# Sitagliptin phosphate monohydrate

**Cat. No.:** HY-13749B

**CAS No.:** 654671-77-9

**Molecular Formula:** $C_{16}H_{20}F_6N_5O_6P$

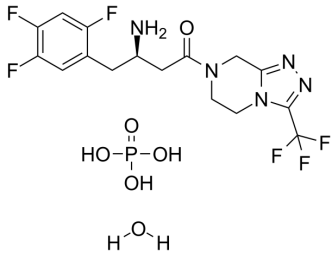
**Molecular Weight:** 523.32

**Target:** Dipeptidyl Peptidase; Autophagy

**Pathway:** Metabolic Enzyme/Protease; Autophagy

**Storage:** 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



## SOLVENT & SOLUBILITY

**In Vitro**

$H_2O$ : ≥ 33 mg/mL (63.06 mM)

* "≥" means soluble, but saturation unknown.

**Preparing Stock Solutions**

| Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 1 mM | 1.9109 mL | 9.5544 mL | 19.1088 mL |
| 5 mM | 0.3822 mL | 1.9109 mL | 3.8218 mL |
| 10 mM | 0.1911 mL | 0.9554 mL | 1.9109 mL |

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

**In Vivo**

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (95.54 mM); Clear solution; Need ultrasonic

## BIOLOGICAL ACTIVITY

**Description**

Sitagliptin phosphate monohydrate (MK-0431 phosphate monohydrate) is a potent inhibitor of DPP4 with an $IC_{50}$ of 19 nM in Caco-2 cell extracts[1].

**$IC_{50}$ & Target**

IC50: 19 nM (DPP4, in Caco-2 cell extracts)

**In Vitro**

Sitagliptin phosphate exhibits a potent inhibitory effect on DPP-4 with $IC_{50}$ of 19 nM from Caco-2 cell extracts[1]. Sitagliptin reduces in vitro migration of isolated splenic CD4 T-cells through a pathway involving cAMP/PKA/Rac1 activation[2]. A recent study demonstrates that sitagliptin exerts a novel, direct action in order to stimulate GLP-1 secretion by the intestinal L cell through a DPP-4-independent, protein kinase A- and MEK-ERK1/2-dependent pathway. It therefore reduces the effect of autoimmunity on graft survival[3].

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

**In Vivo**

In vivo, the $ED_{50}$ value of sitagliptin phosphate for inhibition of plasma DPP-4 activity is calculated to be 2.3 mg/kg 7 hour

| | |
|---|---|
| | postdose and 30 mg/kg 24 hour postdose in freely fed Han-Wistar rats[1]. The streptozotocin-induced type 1 diabetes mouse model exhibits elevated DPP-4 levels in the plasma that can be substantially inhibited in mice on an Sitagliptin phosphate diet. This is achieved by a positive effect on the regulation of hyperglycemia, potentially through prolongation of islet graft survival[4]. The plasma clearance and volume of distribution of Sitagliptin phosphate are higher in rats (40-48 mL/min/kg, 7-9 L/kg) than in dogs (9 mL/min/kg, 3 L/kg); and its half-life is shorter in rats,2 hours compared with 4 hours in dogs[5].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## PROTOCOL

| | |
|---|---|
| **Cell Assay** [2] | CD4T-cells are plated on membrane inserts in serum-free RPMI 1640, and cell migration is assayed using Transwell chambers (Corning), in the presence or absence of purified porcine kidney DPP-4 (32.1 units/mg; 100 mU/mL final concentration) and DPP-4 inhibitor (100 μM). After 1 hour, cells on the upper surface are removed mechanically, and cells that have migrated into the lower compartment are counted. The extent of migration is expressed relative to the control sample.<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |
| **Animal Administration** [1] | Mice: Overnight fasted C57BL/6J mice are challenged 45 min after compound administration with an oral glucose load (2 g/kg). Blood samples for glucose measurement are obtained by tail bleed predose and at serial time points after the glucose load. To evaluate the duration of the effect on glucose tolerance, vehicle or DPP-4 inhibitors are administered 16 h before the glucose challenge.<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## CUSTOMER VALIDATION

- Cell Death Dis. 2021 Oct 11;12(10):928.
- Biomed Pharmacother. 2023 Mar 24;162:114555.
- Biochem Pharmacol. 2023 Oct 5:115846.
- iScience. 2023 Feb.
- J Biol Chem. 2018 Dec 7;293(49):18864-18878.

See more customer validations on www.MedChemExpress.com

## REFERENCES


[1]. Thomas, L., et al. (R)-8-(3-amino-piperidin-1-yl)-7-but-2-ynyl-3-methyl-1-(4-methyl-quinazolin-2-ylm ethyl)-3,7-dihydro-purine-2,6-dione (BI 1356), a novel xanthine-based dipeptidyl peptidase 4 inhibitor, has a superior potency and longer duration of acti

[2]. Kim, S.J., et al., Dipeptidyl peptidase IV inhibition with MK0431 improves islet graft survival in diabetic NOD mice partially via T-cell modulation. Diabetes, 2009. 58(3): p. 641-51.

[3]. Sangle, G.V., et al., Novel biological action of the dipeptidylpeptidase-IV inhibitor, sitagliptin, as a GLP-1 secretagogue. Endocrinology, 2012. 153(2): p. 564-73.

[4]. Kim, S.J., et al., Inhibition of dipeptidyl peptidase IV with sitagliptin (MK0431) prolongs islet graft survival in streptozotocin-induced diabetic mice. Diabetes, 2008. 57(5): p. 1331-9.

[5]. Beconi, M.G., et al. Disposition of the dipeptidyl peptidase 4 inhibitor sitagliptin in rats and dogs. Drug Metab Dispos, 2007. 35(4): p. 525-32.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA