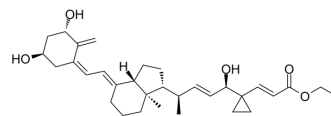


## ZK168281

Cat. No.:	HY-12407
CAS No.:	186371-96-0
Molecular Formula:	C <sub>32</sub> H <sub>46</sub> O <sub>5</sub>
Molecular Weight:	511
Target:	VD/VDR
Pathway:	Vitamin D Related/Nuclear Receptor
Storage:	4°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 100 mg/mL (195.69 mM; Need ultrasonic)

Concentration	Mass		
	1 mg	5 mg	10 mg
1 mM	1.9569 mL	9.7847 mL	19.5695 mL
5 mM	0.3914 mL	1.9569 mL	3.9139 mL
10 mM	0.1957 mL	0.9785 mL	1.9569 mL

Please refer to the solubility information to select the appropriate solvent.

### BIOLOGICAL ACTIVITY

#### Description

ZK168281 is a 25-carboxylic ester 1α,25(OH)<sub>2</sub>D<sub>3</sub> analog and a pure VDR antagonist with a K<sub>d</sub> value of 0.1 nM. ZK168281 is an effective inhibitor of the coactivator (CoA) interaction of its receptor<sup>[1]</sup>.

#### IC<sub>50</sub> & Target

Kd: 0.1 nM (VDR)<sup>[1]</sup>

#### In Vitro

ZK168281 resembles more the mouse constitutive androstane receptor (CAR) inverse agonist Androstanol in its ability to recruit corepressor (CoR) proteins. A salt bridge between the CoR and a conserved lysine in helix 4 of the nuclear receptor (NR) is central to this interaction, but also helix 12 was stabilized by direct contacts with residues of the CoR. Fixation of helix 12 in the antagonistic/inverse agonistic conformation prevents an energetically unfavorable free floatation of the C terminus<sup>[1]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### REFERENCES

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[1]. Lempiäinen H, et al. Antagonist- and inverse agonist-driven interactions of the vitamin D receptor and the constitutive androstane receptor with corepressor protein. Mol Endocrinol. 2005 Sep;19(9):2258-72.

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

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