

Product Name: Saxagliptin hydrochloride

Catalog No.: 6507

Batch No.: 1

CAS Number: 709031-78-7

IUPAC Name: (1S,3S,5S)-2-[(2S)-Amino(3-hydroxytricyclo[3.3.1.1^{3,7}]dec-1-yl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₅N₃O₂.HCl.¾H₂O

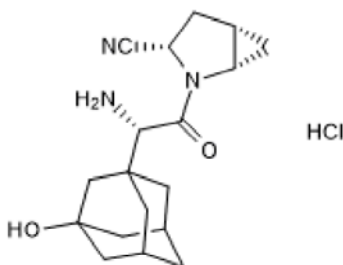
Batch Molecular Weight: 365.38

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.17	7.59	11.5
Found	59.36	7.6	11.48

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Description:

High affinity DPP-IV inhibitor ($K_i = 0.6$ nM). Inhibits plasma DPP-IV (87%). Elicits enhanced glucose clearance in Zucker^{fa/fa} rats.

Physical and Chemical Properties:

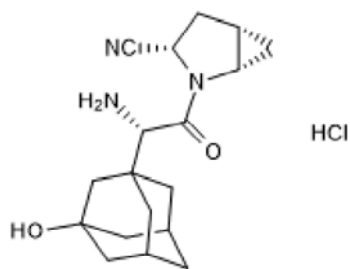
Batch Molecular Formula: C₁₈H₂₅N₃O₂.HCl.¾H₂O

Batch Molecular Weight: 365.38

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

ethanol 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:

Augeri et al (2005) Discovery and preclinical profile of Saxagliptin (BMS-477118): a highly potent, long-acting, orally active dipeptidyl peptidase IV inhibitor for the treatment of type 2 diabetes. *J.Med.Chem.* **48** 5025. PMID: 16033281.

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