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:**

λ_{max}: 213, 239, 326 nm UV/Vis.: Supplied as: A crystalline solid Storage: Room temperature

≥4 years Stability:

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. SR-12813 is also a high affinity ligand for human and rabbit pregnane X receptors ($K_d = 41 \text{ nM}$; $EC_{50} = 137 \text{ nM}$ 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).

WARNING
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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