TOCRIS
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Print Date: Feb 25th 2019

Certificate of Analysis

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Product Name: **Sitagliptin phosphate** **Catalog No.: 6816** **Batch No.: 1**

CAS Number: 654671-78-0

IUPAC Name: (3*R*)-3-Amino-1-[5,6-dihydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazin-7(8*H*)-yl]-4-(2,4,5-trifluorophenyl)-1-butanone phosphate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{15}F_6N_5O.H_3O_4P.H_2O$

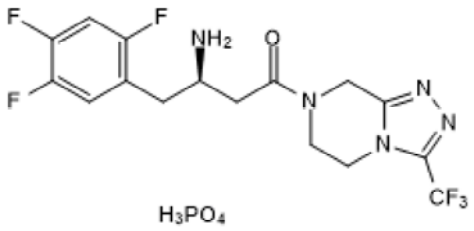
Batch Molecular Weight: 523.33

Physical Appearance: White solid

Solubility: water to 50 mM
DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -22.6 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	36.72	3.85	13.38
Found	36.84	3.8	13.3

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Product Information

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Description:

Potent and selective DPP IV (DPP4) inhibitor (IC_{50} = 18 nM). Displays >2600-fold selectivity for DDP IV over other proline specific peptidases. Reduces blood glucose and increases GLP-1 levels after oral glucose tolerance test in normal and diet-induced obese mice.

Physical and Chemical Properties:

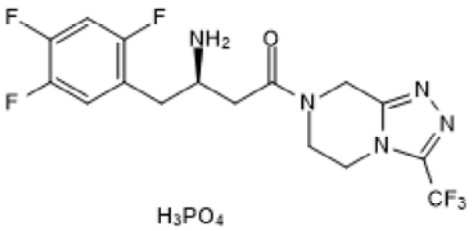
Batch Molecular Formula: $C_{16}H_{15}F_6N_5O.H_3O_4P.H_2O$

Batch Molecular Weight: 523.33

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 50 mM
DMSO to 50 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Kim *et al* (2005) (2*R*)-4-oxo-4-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,3-α]pyrazin-7(8*H*)-yl]-1-(2,4,5-trifluorophenyl)butan-2-amine: a potent, orally active dipeptidyl peptidase IV inhibitor for the treatment of type 2 diabetes. J.Med.Chem. ***48*** 141. PMID: 15634008.