

Data Sheet

Product Name: Ercalcidiol
Cat. No.: CS-0393
CAS No.: 21343-40-8
Molecular Formula: C28H44O2
Molecular Weight: 412.65

Target: Endogenous Metabolite; VD/VDR

Pathway: Metabolic Enzyme/Protease; Vitamin D Related

Solubility: DMSO : \geq 100 mg/mL (242.34 mM)

BIOLOGICAL ACTIVITY:

Ercalcidiol is a metabolite of **vitamin** D_2 , is regarded as an indicator of vitamin D nutritional status. IC50 & Target: Vitamin $D_2^{[1]}$ **In Vitro**: Differentiation between Ercalcidiol (25(OH)D₂) and 25(OH)D₃ is important for monitoring vitamin D therapy, as vitamin D₂ is the predominant prescription form. The half-life of Ercalcidiol is shorter than that of 25(OH)D₃ and it binds less well to the vitamin D binding protein, making it less potent and, therefore, required to be administered at much higher doses than vitamin D₃. Some currently used assays have a diminished capacity to detect Ercalcidiol, which can lead to dangerous overdosing when attempting to monitor therapy with vitamin $D_2^{[2]}$.

References:

[1]. Li L, et al. Performance evaluation of two immunoassays for 25-hydroxyvitamin D. J Clin Biochem Nutr. 2016 May;58(3):186-92.

[2]. Newman MS, et al. A liquid chromatography/tandem mass spectrometry method for determination of 25-hydroxy vitamin D2 and 25-hydroxy vitamin D3 in dried blood spots: a potential adjunct to diabetes and cardiometabolic risk screening. J Diabetes Sci Technol

CAIndexNames:

 $\label{lem:cyclohexanol} Cyclohexanol, 4-methylene-3-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R,2E,4S)-5-hydroxy-1,4,5-trimethyl-2-hexenyl]-7a-methyl-4H-inden-4-ylidene]-, (1S,3Z)-\\$

SMILES:

 $C = C1CC[C@H](O)C/C1 = C/C = C2[C@]3([C@@](C)([C@H](CC3)[C@@H](/C = C/[C@@H](C(C)(O)C)C)CCC/2)[H] \\ = C1CC[C@H](O)C/C1 = C/C2[C@@H](C(C)(O)C)CCC/2)[H] \\ = C1CC[C@H](O)C/C1 = C/C2[C@](C(C)(O)C)CCC/2)[H] \\ = C1CC[C@H](O)C/C1 = C/C2[C@](C(C)(C)CC/2)[H] \\ = C1CC[C@H](O)C/C1 = C/C2[C@](C(C)(C)CC/2)[H] \\ = C1CC[C@H](O)C/C1 = C/C2[C@](C(C)(C)C2CCC/2)[H] \\ = C1CC[C@](C(C)(C)CC/2)[H] \\ = C1CC[C@](C(C)(C)(C)CC/2)[H] \\ = C1CC[C@](C(C)(C)(C)CC/2)[H] \\ = C1CC[C@](C(C)(C)(C)CC/2)[H] \\ = C1CC[C@](C(C)(C)CC/2)[H] \\ = C1CC[C](C(C)(C)CC/2)[H] \\ = C1CCCC(C)CC(C)CC/2 \\ = C1CCCCC/2 \\ = C1CCCCC/2 \\ = C1CCCCC/2 \\ = C1CC$

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

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