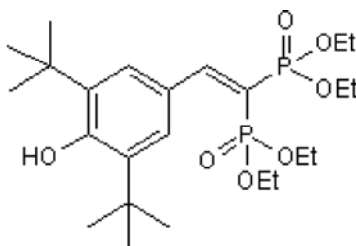
Batch No.: 1

CAS Number: 126411-39-0

IUPAC Name: [[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]ethenylidene]bis-phosphonic acid tetraethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₄ H ₄₂ O ₇ P ₂
Batch Molecular Weight:	504.53
Physical Appearance:	Beige solid
Solubility:	DMSO to 100 mM ethanol to 100 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.4 (Chloroform:Methanol [95:5])
HPLC:	Shows >99.9% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	57.13	8.39	
Found	57.12	6.8	

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Pregnane X receptor (PXR) agonist (EC₅₀ values are 200 and 700 nM for human and rabbit PXR respectively). Activates the farnesoid X receptor (FXR) at μM concentrations. Displays hypocholesterolaemic activity via enhanced degradation of HMG-CoA reductase.

Physical and Chemical Properties:

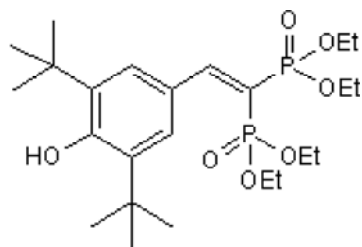
Batch Molecular Formula: C₂₄H₄₂O₇P₂

Batch Molecular Weight: 504.53

Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Lemaire et al (2007) Discovery of a highly active ligand of human pregnane X receptor: a case study from pharmacophore modeling and virtual screening to "in vivo" biological activity. *Mol.Pharmacol.* **72** 572. PMID: 17573484.

Jones et al (2000) The pregnane X receptor: a promiscuous xenobiotic receptor that has diverged during evolution. *Mol.Pharmacol.* **14** 27.

Berkhout et al (1996) The novel cholesterol-lowering drug SR-12813 inhibits cholesterol synthesis via an increased degradation of 3-hydroxy-3-methylglutaryl-coenzyme A reductase *J.Biol.Chem.* **271** 14376. PMID: 8662919.

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