

Certificate of Analysis

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Product Name: PK 44 phosphate

Catalog No.: 4145

Batch No.: 1

CAS Number: 1017682-66-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₆F₅N₇O.H₃PO₄.H₂O

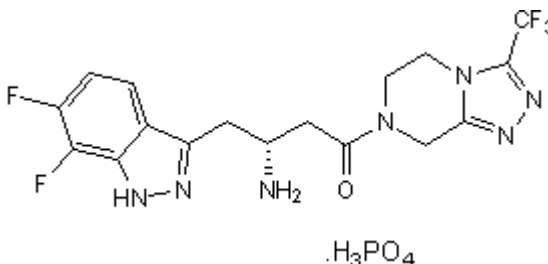
Batch Molecular Weight: 545.36

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 191 - 196°C

HPLC: Shows 98% purity

Chiral HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	37.44	3.88	17.98
Found	37.46	3.54	17.84

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Description:

Potent inhibitor of dipeptidyl peptidase IV (DPP-IV) ($IC_{50} = 15.8$ nM). Displays >1000-fold selectivity for DPP-IV over DPP-8 and DPP-9. Improves glucose tolerance in a mouse oral glucose tolerance assay.

Physical and Chemical Properties:

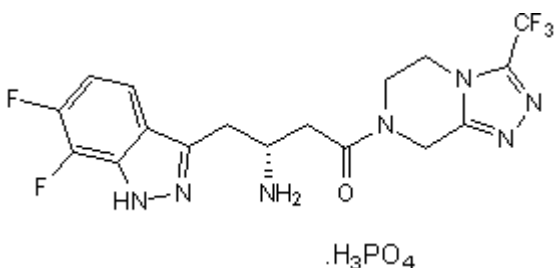
Batch Molecular Formula: $C_{17}H_{16}F_5N_7O \cdot H_3PO_4 \cdot H_2O$

Batch Molecular Weight: 545.36

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM
DMSO to 100 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:

Tozer *et al* (2010) Indole- and indazole-based inhibitors of dipeptidyl peptidase IV for the treatment of type 2 diabetes. 32nd Annual National Medicinal Chemistry Symposium Poster 52.

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