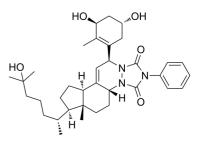


Building Blocks, Pharmaceutical Intermediates, Chemical Reagents, Catalysts & Ligands www.ChemScene.com

Data Sheet

Product Name:	Impurity C of Calcitriol
Cat. No.:	CS-1177
CAS No.:	86307-44-0
Molecular Formula:	$C_{35}H_{49}N_3O_5$
Molecular Weight:	591.78
Target:	VD/VDR
Pathway:	Vitamin D Related/Nuclear Receptor
Solubility:	DMSO : 50 mg/mL (84.49 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Impurity C of Calcitriol, Calcitriol(1,25-Dihydroxyvitamin D3; Rocaltrol) is the hormonally active form of vitamin D, Calcitriol is the active metabolite of vitamin D3 that activates the vitamin D receptor (VDR). IC50 value: Target: vitamin D receptor Calcitriol(1,25-Dihydroxyvitamin D3; Rocaltrol) displays calcemic actions. Calcitriol stimulates intestinal and renal Ca2+ absorption and regulates bone Ca2+ turnover. Calcitriol (1,25-Dihydroxyvitamin D3; Rocaltrol) exhibits antitumor activity; Calcitriol(1,25-Dihydroxyvitamin D3; Rocaltrol) inhibits in vivo and in vitro cell proliferation in a wide range of cells including breast, prostate, colon, skin and brain carcinomas and myeloid leukemia cells.

References:

[1]. Canalejo et al (2000) The in vitro effect of calcitriol on parathyroid cell proliferation and apoptosis. J.Am. Soc. Nephrol. 11 1865. Beer and Myrthue (2004)

[2]. Calcitriol in cancer treatment: from the lab to the clinic. Mol.Cancer Ther. 3 373.

[3]. Krishnan AV, Swami S, Feldman D.Equivalent anticancer activities of dietary vitamin D and calcitriol in an animal model of breast cancer: Importance of mammary CYP27B1 for treatment and prevention.J Steroid Biochem Mol Biol. 2012 Aug 23.

[4]. Alkharfy KM, Al-Daghri NM, Yakout SM, Ahmed M. Calcitriol Attenuates Weight-Related Systemic Inflammation and Ultrastructural Changes of the Liver in a Rodent Model.Basic Clin Pharmacol Toxicol. 2012 Aug 21.

CAIndexNames:

 $1H,5H-Cyclopenta[f][1,2,4]triazolo[1,2-a]cinnoline-1,3(2H)-dione, 11-(3,5-dihydroxy-2-methyl-1-cyclohexen-1-yl)-4a,6,6a,7,8,9,9a,11-octahydro-7-(5-hydroxy-1,5-dimethylhexyl)-6a-methyl-2-phenyl-, [4aR-[4a\alpha,6a\alpha,7\alpha(R*),9a\beta,11\alpha(3S*,5R*)]]- (9CI)$

SMILES:

O[C@@H](C[C@@H]1O)CC([C@@H]2C=C3[C@@](CC[C@]4([H])[C@@H](CCCC(C)(O)C)C)([H])[C@]4(C)CC[C@@]3([H])N(C(N5C6=CC=CC=C6)=O) N2C5=O)=C1C

Caution: Product has not been fully validated for medical applications. For research use only.

 Tel: 610-426-3128
 Fax: 888-484-5008
 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA