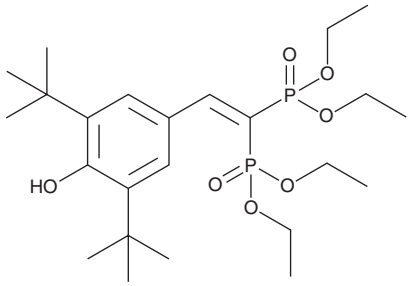
PRODUCT INFORMATION

SR-12813

Item No. 18115

CAS Registry No.:	126411-39-0
Formal Name:	P,P'-[[3,5-*bis*(1,1-dimethylethyl)-4-hydroxyphenyl]ethenylidene]*bis*-phosphonic acid P,P,P',P'-tetraethyl ester
Synonym:	GW 485801
MF:	$C_{24}H_{42}O_7P_2$
FW:	504.5
Purity:	≥98%
UV/Vis.:	λ_{max}: 213, 239, 326 nm
Supplied as:	A crystalline solid
Storage:	Room temperature
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

SR-12813 is supplied as a crystalline solid. A stock solution may be made by dissolving the SR-12813 in the solvent of choice, which should be purged with an inert gas. SR-12813 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of SR-12813 in these solvents is approximately 5, 1, and 15 mg/ml, respectively.

Description

SR-12813 is a 1,1-bisphosphonate ester that exhibits hypocholesterolemic activity by enhancing the degradation of HMG-CoA reductase in various animal models.[1] SR-12813 is also a high affinity ligand for human and rabbit pregnane X receptors (K_d = 41 nM; EC_{50} = 137 nM for hPXR *in vitro*) and can induce cytochrome P450 3A expression in human and rabbit hepatocytes.[2-4]

References

1. Berkhout, T.A., Simon, H.M., Patel, D.D., *et al*. 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(24)**, 14376-14382 (1996).
2. Watkins, R.E., Wisely, G.B., Moore, L.B., *et al*. The human nuclear xenobiotic receptor PXR: Structural determinants of directed promiscuity. *Science* **292(5525)**, 2329-2333 (2001).
3. Lemaire, G., Benod, C., Nahoum, C., *et al*. 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(3)**, 572-581 (2007).
4. Jones, S.A., Moore, L.B., Shenk, J.L., *et al*. The pregnane X receptor: A promiscuous xenobiotic receptor that has diverged during evolution. *Mol. Endocrinol.* **14(1)**, 27-39 (2015).

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